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PHYSICAL PROPERTIES OF THE 1D MAGNET $\beta - VOSO_4$

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0.2 Abstract

In this work the β phase of Vanadiumoxosulphate (VI) ($\beta - VOSO4$) crystal was used to study the physical properties of low dimensional magnetism in spin $\frac{1}{2}$ chains. Structural analysis from X-ray diffraction and neutron diffraction performed on the sample, confirm that it crystallizes in the Pnma (62) space group. $\beta - VOSO4$ has V4+ bounded to six oxygen that gives it an octahedral configuration with one unpaired electron, thus with a total spin 1/2. The V-O-V bound running parallel to the a-axis form a spin $\frac{1}{2}$ chain. The physical effect of this spin chain on the magnetic susceptibility and heat capacity was examined and it shows that the magnetic moment is isotropic and the intra-chain magnetic interaction is antiferromagnetic. This magnetic behavior has a significant effect on the susceptibility and heat capacity at temperatures below 60K. The magnitude of the magnetic exchange interaction between the spins was calculated to range from 45.4(3) K to 43.9(5)K but from fits to the magnetic susceptibility curve the exchange interaction was model to be approximately 25.05(99)K in all direction. The magnetic contribution to the internal energy of the crystal was found to be approximately $4.5 JK^{-1}mol^{-1}$ at 50K.

Contents

Chapter 1

Theoretical Background

1.1 Introduction

The field of quantum magnetism has received a wide range of attention over the years. Supper conductors and the notion of storing information in the form of spin orientation is a frontier of science, the theoretical framework of one-dimensional magnetism is a fascinating work of numerical analysis and theoretical computational physics as is seen in the work of Bonner and Fisher (1964), but the existence of material that exhibit such property moves one to try to confirm and investigate the true nature of this material and see how to characterize their behaviour under certain conditions as well as looking at the structural architecture that permits the existence of such phenomena in reality. The crystal $\beta - VOSO_4$ has been studied over the years, Paufler et al. (2014), studied the thermal behaviour of the crystal, Boghosian et al. (1995) studied the spectral and structure of the crystal, but the magnetic contribution of the spin system in the crystal was not given much attention.

In view to understanding the magnetic nature, strength and contribution to the internal energy of the crystal we embark on this journey hoping to find answers.

Generally, this project aims to investigate the magnetic properties of 1D magnetism in $\beta - VOSO_4$, to have an insight into the physical property of 1D magnetism and the peculiarity of the one-dimensional magnetism in $\beta - VOSO_4$ if any.

this thesis is structured as follows: The first chapter introduced the background theories, chapter two the theories and experimental procedures used in the project are discussed in brief, chapter three and four are result presentations and analysis.

To achieve this we will take the following steps: The procedure for this

project will be preparation of the sample followed by series of confirmation processes then finally the bulk property examination, these are itemized below in steps.

- physical examination, looking at the texture colour and nature of crystal under the microscope.
- perform a TGA experiment for the heat capacity of the crystal to check for residual water of crystallization in the crystal. This is done because the water of crystallization is not visible in the neutron and x-ray diffraction experiments as they appear as background noise in the plots.
- perform Rietveld refinement on the x-ray and neutron diffraction result and generate the crystalline structure of $\beta - VOSO_4$.
- perform and analyse the Raman spectroscopy experiment.
- Analyse the heat capacity experimental result.
- Analyse the magnetic susceptibility experimental results.
- analyse the magnetic contribution of the spin chain to heat capacity.

Before we look at the experiments and result from the analysis of the various steps listed above a quick look at the background theories of the processes used in the experiments and result analysis will be discussed in brief in chapter two. In chapter three the structural analysis and Raman spectroscopy will be studied. In chapter four the bulk property of the crystal will be studied and finally, our conclusions will be drawn based on our results from the analysis of the data available to us.

1.2 Magnetism in Solids

Solids are define as materials which are rigid and the relative positions of the atoms that make up the solids are constant with respect to a given reference point (Goldstein, 2014). On the other hand magnetism is a material property that has its origin from the subatomic level and hence can be best described quantum mechanically (Stephen, 2001). As an overview magnetism can be regarded as the interplay of magnetic moments resulting from electron movements and spin orientation. A moving charge has an associated magnetic field, and solids are made of atoms which have orbiting electrons, each

of these moving electrons in the solid has an associated magnetic moment. This magnetic moment is a combination of the electron's intrinsic magnetic moment known as spin moment S and orbital magnetic moment L. Each atom of a solid can have more than one electron and there are $6.03 * 10^{23}$ molecules in a mole of a solid, hence $N * 6.03 * 10^{23}$ electrons where N is the sum of the atomic number of the elements of the solid; this is a large number of electrons.

The magnetic contribution of the electron in the solid is dependent on the electronic configuration and not the total number of the electrons in the solid (dacollege.org, 2021). Hence magnetism in solids has an orbital dependence and electron pair dependence. Materials which have paired electrons in a filled orbit are generally nonmagnetic. For example noble gases like Argon ($1s^2 2s^2 2p^6 3s^2 3p^6$) and Neon ($1s^2 2s^2 2p^6$) are non magnetic, but solids like sodium($1s^2 2s^2 2p^6 3s^1$) and magnesium($1s^2 2s^2 2p^6 3s^2$) (metals) have unpaired electrons in their electronic orbit, with weak nuclear influence on them. Not only pure elements that are magnetic solid, some solids compounds are also magnetic even though their constituent elements are nonmagnetic as pure elements, some elements are nonmagnetic as an atom but become magnetic at the molecular level for example Oxygen (Merzbacher, 1998). This in order words points to the type of bound formed by these compounds as the determining factor as to the magnetic nature of such compounds. Some compounds form crystalline solids, and these crystalline solids can also be magnetic depending on the bounding structure of the crystal and the presences of unpaired electrons. For example $\beta - VOSO_4$, this crystal has a vanadium atom which has an unpaired electron therefore exhibits a magnetic behaviour (configuration).

The nature of this magnetic behavior depends on how this electrons are arranged in the material or crystal, this arrangement can occur in various space and dimension like 3D, 2D and even as low as 1D. the Dimension of the ordering of this electron spins define the complexity of the magnetic properties in the material. In 1D the the electron spins arranged in a line called spin chain, this chains can be half integer spins or whole number spins for example a spin chain made up of spin 1/2 electrons is called spin half chain written as spin1/2.

In Summary, the main contribution to magnetism is from unpaired electrons which has two magnetic components the magnetic spin moment and the orbital magnetic moment. Let first look at what is an electron spin moment?

1.2.1 Electron Spin:

Spin is an intrinsic form of angular momentum carried by elementary particles **(Merzbacher, Eugen ,1998),** electrons are fermions hence obey Pauli exclusion principle, this implies that electrons in a given orbit can either be singular or in pairs when their intrinsic moments are not the same. The intrinsic moment of electrons known as spin is quantized and has an associated spin quantum numbers,the spin quantum number can have only two possible values $\pm\hbar/2$ **(Blundell S. , 2001)**. The magnetic moments associated with this spin quantum numbers $Ms = \pm\hbar/2$ for a given direction.

The magnitude of the spin angular momentum is given by

$$Ms = \sqrt{(s(s+1))}\hbar \tag{1.1}$$

From Pauli exclusion principle, if the electronic orbit has a pair of electrons, these electrons must not have the same four quantum numbers. This means that the electrons must have different spin quantum number hence different magnetic spin moment which is either $+\hbar/2$ or - $\hbar/2$. These magnetic moments are anti parallel and spontaneously cancel each other out resulting in a zero net magnetic moment, thus, even though electrons are magnetic in nature, two electrons with the same energy in a given orbital have zero magnetic contribution. The magnetic nature of a material is dependent on the number of unpaired electrons it has. By this argument one may be tempted to say that atoms that have even number of electron in their outermost shell are nonmagnetic, for example Calcium ($(1s^2 2s^2 2p^6 3s^2 3p^6 4s^2)$), but one has to take into account the available orbits to these electrons. The 4s orbit has lower energy due to orbital overlap, the 4s orbit can hybridize with the 3d orbit to form a hybrid orbit and the electrons take $4s^1$ and $3d^1$ configuration hence resulting in a magnetic atom. This is called high spin configuration.

1.2.2 Orbital contribution

The orbital angular momentum of the electron is related to the magnetic moment µ generated by the orbiting electron as follows:

$$\mu = \mu_B \, \mathbf{L} \tag{1.2}$$

magnetic moment μ is the resultant effect of the combination of magnetic spin moment s and orbital magnetic moment L of an electron in an atom. The orbital moment $\mathbf{L}$ is related to the magnetic moment μ by equation 1.2 where $\mathbf{L}$ is a dimensionless operator and μ_B is Bohr magnetron measured in Joule per Tesla.

Magnetic moment μ from euation 1.2 is dependent on the electron. the electron dependence is introduced by μ_B, which is defined on the spin moment and orbital motion of the electron, which in quantum mechanical terms is a probability function dependent on other constrains in the system. These constrains arising from the orbital motion of the electron are better defined by a quantum mechanical operator **L** which is of the form **L(L+1)** similarly the spin constrains on the electrons are defined by the spin quantum operator s which is of the same form as the orbital operator. hence the magnetic moment of the electron can be written as a combination of these quantum operators as shown in equation 1.4.

Orbital is the space within which the probability of electrons being found is high, and the magnetic moment of a dipole is dependent on the radius of this space. Hybrid orbits have different energy compared with the unhybridized orbits, for electrons in the hybrid orbits their spin and orbital momentum interact in what is know as spin orbital coupling. This effect results in the change of the magnetic moment of the material. This is seen in the change in the magnetic moment generated by the spin moment alone given by

$$\mu = \sqrt{(4S(S+1))} \tag{1.3}$$

to

$$\mu = \sqrt{((4S(S+1) + L(L+1))} \tag{1.4}$$

resulting from orbital contribution to the magnetic moment of the material. The orbital contribution is more pronounced in material where there is hybridization of the orbits into orbits of equal energy and symmetry that permit mobility of the electrons into the other hybrid orbits. The spin orbital coupling plays a key role in the magnetic property of d and f block metals in a compound. This effect is captured in the crystal field theory.A material exhibit magnetic behavior based on the nature of the interaction between all the compounds of the magnetic moments of the material, these interactions include magnetic dipole interaction and exchange interactions The total magnetic moment in a paramagnetic material is the sum of the magnetic orbital angular momentum and the Magnetic spin angular momentum written as $J = \hbar(L + S)$ (Blundell S. , 2001).

1.3 Magnetic Interactions and long-range magnetic order:

Magnetic ordering (alignment) give rise to magnetic properties and this order results from the interaction between the spins in the material.These interac-

tions include

- Magnetic dipolar interaction
- Exchange interaction

Magnetic dipole interaction is a measure of the force of attraction or repulsion between two magnetic dipoles in a material separated by a distance r, the energy of the type of interaction is given by

$$E = \frac{mu_0}{4\pi r^3}(\mu_1.\mu_2 - 3r^2\mu_1.r\mu_2.r) \tag{1.5}$$

where μ_1, μ_2 are magnetic dipoles and r is the distance separating the two dipoles, the energy contribution of this type of interaction is of the order of 1K, (Blundell S. , 2001). This contribution does not consider the mobility of the electrons. The energy contribution is very small in comparison to other types of interaction.

1.3.1 Magnetization:

A material is said to be magnetized when an external magnetic field force most of the magnetic dipoles in the material to have a common orientation in space, or simply put, align in the same direction. Mathematically magnetization can be defined as the number of magnetic dipoles per unit volume of a material that are aligned (Stephen, 2001). Magnetization is a vector that is associated with a material, and its influence can be felt outside the material, the area where this field can be felt is known as the magnetic field of the material. Magnetic field of a material can be described using two vector fields the magnetic flux density B and magnetic field strength H, hence magnetization can be written as

$$M = \frac{B}{\mu_o} + H$$

where μ_o is the permeability due to free space,

1.4 Magnetic Susceptibility:

Magnetic susceptibility is the measure of the magnetic responds of a material to an external magnetic field, it also describes the ratio of magnetization of a material to the applied magnetic field the material is placed in.

Magnetic susceptibility is given by the equation

$$\chi = \frac{M}{H} \tag{1.6}$$

Where χ is magnetic susceptibility, M is magnetization and H is magnetic field strength. Magnetic susceptibility describes the nature of the interaction between the magnetic dipoles in a material (with respect to their orientation or alignment,) as well as the force exchanged between the magnetic dipoles in a material or crystal, in the presences of an external magnetic field. The nature of the alignment of the magnetic dipoles or spins defines the type of magnetic behavior the crystal will have. The magnetic susceptibility of a material in a external field is affected by the nature of the inherent magnetic dipole alignment pre existing in the material. This alignment that is spontaneous in the material define the magnetic property of the material known as the magnetic ground states of the material as:

1.5 Exchange interaction:

Is a quantum mechanical concept as it is not electrostatic but depends on the wave nature of electrons. It accounts for the effects of electrons on one another, based on their quantum states considered simultaneously. Here the quantum states of these electrons is represented by a wave function that is antisymmetric in the spatial and symmetric in spin states. Following this logic when the spatial state is symmetric the spin state is an antisymetic singlet state, while the spin state is symmetric the spatial state is antisymmetric triplet state (Stephen, 2001).

From the Hamiltonian of the electrons the energy of the states can be calculated, the Hamiltonian has to account for the probability of all the electron states and exchange interaction between the states. the Hamiltonian for spin exchange interaction for a two spin system (dimer) is given by the effective Hamiltonian written as

$$H_{eff} = -2JS_1.S_2 \tag{1.7}$$

Where H_{effis} the effective Hamiltonian of the spins and $S_1.S_2$ is the spin quantum state of electron 1 and 2 respectively and J is called the exchange constant or exchange integral (Stephen, 2001).

In general there are many electrons in an atom and many atoms in a solid, hence the exchange interaction which is the major determinant of magnetic order can be given as a summation of all the exchange interaction between the i^{th} and j^{th} electrons in the system and it is given by the Werner Heisenberg

model. This model assumes electrons to have unrestricted degree of freedom that is the electron can have any spin direction and it is written as follows

$$H = \sum_{ij} -J_{ij} S_i S_j \tag{1.8}$$

These interactions between the electrons in a material can be in many forms and they include:

- Direct exchange interaction: this describes the interaction between next neighbor spins
- Double exchange: this interaction where an atom can have two types of interaction because the electron can exist in two states with each state having an interaction energy different from the other, when these two interactions occur simultaneously in a system it called double exchange interaction
- Anisotropic exchange: this the exchange interaction in which the indirect exchange use the spin orbital coupling as its exchange path

The magnetic ground state and excited states of a crystal or any material defined by the net configuration of the spins resulting from the exchange interactions in the system. If this net configuration has a pattern that is repeated over a short interval between few atoms, we say the system has a short range order. But if such pattern of arrangement/orientation repeats over a long range with out a break in order the material is said to have long range order.

This long range order give rise to any of the following type of magnetic ground state:

- Ferromagnetic ground state.
- Antiferromagnetic ground state.
- Ferrimagnetic ground state.

1.5.1 Ferromagnetic materials:

This materials have an inherent magnetic orientation where many of the magnetic dipoles point in a given direction, this magnetic alignment arise from the magnetic interaction between neighboring magnetic moments and this interaction is called exchange interaction. Exchange interaction defines

the influence of other magnetic dipoles on a given dipole, the picture of exchange interaction is better seen using quantum wave mechanics. The exchange interaction of ferromagnetic materials is large and is responsible for long range order in the material. Ferromagnetic materials also have a positive magnetic susceptibility respond to external magnetic field. fig1.3b sow the nature of the inverse magnetic susceptibility responds of this material with increase in temperature. this sketch shows that the material has a positive temperature intercept, this imples thet from **equation 1.2** that at some temperature θ_{cw} some thing interesting happen that indicate a change in regime, below this temperature.

In ferromagnets the magnetic moments of a ferromagnet point in one direction and takes the direction of an external magnetic field when placed in such field and retain this direction in the absence of the external magnetic field.

In a magnetic filed **B** the magnetic moments experience two influences, the influence from other electrons and the influence from the magnetic field **B**, and hence a suitable Hamiltonian while be the one that combines the exchange interaction Energy and the Zeeman energy (Stephen, 2001)and it can be written as follows

$$H = \sum_{ij} -J_{ij} s_i s_J + g\mu_B \sum_{ij} s_j.\mathbf{B} \tag{1.9}$$

where is the g tensor Solving this Hamiltonian gives the ground state and excited states of the material. According to the Weiss model which assumes that the interactions from other electrons or dipole moments build up into a field known as molecular field B_{mf}. This molecular field act as an external magnetic field when it encounters the i^{th} electron in the material hence aligning the i^{th} spin to the direction of the molecular field spin, this influence of the molecular field at higher temperatures is restricted by the thermal excitations but dominate within a short distance there by forming a domain, at this temperature in the absence of external field the material has a short range ordering (Carlin, 1986). At certain temperature known as the curie temperature of the material a magnetic and thermodynamic anomaly occurs and the molecular field effect become long range and there is a spontaneous alignment of the magnetic moments, and the magnetic behavior of the material becomes fully ferromagnetic.

Replacing the spin contribution from the j spin as that from the molecular field, the Hamiltonian can then be written as follows

$$-2S_i \sum_i -J_i j S_J = -g\mu_B.S_i B_{MF} \tag{1.10}$$

Where $2\sum_{ij} J_{ij}S_j$ is the sum of the exchange interaction from other spins that, this produce the molecular filed B_{mf}. Substituting into Hamiltonian above gives

$$H = -g\mu_B.S_iB_{MF} + g\mu_B \sum_{ij} S_j.B \tag{1.11}$$

$$H = g\mu_B \sum_{ij} S_i(B_{MF} + B) \tag{1.12}$$

1.5.2 Antiferromagnetic materials:

These are materials which have an inherent magnetic dipole alignment in which each magnetic dipole has an antiparallel alignment to its next neighbors, that is the dipoles have an antiparallel spin to each other hence the material is nonmagnetic and oppose external magnetic field, this material have a negative magnetic susceptibility, The inherent magnetic alignment in the material is also as a result of exchange interaction in the material, and it is responsible for long range order in such material. Antiferromagnetic materials are similar to the ferrimagnetic materials, the difference is that below Neil temperature T_N the magnetic susceptibility of this materials start to rapidly decrease to zero at temperatures below the knee temperature. This decrease with temperature can be attributed to the antiparallel alignment of the spins or dipoles in the material resulting in a zero net magnetic moment. The graph of inverse susceptibility of this materials have a negative intercept on the temperature axis, at this temperature the material loss all it magnetic susceptibility because the antiparallel dipole moments completely cancel each other out and their orientation at this temperature is frozen, hence the material does not respond to external magnetic field.

1.5.3 Diamagnetic materials

These are materials that their magnetic responds to an external magnetic field is to align its magnetic moment in a Manner that the field generated by materials dipoles screen the external magnetic field and prevent the field from pass through the material. The material repel external magnetic fields this type of material have negative magnetic susceptibility in that, the alignment is against the field causing it, and in the absent of the field the material loss this alignment.

1.5.4 Paramagnetic material:

these are materials that their magnetic dipoles in the absence of external magnetic field has no alignment, and are generally nonmagnetic as the net magnetic moment of the material is zero, but when an external magnetic field is applied to them the magnetic moments of the material align themselves parallel to the external magnetic field, this type of material are said to have positive susceptibility to external magnetic field, the magnetization of a material is affected by the temperature of the material, because when the thermal energy of the material increases the entropy of the atoms, electrons and magnetic dipoles increase and this favours randomness, hence magnetization of paramagnetic material is directly proportional to the magnetic field and inversely proportional to temperature (Stephen, 2001). the magnetic susceptibility of these material is shown as the left sketch in fig1.2. The magnetic susceptibility of these materials increases non linearly with decrease in temperature. The plot of their inverse susceptibility shows that the follow the curies law $\frac{C}{T}$ where the plot has a zero intercept as it shown in fig1.3a.

1.5.5 Ferrimagnetic materials:

These materials have similar magnetic property to antiferromagnetic material in the sense that the magnetic dipoles point in an antiparallel direction to each other but the difference is in ferrimagnetic materials the magnetic moment is stronger in one direction than the other as shown in the figure below. Ferrimagnetic materials their magnetic susceptibility responds deviates from the paramagnetic trend at temperature T_N known as the Neil temperature, at temperatures below the Neil temperature the magnetic susceptibility of the material starts decreasing slowly and will have a positive intercept on susceptibility axis at T = 0 as shown in the center figure in fig1.2.

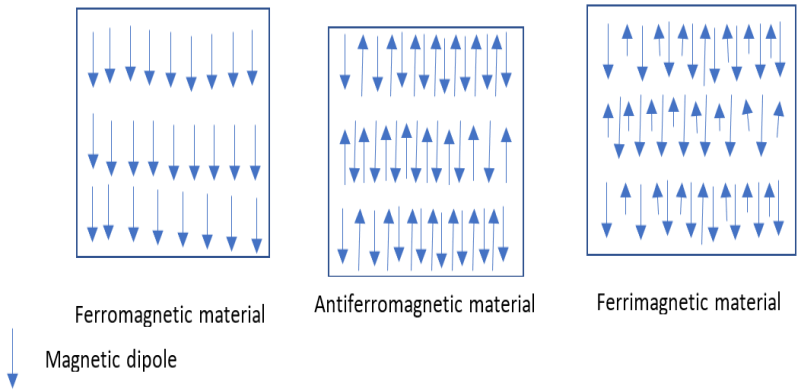


Figure 1.1: Magnetic ground states

The responds of this materials magnetic susceptibility to temperature can be explained using the graph in fig 1.2

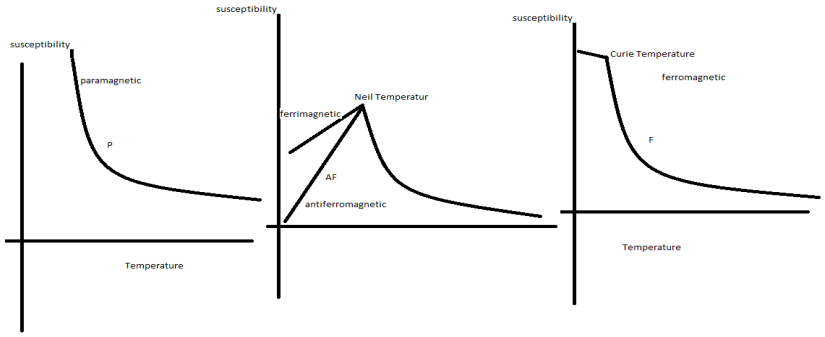


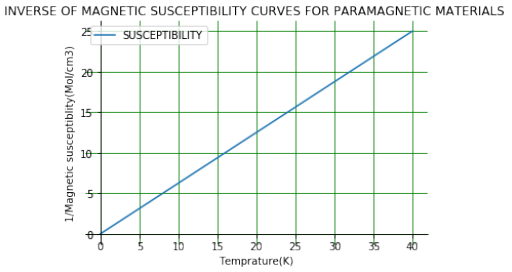
Figure 1.2: Magnetic susceptibility

From fig 1.2 it can be seen that at higher temperatures all magnetic materials has a characteristic magnetic susceptibility respond that is similar to that of paramagnetic materials. In ferromagnetic materials F the magnetic susceptibility is seen to have a sharp rapid increase in magnetic susceptibility at lower temperatures below the curie temperature. At this temperature these materials magnetization rapidly saturates to a fixed value, this is because the material has totally become magnetic, and tend to retain this magnetism even when the external magnetic field is removed. The graph of the inverse magnetic susceptibility of this material deviate from the curie

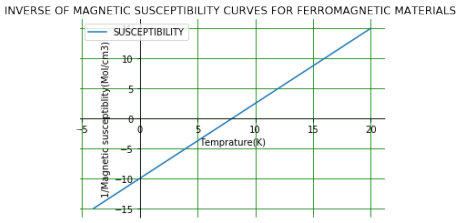
law($\chi = C/T$) , which is a straight line through the origin, instead for ferromagnetic materials the straight line has a positive intercept on the temperature axis, this behavior is properly accounted for by the curie Weiss law.

Curie Weiss Law: This law describes the magnetic responds of a material to external magnetic field at a given temperature, it is written as

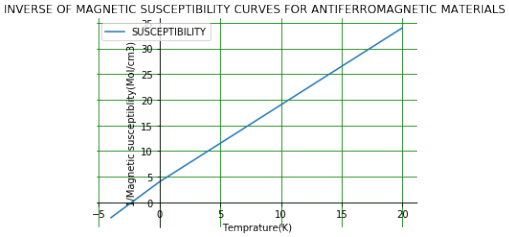
$$\chi = \frac{C}{(T - \theta cw)} \tag{1.13}$$



(a) starts from origin



(b) has positive intercept on temperature axis



(c) has negative intercept on temperature axis

Figure 1.3: Curie Weiss behavior of various material expressed as a plot of inverse susceptibility

1.6 One dimensional magnetism:

This is the term used to describe the magnetism that occur along a line or chain. This generally is a line of spins connected through atomic bonds, electrostatic interaction and/or exchange interaction, a line of such spin is known as spin chain (Stephen, 2001) This spin chain can be either Ising spins chain if they can only be oriented up or down or Heisenberg spin chain if the spins can point in any direction with no restriction. In the case of 1D Heisenberg system the major part of the interaction energy is accounted for by the various exchange interaction in the material. The magnetic part of

these exchange interactions is a major source of magnetic behaviour, and for a simple system where the orbital contribution to the magnetic moment can be ignored the Hamiltonian can be written in terms of spin only contribution for example in a Heisenberg spin 1/2 chain the magnetic part of the exchange interaction can be written as shown in (Stephen, 2001) Generally, a spin chain is named based on the sum of the spin value of the unpaired electrons in the magnetic atom/ion/unit in the crystal or material, for example a compound with a atom with one unpaired electron form a spin $\frac{1}{2}$ chain, and those with atoms with two unpaired electrons has a spin 1 chain and so on.

Bonner and Fisher (1964) described a general Hamiltonian in terms of the spins only as

$$H = 2J(\gamma s_i s_j + (1-\gamma)s_i^z s_j^z) \tag{1.14}$$

where $\gamma = 0, 1, 2, 3$, determine the spin model, the numerical analysis by **Bonner and Fisher** provided a good refrence point to the various investigation to this lower dimensional quantum magnetic systems. The Hamiltonian of interest to us is that of $\gamma = 1$. This model have two possible type of chains the halve integer spin chain (Heisenberg) and the whole number spine chains (Haldane) chains. The correlation between the spins in a chain can be ferromagnetic if the exchange integral **J** is negative or antiferrromagnetic if **J** is Positive. The magnitude of **J** defines the strength of the magnetic property of thee spin chain. This can be calculated from the magnetic susceptibility and heat capacity as a function of temperature graphs of the material. Calculating for **J** from the magnetic susceptibility curve the equation 1.15 can be used.

$$|J| = \frac{T_{max}}{0.640851.|K_B|} \tag{1.15}$$

(Bonner and Fisher, 1964 as in Savina et al., 2011) Where T_{max} is the temperature at which the material has maximum susceptibility and K_B is the Boltzmann constant

J can also be calculated from the peak of the magnetic susceptibility of the material by fitting the magnetic susceptibility peak of a material to the expression

$$\chi = \frac{(N(g\mu_B)^2)}{(K_B T)}\left(\frac{(0.25 + 0.14995\frac{J}{T} + 0.30094(\frac{J}{T})^2)}{(1 + 1.982\frac{J}{T} + 0.68854(\frac{J}{T})^2 + 6.0626(\frac{J}{T})^3)}\right) \tag{1.16}$$

Where $J = |J|/K_B(K)$. where J is the exchange interaction of the nearest neighbor, N is the number of chains g is the g tensor K_B is the Boltzmann constant and T is temperature . J can also be calculated from the heat capacity as a function of temperature in the material using the expression

by **Bonner and Fisher**

$$C = 0.35NK_B(\frac{K_BT}{|J|}) \tag{1.17}$$

for a Heisenberg system. where C is the heat capacity and K is Boltzmann constant and N is the number of chains. This numerical approximations provides an insight into what to expect when investigating a given spin chain and the equations can be used in combination with experimental results to estimate the exchange interaction in the chain.

The magnetic susceptibility curve of low dimensional magnetism show a broad peak at low temperature (Boghosian et al., 1995)

Example of materials that have the spin 1/2 chain include V^{+4} compounds like $\beta - TeVO_4$, Cr^{+5} compounds etc (Boghosian et al., 1995).

1.7 Heat capacity:-

Heat is a form of energy that is attributed to the kinetic energy of the molecules/atoms of a material. In solids this kinetic energy results from the vibration of the atoms of the solid about a mean position and the amplitude of this vibration is proportional to the amount of heat in the solid. In other words heat can be attributed to the internal energy of the solid. In crystals where the atoms are in periodic arrangements and joined by bonds. The atoms and bonds set up, build up in to a mesh or network of atoms bonded together into a solid such that the vibration of one atom set other atoms into some kind of vibration too. The frequency of this vibrations depends on the internal energy of the system, this internal energy is heat energy, the amount of heat need to rise the internal energy of a crystal by 1K is known as the heat capacity of the system at the initial temperature. the amount of heat required to increase the frequency of vibration of the atoms of a crystal varies non linearly with temperature. the theoretical frame work on how this vibrations defines the amount of heat required to rise the temperature of a material was put forward by **Einstein and Debye** thus:

1.7.1 Einstein Model:

Einstein assumed that all the natural modes of vibration or phonon modes have the same frequency and independent of each other, each of the N modes has three degree of freedom, hence there are $3N - 6$ modes of vibration for a system with N independent particles where 6 represent the translational and rotation degree of freedom of the entire solid, in a typical system this number

of mode is appriximatle 3N, for a large N (Blundell & Blundell, 2009). The energy distribution of the system can be written as a sum of all the partition function of each mode in the crystal as shown below, written as presented by (Blundell & Blundell, 2009)

$$Z = \Pi_{i=1}^{3N} Z_i \tag{1.18}$$

Where Zi is the partition function of the individual mode, hence taking the log of both sides gives

$$Z = \sum_{i=1}^{3N} lnZ_i \tag{1.19}$$

where Z_i is given by

$$Z_i = \sum_{n=0}^{\infty} e^{-(n+\frac{1}{2})\hbar\omega_E\beta} \tag{1.20}$$

$$lnZ = 3N(-\frac{1}{2}\hbar\omega_E\beta - ln(1 - e^{\hbar\omega_E\beta})) \tag{1.21}$$

Differentiating the equation above with respect to the β, the internal energy of the solid is given b y

$$U = \frac{3N}{2}\frac{h}{2\pi}\omega_E + \frac{3Nh\omega_E}{2\pi e^{h\omega_E} - 1} \tag{1.22}$$

Writing the internal energy in terms of temperature by replacing $\hbar\omega = K_B\Theta_E$ where Θ_E is the Einstein Temperature of the of the system. The specific heat capacity of the material can be calculated by differentiating the internal energy of the material with respect to the thermodynamic temperature.

$$U = 3R\Theta_E([\frac{-1}{e^{\frac{\Theta_E}{T}} - 1}]e^{\frac{\Theta_E}{T}}[\frac{\Theta_E}{T^2}]) \tag{1.23}$$

From the equation above taking limits we see that specific heat capacity approaches $3R$ as temperature approaches infinity or becomes larger and specific heat capacity approaches

$$(\ 3R(\Theta_E/T)^2 exp(-\Theta_E/T) \tag{1.24}$$

as Temperature becomes smaller.

1.7.2 Debye Model:-

In this model the Einstein assumption of common frequency for all natural modes was adjusted to account for other possible frequency by assuming a range of frequencies for the natural modes of vibrations in the crystal sums ups to 3N the limit of this frequency range is known as the Debye frequency. Secondly Debye model assumes that all the lattice vibrations have the same speed and a wave vector, combining the wave vector and density of state of the natural modes and integrating over that range of frequencies to obtain the internal energy of the system In summary the Einstein and Debye model of specific heat capacity are theoretical approximation to the behaviour of specific heat capacity of materials with increase in temperature. these theories tries to connect thermal vibrational frequencies to the internal energy which in turn define the specific heat capacity of the material, in clear terms the Einstein and Debye model connect the vibrational mode of a crystal to the specific heat capacity of the crystal. but in practical terms the experimental results do not march the theoretical models because of other factors, for instances the assumption that all the vibrational models in Einstein have the same frequency is often not true as is shown in the Raman spectrum of the same crystal. as the Raman active modes have different frequencies and energy.

Chapter 2

Experimental methods

2.0.1 Sample Preparation Of $\beta - VOSO_4$:

The $\beta - VOSO_4$ used in this studies was prepared by ***Katrin Mayer-Kirchner and Angela Benitez Castro and D. L Quintero-castro****, at Helmholtz Zentrum Berlin (HZB).*

$\beta - VOSO_4$ was prepared by heating 3g of V_2O_5 in 100ml of H_2SO_4 up to a temperature below the boiling point of 290^{o}C in a conical flask and the vapour from the flask is condensed using fractional column. The equation of the reaction is given below

$$V_2O_5 + 2H_2SO_4 - 2\beta VOSO_4 + 2H_2O + 0.5O_2$$

The reaction was slowly heated and cold at a rate of $135^oC/h$ and $300^oC/h$ respectively. The crystals were allowed to grow for 3 months which result in a dark green needle-like single crystals which grow up to 6mm, the crystals were washed in ice water bad multiple times and dried at 110^oC for 12 hours.

2.1 X-ray Diffraction:

This experimental technique is employed in the investigation of structural features of materials like crystals. The technique basically uses x-rays which are electromagnetic waves of wavelengths of magnitude 1Å to 2Å. X-rays wavelength is equivalent to the atomic spacing between atoms in a crystal. x-ray diffraction technique use the wave property of x-ray known as diffraction (which is the ability of waves to bend around obstacles, in this case, atoms of a crystal). When a monochromatic x-ray beam is incident on a crystal the x-ray interact with the electron cloud around the atoms of the crystal, this interaction results in what is known as atomic scattering. The periodic

arrangements of atoms in a crystal implies a periodic sites of interaction with the x-ray and periodic arrangement of scattered rays since the atoms of the crystals have periodic arrangements this implies that the atoms are arranged in planes. the planes of a crystal is defined by it (hkl) (miller indices) . The position of the atoms in the crystal is related to (hkl) value, since these planes are periodic the distance between parallel planes is known as d_{hkl}, the scattered x-rays from the periodic atoms of the crystal interfere as the travel in a given direction, the nature of the interference observed is dependent on the angle of incident of the x-ray and the path difference between the scatted rays. From Bragg's law constructive interference are observed when the incident angle on a given plane θ (Bragg angle), the wavelength λ, of the x-ray and the distance between the parallel plans d_{hkl} satisfies the the relation

$$\lambda = 2d_{hkl}sin\theta \tag{2.1}$$

Depending on the crystal class and space group certain planes in the crystals produce reflections while others do not. The intensity of the diffracted x-ray detected can be calculated using various equations depending on the type of method used in the experiment and the size of the sample been irradiated with the x-ray. For the purpose of these work we will only focus on powder x-ray diffraction.

The powder sample of the crystal is use, this powdered sample have the crystals randomly arranged such that in a give small ring large number of the crystals are oriented such that they satisfy the Bragg law for all the possible plans. the method of illumination can be either rotating source where the x-ray source rotated round the sample or rotating sample technique. The x-ray detector is mounted at angle 2θ to the source this relation is Maintain by the goniometer. The intensity of the x-ray is calculated using equation 4.10 in (Waseda et al., 2011), of the x-ray is fitted through Rietveld refinement

From the intensity values the atomic position of the sample can also be obtain and the general crystal structure can be plotted, this is also automated and several computer applications like VESTA can solve.

2.1.1 X-ray Diffraction Experimental procedure:

X-ray diffraction of $\beta - VOSO_4$ used in the work was performed by ***Pavel Karen and Diana Quintero-castro,*** *L at the university of Oslo (RECX)*

the x-ray instrument was calibrated as follows:

- The geometry of the transmission diffractometer was calibrated at 296K on a NIST Standard Si of a= 5.431201A.

- The refined diffractometer parameters K to fit the standard were lamdda = 1.54397Å, Z=-11.27(the Z is the true position of zero in centidegrees on the 2 theta scale of the diffractometer).
- The wave length of the x-ray used is 1.54397Å.
- 7.021mg of $VOSO_4$ were grinded into powder and placed in the sample holder of the x-ray diffractometer.
- $CuK\alpha$ x-ray of wavelength 1.543120Å was used to illuminate the sample as it is rotated to vary the angles of .
- The brag angle 2θ and the intensity of the diffracted x-rays was measured and analyzed.

2.2 Neutron diffraction:

Neutron diffraction time of flight experimental technique is an experimental technique in which neutrons are generated and pass through a pulse generating mechanism before getting to the experimental sample, which then diffract the neutrons onto a detector from which the energy and intensity of the diffracted neutron is measured. (Voss et al., 2007). A typical neutron diffractometer as was described in (Copley & Udovic, 1993) should have the following essential components

- **Neutron source:** the neutrons are generated in the reactor and passed onto crystal monochromater
- **Monochromator:** consist of layers of crystal incline at angle to the incident neutrons such that only neutrons with wavelength and energy that satisfies the Bragg's relationship $\lambda = 2dsin\theta$ where d is the distance between the layers of the monochromator. The set up is such that the diffracted neutrons are incident on the chopper which is a pulse generating mechanism.
- **Chopper:** this a mechanical component that has gears that open at regular intervals to create the pulsing effect, the opening time help in the timing of the travel time of the neutron from the chopper to the sample and to the detectors which is very important part of the parameter used for calculating the time of flight of the neutron.(Copley, J. R., and Udovic, T. J. 1993)

- **Sample holder:** this is where the sample is placed and position on the path of the neutrons .
- **Detector:** systems is is made of detector banks where the Q factor of the neutrons are measured.

The time of flight of the neutrons from the chopper to the detector = time of flight from chopper to sample + time of flight from sample to detector, because of the diffraction of the neutrons at the sample the energy, wavelength, wave vector of the neutrons also changes depending on which layer or atom a particular neutron ray was diffracted at. The intensity and corresponding time of fight of each neutron ray is measured these data are then fitted and the corresponding atomic positions and lattice parameters of the sample are evaluated by Rietval refinement.

2.2.1 Neutron scattering procedure:

The neutron scattering measurement of $\beta - VOSO_4$ was done with the ISIS high resolution powder diffractometer HRPD by ***Alexandra Gibbs****.*

- The instrument calibration was confirmed to be in range.
- The profile was set to back-to-back expolation pseudo-potential Voigt
- The sample was placed in the sample holder of HRPD.
- The minimum and maximum time of flight was also set for each of the profile.

2.3 Rietveld Refinement:

Rietvel Refinement is the art of fine-tuning the model to the experimental results obtained to a close match to existing data on same compound, to a meaningful values that has realistic implications. Basically it the act of matching curves and analysing the match, The computer program fullprof was used for this refinement, fullprof is an integrated software with various subapplications like the PCR editor,winprof etc. The PCR file is loaded into the software and the non constant parameters of the model (x-ray, neutron diffraction) are numerically minimized toward the matching curve value from the crystals in the given space group this act of minimizing deviation or error is known as Refinement. Refinement of a given set of data is down with strategy to avoid creating a wide divergence that makes your minimization

impossible to converge. The steps used is dependent on the user and the nature of the parameters you want to refine and the information one knows about the crystal space group. PCR file is the information file where all the parameters of crystal are written, it holds information such as links to other information files like the instrument resolution file rif file, x-ray intensity files, the background file. One common strategy to refinement is to refine one parameter at a time. For instance start with the instrument related refinement to get the true instrument parameters into the pcr, the refine the scales to get your matching curves and the experimental result on the same level, Next the scale of the profile is refined not forgetting the zero of the instrument. When all this background information are in range and have selected the appropriate experimental mode for each of the experiment one can the proceed to refine very important parameters like the atomic positions the cell parameters this is done with key focus on on how the outcome minimizes the error and gap between the model and the experimental result, these convergence can be readout as the chi square value, R factor and Bragg R factor of the refinement.

2.4 Magnetic susceptibility:

The nature of the magnetic susceptibility curve also holds typical information for the confirmation of the type of the spin chain the crystal has and from the peak values of such graph and the graphs of inverse magnetic susceptibility the exchange interaction can be calculated, hence the need for a magnetic susceptibility experiment. The magnetic susceptibility experiment was performed at ISSP Tokyo by **D, Quintero-castro**, using MPMS3 Superconducting Quantum Interference Device (SQUID) which is a multipurpose device that can measure magnetic susceptibility of a sample at various temperature and magnetic field strength with high resolution results. MPMS3 SQUID can measure magnetic susceptibility of a sample at the temperature range of 1.8K to 400K, and has a cooling rate of 30K/min the temperature of the device is regulated using liquid helium. The liquid helium is use to cool the sample and probe. SQUID MPMS3 has the magnetic sensitivity of the order of $10-8$ emu and has a maximum magnetic field range 7 Tesla and minimum of 0.4mT. MPMS3 SQUID can be operated in DC scan mode and AC scan mode. In the DC mode as the sample is scan through the gradiometer a screening current is induced in the gradiometer which has the SQUID attached to it, the screening current generated a voltage wave form in the gradiometer, the magnetic moment in the sample at that condition of the sample can then be 3calculated from the voltage induced in the super con-

ducting coil in the SQUID. In this device the sample is loaded onto a sample probe which is then set into vertical oscillated in a closed superconducting chamber. The motion of the sample (if magnetic) generates an induced emf in the coils in the chamber and the magnitude of this emf is proportional to the amplitude of the vibration of the sample in the probe. The induced current is the measured by the SQUID located at the base of the probe. The SQUID is a good linear current to voltage converter.

The case of our sample which is $VOSO_4$, (V^{+4}), which has a nonmagnetic singlet ground state, the present of the unpaired electron in the spin $\frac{1}{2}$ chain with a low exchange interaction energy, the temperature variation excite the electrons spins hence inducing current signal in the super conducting coil. In our experiment 7.021g of $\beta - VOSO_4$ was placed in the sample holder inside the probe and the magnetic susceptibility and temperature of $\beta - VOSO_4$ was measured and the result contained in the data file is saved for the three magnetic field directions.

2.4.1 TGA/DSC

The question of weather the sample has water of crystallization was investigated using a metter toledo's Thermogravimetric Analyzer TGA machine at UiS, The TGA experiment was performed using a thermodynamic profile with heating rate of 10^oC per minute starting from 25^oC to 500^oC, The change in weight of the sample with increase in temperature and amount of heat flow was measured and recorded. The initial and final mass of the sample was measured and analyzed to confirm the the existence of water of crystallization. For each sample loaded into the TGA machine the measurement is done twice, first heating the sample up to 500^oC, normally if the sample has any water of crystallization it will evaporate at this high temperature leaving the dry sample behind. after cooling the supposed dried sample is heated again, if the sample had water of crystallization from the onset the second TGA graph will differ greatly from the first one both in initial mass and final mass. the second profile which is stable will have little or no variation in the mass of the sample at the end of the experiment and the mass different will be larger than the instrument error range. in this thesis a set of 6 TGA experiments where performed two under nitrogen and four with air environment. DSC experiment was conducted using sapphire method to measure the the heat capacity of the sample measured as a function of temperature.

2.5 Raman Spectroscopy:

Raman Spectroscopy is the study of light resulting from Raman effect. The Raman effect is an inelastic light scattering effect in which an incident light radiation gets absorbed by an atom/electron and the atom/electron emits light radiation of different energy from the incident absorbed ray. This effect involves electrons of an atom initially at a stable energy level En before absorbing photons of the incident radiation which excites the electron to a higher unstable energy state E, from which this electron drops from to a new stable energy level that can be En±x. If the electron drops to a lower energy level the photon emitted has higher energy than those of the incident photon and this is known as anti stocks scattering but if the electron returns to an energy level higher than En the photon emitted is of lower energy than the incident ray that is known as stocks scattering. Reman spectroscopy is plot of the shift in wavelength of the incident ray against the intensity of the scattered radiations, the intensity of reman scattered radiations is proportional to the population of electrons having the same energy change to this energy level, this has statistical dependence and best described by boltzman distribution. The intensity of the raman scatter radiation is related to the change in wave number thus:

$$I\alpha(1/\lambda_0 - 1/\lambda_f)^4 \tag{2.2}$$

The Raman scattering just like x-ray scattering is a characteristic scattering and hence hold the finger print of the compound or material, Raman spectroscopy can be use to identify crystals and even differentiate crystal phases of the same compound. Raman spectroscopy experiment generates a plot, showing the intensity of raman scattered lasers agent the frequence shift of the laser in wave number,

Raman active modes: this describes mode of vibrations in the molecule or crystal that favours Raman scattering because the result in the deformation of the polarizability ellipsoid. This deformations increases the probability of electrons been excited to the virtual states returning to an electronic state of different energy. Since Raman effect is a photon effect it involves the excitation of surface electrons, which are mostly involve in bound formation hence the electronic bonds in a compound is a site of interest in Raman spectroscopy. Raman lines are assign to bonds between atoms or groups in a crystal and the intensity of this lines define the population density of this bounds in the Raman effect, for example in $VOSO_4$the $(V = O)$, (Boghosian et al., 1995)has the highest intensity, this is partly because the number of electrons in the pi bond is higher and the bound is a lot weaker, so the population of electrons in this bound is twice higher than those in the sigma

bounds. the Raman spectroscopy looks at the mode of vibration of the moles at the ground state and also help to confirm the number of mode of vibration in the system that are raman active to a given light of frequency,

Chapter 3

Structural Analysis of $\beta - VOSO_4$

3.1 Atomic structure of $\beta - VOSO_4$

The structural analysis on $VOSO_4$ requires a combination x-ray diffraction and neutron diffraction experiments because the low number of electrons in oxygen atom makes it difficult for x-ray diffraction to pick up their position and considering the number of oxygen in our sample x-ray diffraction alone will be misleading, the neutron diffraction is not good with vanadium because of the large incoherent scattering produced when neutrons interact with vanadium. The x-ray diffraction experiment was performed on $\beta - VOSO_4$, from the result, the graph of the Bragg angle 2θ was plotted against the intensity of diffracted rays. This is shown in figure 3.1

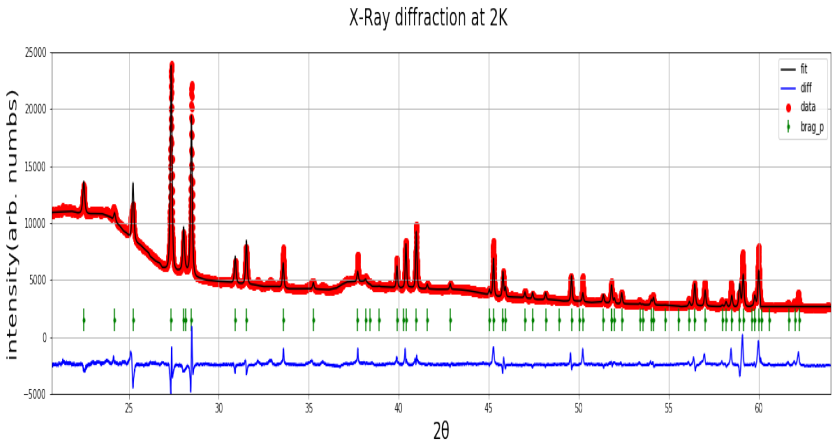


Figure 3.1: X-Ray diffraction

Fig 3.1 shows three graphs and the Bragg positions of the peaks in green. the experimentally measured data shown in red label "data" the black graph is the calculated values while the blue graph is the difference between the calculated and measured values or the matching curve. From the graph, the maximum intensity was observed at the crystal plane (201), the lift in the zero of the x-ray plot is the background noise from the glass slate used, hence the variations seen in the fitting curve in black. The intensities measured in the graph are relative intensities of the diffracted rays observed. Fig 3.2 show the neutron diffraction graph for $\beta - VOSO_4$, it is a graph intensity of diffracted neutrons against the lattice spacing d(Å)

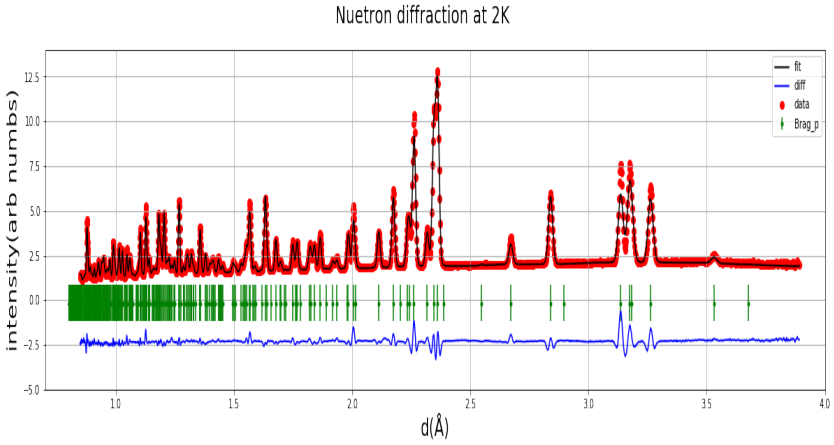


Figure 3.2: Neutron diffraction

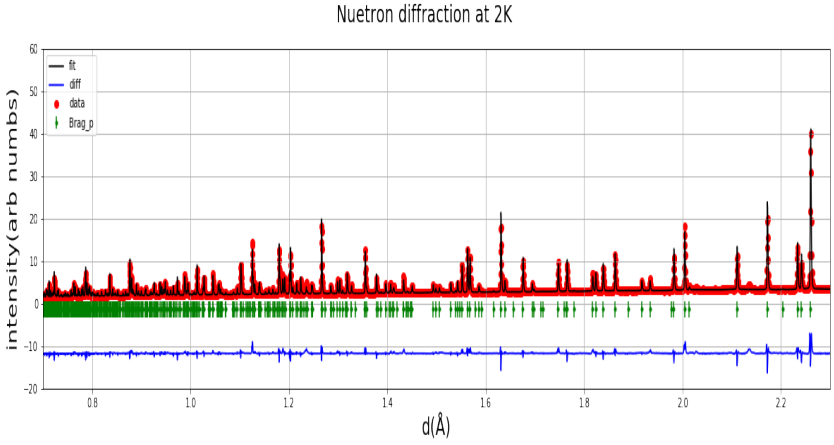


Figure 3.3: Neutron diffraction

Rietveld refinement of the results from the experiments gives the crystallographic parameters as well as the atomic positions of the atoms in the crystal as is shown in table 3.1,

atom	x(Å)	y(Å)	z(A)	b(Å)	occupation
V1	0.16364(127)	0.25(0)	0.23748(140)	0.05(0)	0.5
S1	0.87406 (126)	0.25(0)	0.87408(92)	0.05(0)	0.5
O1	0.71441(53)	0.25(0)	0.98821(70)	0.05(0)	0.5
O2	0.04463(54)	0.25(0)	0.97938(67)	0.05(0)	0.5
O3	0.37423(79)	0.25(0)	0.16946(49)	0.05(0)	0.5
O4	0.11908(86)	0.56241(36)	0.25824(40)	0.05(0)	1.0

Table 3.1: Atomic Positions extracteed from combine refinement of x-ray and neutron data at 2K

lattice parameter	length (Å)	reff1(Å)	reff2(Å)
a	7.36022(11)	7.3789(14)	7.376(3)
b	6.27603(12)	6.282(2)	6.269(5)
c	7.06650(12)	7.0761(8)	7.082(3)

Table 3.2: Lattice parameters, reff1: (Paufler et al., 2014),reff2: (Boghosian et al., 1995)

Atomic structure is a detailed description of the atomic positions and bonds between different atoms of elements in a unit cell of a crystal, these positions are measured relative to a reference point in the crystal. $\beta - VOSO_4$ has been described as a single crystal which has lattice parameter $a = 7.3789(14)\mathring{A}$, $b = 6.282(2)$Å, $c = 7.0761(8)$Å, and unit cell volume of $328.0(1)\mathring{A}^3$. Formed from a chain of corner sharing VO_6 octahedra arranged along the a and c axis connected through SO_4 tetrahedra (Paufler et al., 2014) $VOSO_4$ was stated to have a slightly different values in lattice parameters of a=7.376(3)Å, b=6.269(5), c=7.082(3)Å, formed from the bonding of distorted VO_6 zigzag chains parallel to the a axis with SO_4 group referred to as bridging Sulphur group (Bocquet et al., 2001). All the reference in the literatures on $VOSO_4$ all agree that it an orthorhombic crystal belonging to the space group pnma 62.

From the refined data of the combine x-ray and neutron diffraction shows that $\beta - VOSO_4$ has the lattice parameter show in **table 3.2** and unit cell volume of $326.491\mathring{A}^3$. The structure and bounding of $\beta - VOSO_4$ was described

to have two zig zag spin 1/2 chain formed by Vanadium-Oxygen-Vanadium (V-O-V) is surrounded by four SO_4 group, thus completely isolating the chains from each other (Boghosian et al., 1995). Each Vanadium atom is directly bonded to six Oxygen atoms with a slightly varying bound length in all four equatorial directions on the bc plane, ranging from 1.965Å to 1.99Å, (Boghosian et al., 1995). This distance is close to 1.99 to 2.02Å that was found by Paufler et al., 2014 measured at $300K$. Fig 3.4 shows a unit cell of $\beta - VOSO_4$. the vanadium atoms are coloured blue marked V1, Sulphur is coloured yellow and marked S1 while oxygen is coloured red and marked O1 to O4. The chain described as zig zag in (Boghosian et al., 1995) is the V1-O3-V1 seen in fig 3.4. the building block of the crystal is the $VOSO_4$ unit which has the chemical structure shown bellow, where the VO group is attached to the SO_4 group. Though the crystalline structure of $VOSO_4$ is different from the chemical structure, in the crystal structure the building unit can be ordered to show VO_5S. A close look at table 3.2 and comparing the values we got with the once in reff1 and reff2 from (Paufler et al., 2014) and (Boghosian et al., 1995) paper their is a good correlation between our result and those obtained there.

Fig 3.5 to fig 3.7 shows the unit cell of $\beta - VOSO_4$ viewed from different crystallographic directions.

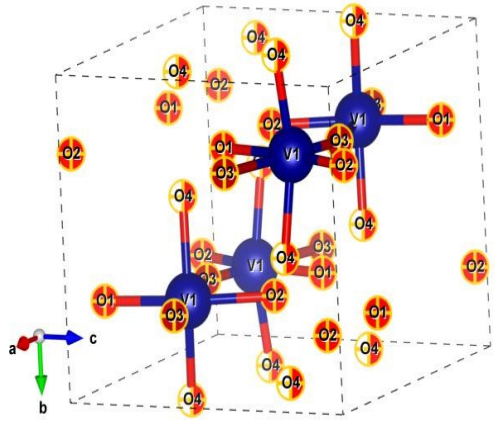


Figure 3.4: unint cell showing oxygens attached to vanadium

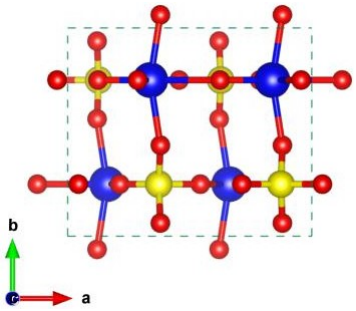


Figure 3.5: unit cell viewed from c axis

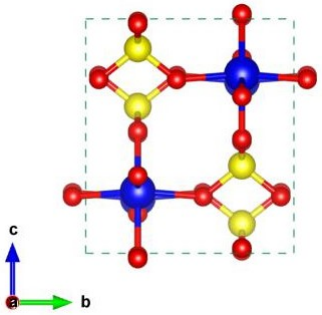


Figure 3.6: unit cell viewed from a- axis, plot generated from VESTA

Each Vanadium atom is bonded directly to six oxygen atoms, one of the oxygen is from the neighboring VO_5 group, the oxygen in V1-O3 that is from a given VO_5‘ group is called the apical oxygen (Boghosian et al., 1995). From our results, There is clear variation in the bond length between the Oxygen-Vanadium-Oxygen (O-V-O) bonds, where the (V1-O3) bond is shorter at a distance of 1.5976(17)Å, while the other (V1-O3) bond is longer at 2.2705(18)

Å, this quite close to the values of 1.61 Å for the short bond and 2.27 Å for the long bond. obtained at 300K by (Paufler et al., 2014), and the same values of 1.598(2)Å and 2.271(2)Å found by (Boghosian et al., 1995). Fig 3.8 show that there two V-O-V chain in a unit cell and are position diagonally on the bc plane or the (100) at a distance of 4.89527(0) Å, the Vanadium atoms are slightly displaced from each other at an angle of $72.73^o(0)$, the V-O-V bound is slightly bended in and out alternatively giving the bond a zig-zag look (Boghosian et al., 1995). This is as a result of the V-O-S-O-V bound between neighboring Vanadium atoms this bond tend to pull the V-O-V chain toward the SO_4 group. The bound occur alternatively on both sides of the chain.

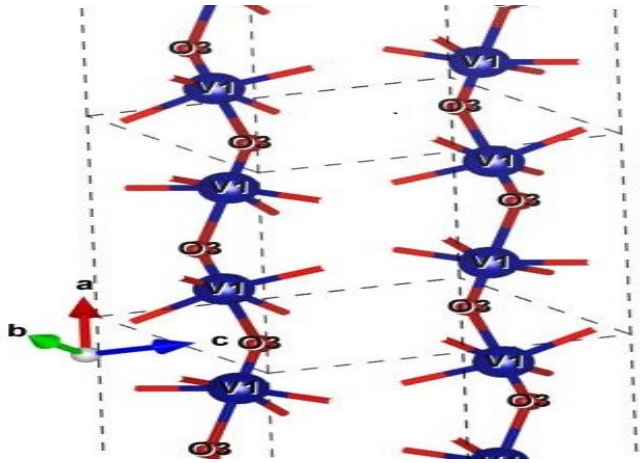


Figure 3.7: V-O-V chain parallel to a

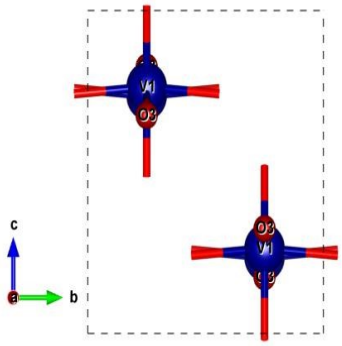


Figure 3.8: bc plan showing chain position

Generally the structure from our analysis is structurally the same as those previously examined at 300K with difference in lattice parameter and bound length which we can attribute to thermal expansion of the crystal.

3.2 Rama Spectroscopy Result

The Raman spectrum of polycrystalline $\beta - VOSO_4$ at room temperature using a laser of wavelength 488.0nm with laser power of 80mW on a spectral slit of width 6cm show that some Raman active bands exist between 1000 – 1220, 580 – 670, and 400 – 500 cm-1, (Boghosian et al., 1995). These ranges correspond to 1438K – 1619K, 834K – 963K, 575K – 719K, the Raman table from (Boghosian et al., 1995) has the lowest phonon energy at 138K, in this work the Raman spectroscopy of $\beta - VOSO_4$ was performed using Renishaw inVia Raman Microscope with Ar 514 laser with a glass slit of width 6cm and laser power of 80mW.

Fig 3.7 shows the Raman spectrum of $\beta - VOSO_4$, the peak position and intensity was fitted to the Gaussian expressions. The peaks are sifted because of the difference in the wave length of the laser used but taking into account that, the peaks appear at same positions and it safe to say that our $\beta - VOSO_4$ is the same as the one analized by Boghosian et al., 1995

$$a * exp(-0.5 * (\frac{(x-b)}{c})^2) \tag{3.1}$$

where a is the intensity of the peak, b is the position of the peak and c is the width of the Gaussian. to fit the entire spectrum 23 Gaussian where used with each fitting a given peak.

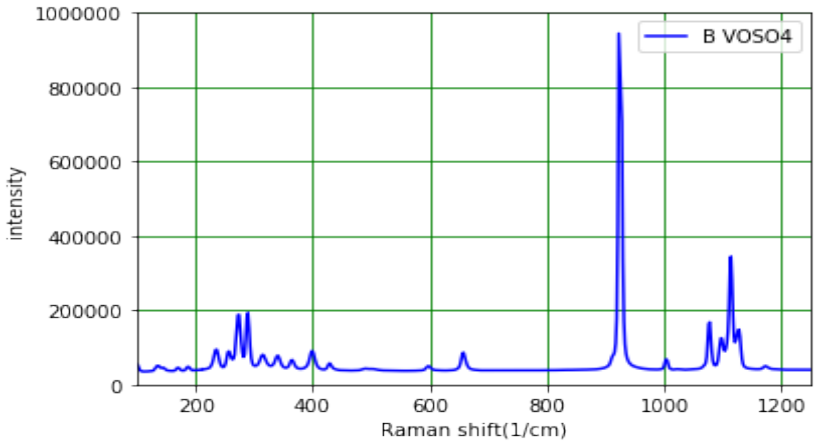


Figure 3.9: Raman spectrum

from which 22 active mode peaks were identified and fitted, as shown below

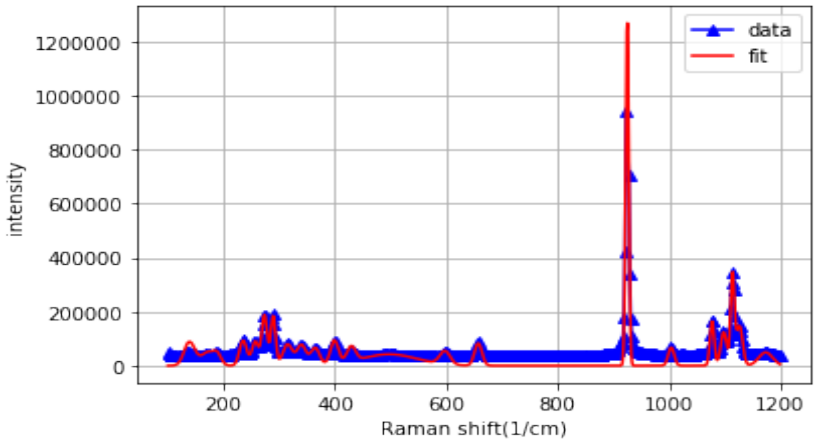


Figure 3.10: Raman spectrum showing fit

Table 3.3 shows the corresponding phonon shifts and the relative strength of the mode. comparing the results obtained and those obtained by (Boghosian et al., 1995) .

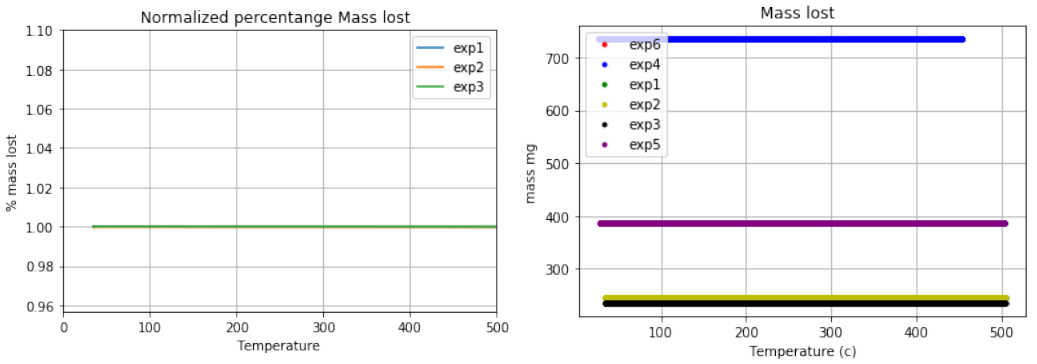
Raman shift (1/cm)	Relative intensity	Relative intensity	reference
135.887633	5.096179e+04	3.995704W	-
144.011365	4.558807e+04	3.574372w	136w
170.089874	4.525474e+04	3.548237w	167w
187.458416	4.819357e+04	3.778659w	184w
235.158753	9.303115e+04	7.294188m	231m
256.885187	8.947872e+04	7.015657m	253w
273.471410	1.868832e+05	14.652742s	269s
289.113289	1.830251e+05	14.350240s	285s
314.904493	7.954225e+04	6.23657m9	311w
339.827481	7.653995e+04	6.00011m	335w
364.342251	6.492138e+04	5.09021m8	361w
398.898434	8.825806e+04	6.919950m	395m
429.061960	5.626659e+04	4.411631w	425w
497.105202	4.231650e+04	3.317862w	488w
597.416719	4.955406e+04	3.885329w	596w
657.292880	8.262376e+04	6.478188m	654m
924.737284	1.275415e+06	100.0000Vs	925vs
1003.723105	6.744972e+04	5.288454	1002s
1077.040837	1.643930e+05	12.889373s	1075s
1097.785322	1.243027e+05	9.746061m	1095m
113.821890	3.338605e+05	26.176624s	1112s
1126.335683	1.465709e+05	11.492021s	1125s
1173.298312	4.940311e+04	3.873494w	-

Table 3.3: Raman bands

3.3 TGA Results

the thermal responds of $\beta - VOSO_4$ to increase in temperature as well as the knowledge of the decomposition temperature, as this information serve as a guide in determining the temperature range in which the compound is stable as well as how the mass of the crystal change with increase in temperature. in order to investigate the stability and reactivity of the $\beta - VOSO_4$ with increase in temperature in the present of oxygen and Nitrogen. fig3.12b show

the change in mas of $\beta - VOSO_4$ as a function of temperature, the mass loss of the compound is normalized and the percentage mass lost is less then 2 percent of the initial mass, when mass lost is measured with reference to the actually mass of the same there is no physical variation in mass see in the graph. these results and observation coupled with calculation for water of crystallization lead to the conclusion that $\beta - VOSO_4$ has no water of crystallization and is stable under heat up to 500^oC



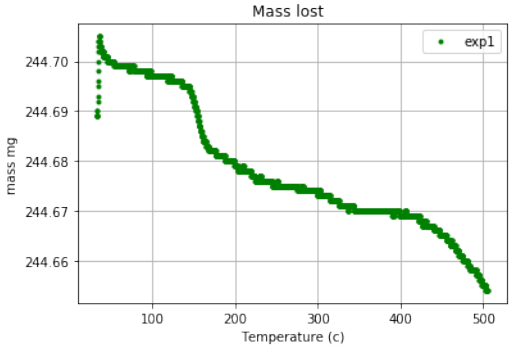
(a) percentage weight lost

(b) mass lost as a function of temperature

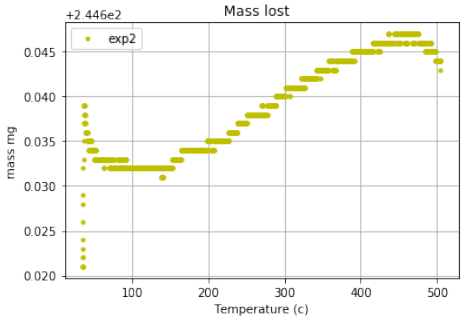
Figure 3.12: Thermogravimetric Analysis (TGA)

Fig3.12 show a constant line in both percentage weight lost and weight lost for each of the experiment, this simple means there is no significant change in mass of the sample or better put the mass of the sample is constant. these goes to confirm finding of Paufler et al. (2014), where the TGA for $\beta - VOSO_4$ remain constant up to the dissociation temperature of 604^oC after which the crystal burn in oxygen to produce V_2O_5 and SO_3.

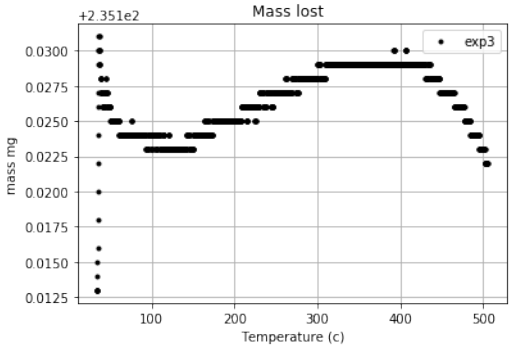
A zoom into the individual experiment at the decimal level a very small variation in the mass of the sample is seen in fig 3.11. This variation is attribute to the mass of the air flowed over the sample as the nitrogen environment experiment has a different trend, indicating a gain in mass of the sample shown in fig3.11b and fig3.11e which are the complimentary experiments. Air environment show an unstable variation in weight, but this variations are within the margin of error, as was stated earlier if they were actual water lost this will be significant and will over shadow the variation seen here. The one to one ratio of water to the vanadium molecule is $\frac{18}{179}$ approximately 10% of the mass, but from what we have seen if fig3.12 it is less than 1% In summary the TGA analysis shows that $\beta - VOSO_4$ is stable under heat up to 500^oC and is a dry solid that has no water of crystallization.



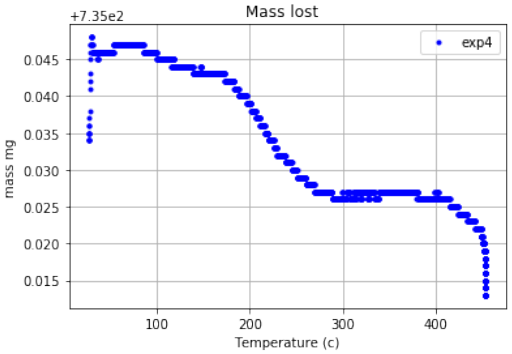
(a) exp1



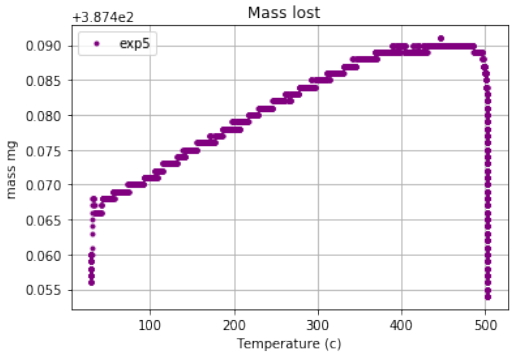
(b) exp2



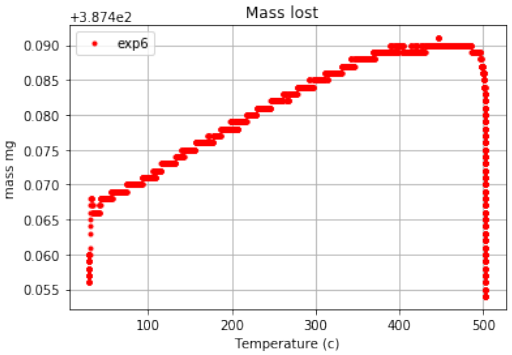
(c) exp3



(d) exp4



(e) exp5



(f) exp6

Figure 3.11: show all the variation in mass recorded by the instrument which are in order of very small fractions of the mass that can be attributed to instrumental error

Chapter 4

Bulk properties of $\beta - VOSO_4$

4.1 Magnetic Susceptibility Results

Fig 4.1a shows the magnetic susceptibility of $\beta - VOSO_4$ for magnetic fields applied parallel to each of the three main crystallographic directions. All the curves have similar behavior with only small deviations. this means that, the material responds to magnetic field in the same way regardless of the orientation of the crystal with respect to the external magnetic field. This implies that the spins in the crystal have no preferred alignment in an external magnetic field, this is one of the characteristic of Heisenberg magnetic chains.

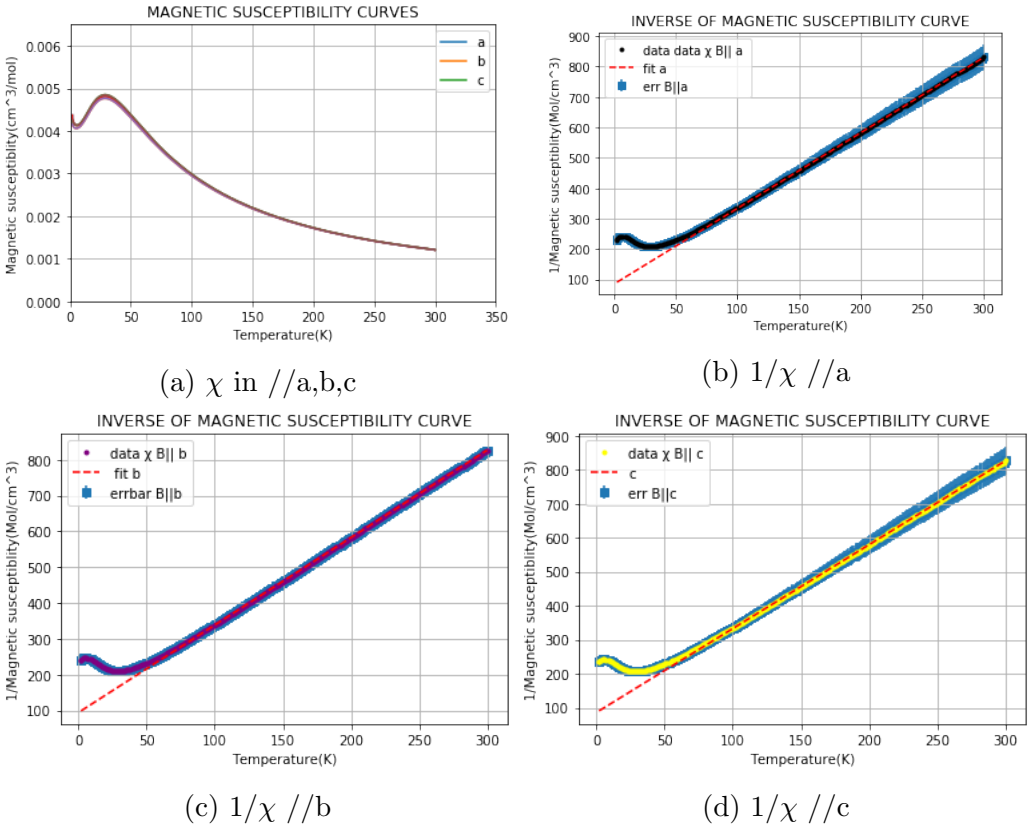
Fig4.1 4.1b,4.1c ,4.1d, show the plots of the inverse magnetic susceptibility for the temperatures above 200K. When these are extrapolated they have a negative intercept on the temperature axis, this temperature is known as Curie Weiss temperature. The values of this intercepts are shown in table 4.3. The negative intercept on the temperature axis is one of the characteristic features of antiferromagnetic correlations. (Stephen, 2001).

The model of inverse magnetic susceptibility shown as red dash lines in fig 4,1(b),(c),(d), has negative intercepts on the temperature axis, this temperature can be interpreted as the temperature where the material has lost all it magnetic properties, the physical implication of this is that the spin or electron in the material is frozen and the material is nonmagnetic. Fig 4.1(b),(c),(d) are plots of inverse magnetic susceptibility against temperature for magnetic fields parallel to the crystallographic directions a,b, c respectively. Fitting the inverse magnetic susceptibility for temperatures above 200K to the Curie Weiss equation

$$\frac{1}{\chi} = \frac{1}{C}(T - \theta_{cw}) \tag{4.1}$$

From the equation above, the Curie constant C for each of the directions

was calculated and tabulated in table 4.2



(a) χ in //a,b,c

(b) $1/\chi$ //a

(c) $1/\chi$ //b

(d) $1/\chi$ //c

Figure 4.1: (a) Isotropy in the magnetic susceptibility in mole per cm^3 (b) $1/\chi$ parallel to a-axis(c) $1/\chi$ parallel to b-axis(d)$1/\chi$ parallel to c-axis

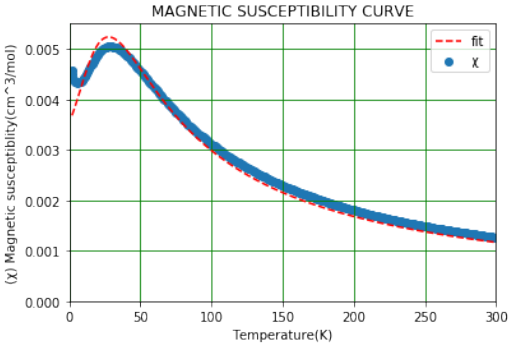
The graphs in fig 4.1a show that the susceptibility of $\beta - VOSO_4$ has a broad peak at low temperature, this is a typical characteristic of magnetic spin chain systems. From fig 4.1a the maximum susceptibility is approximately $0.005cm^3mol^{-1}$ for all crystallographic axis as shown in table 4.3. The magnetic susceptibility of $\beta - VOSO_4$ decreased rapidly from 2K up to 4K, then increased rapidly up to 29.1K where it peaked. From temperatures above 29.1K the magnetic susceptibility of $\beta - VOSO_4$ start to decrease with increase in temperature up to 300K. At temperatures between 4K to 40K the susceptibility curve has a broad peak, The susceptibility curve shows an anomaly between 2K to 4K which can be attributed to paramagnetic impurities in the crystal.

For analysis and fit of the magnetic susceptibility in cm^3/mol against

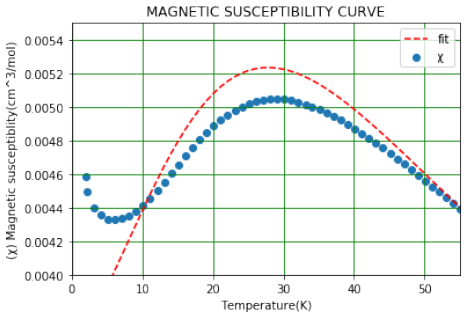
temperature, I modeled it with the **Bonner and Fisher** model

$$\chi = \frac{(N(g\mu_B)^2)}{(K_B T)}\left(\frac{(0.25 + 0.14995\frac{J}{T} + 0.30094(\frac{J}{T})^2)}{(1 + 1.982\frac{J}{T} + 0.68854(\frac{J}{T})^2 + 6.0626(\frac{J}{T})^3)}\right) \tag{4.2}$$

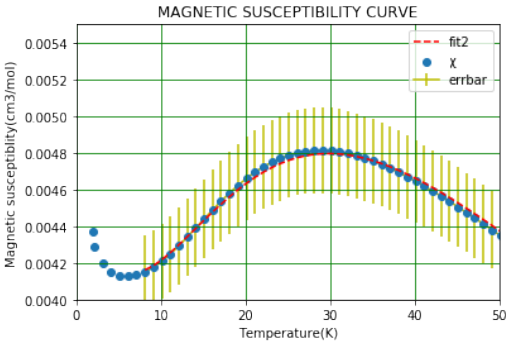
Where $J = |J|/K_B(K)$. where J is the exchange interaction of the nearest neighbor, N is Avogadro's number, g is the g tensor K_B is the Boltzmann constant and T is temperature .



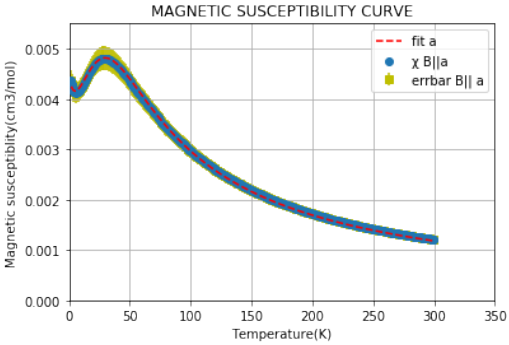
(a) χ in //a, fitted with equation 4.2 show a miss match in the peak and entire curve



(b) χ //a zooming in on the peak

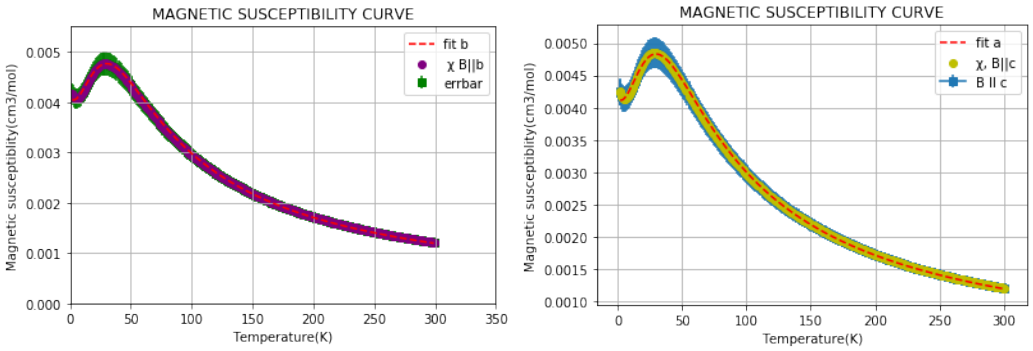


(c) χ //a zoom in to the peak showing matching between the peak and the data



(d) χ //a fitted with equation 4.3 show a miss match in the peak and entire curve

Figure 4.2: magnetic susceptibility for fields along the crystallographic axis a together with fits as it improves with modification of model



(a) χ //b (b) χ //c

Figure 4.3: magnetic susceptibility for fields along the crystallographic axis b and c with fits

Fitting the model with equation 4.2, the model shows a clear resemblance to the experimental data with a miss fit at key areas like the peak and high temperature region of the plot shown in fig 4.2a. The model has a higher peak value compared to the experimentally measured value and at higher temperatures the model is below the experimental plot. At lower temperatures below the peak, there is a clear deviation in the model as the model did not account for the tail of the experimental result. This deviation can be attributed to the impurities in the sample, while around the peak, the model predicted a higher value for the magnetic susceptibility than what was measured experimentally. Both model and experimental result peaked at the same temperature region. If one ignores the higher temperature part of the data, and focus on the peak of the magnetic susceptibility, at temperatures below 100K, the correlation between the experimental data and the model have a close relation with the error range of $0.0002 cm^3/mol$.This is shown in fig 4.2c as zoomed into the peak. The deviation from experimental data at high temperature suggest a deviation from the magnetic behavior exhibited at lower temperature, so in order to account for the higher temperatures the Curie Weiss term $\frac{C}{T-\theta_{cw}}$, is added to the equation4.2 above

$$\chi = \frac{(N(g\mu_B)^2)}{(K_B T)}\left(\frac{(0.25 + 0.14995\frac{J}{T} + 0.30094(\frac{J}{T})^2)}{(1 + 1.982\frac{J}{T} + 0.68854(\frac{J}{T})^2 + 6.0626(\frac{J}{T})^3)} + \frac{C}{(T-\theta_{cw})}\right). \tag{4.3}$$

This further improved the model or fit shown in doted red lines in the graphs in fig 4.2d, the model agrees with the experimental plot at both the lower and higher temperature regions, The model gives the exchange interaction $|J|/K_B$ value of 24.510(99)K and the Curie Weiss constant of

$0.0086(5) cm^3/mol$, along the a direction. the table 4.1 below shows the value of the exchange interaction estimated by the fit for the other directions.

direction	$\|J\|$ (K)
a	24.510(99)
b	25.166(73)
c	25.097(50)

Table 4.1: J from peak fit

Combining the values for the maximum susceptibility obtain from the peak of the curves, and the corresponding temperatures for each direction, the g tensors can be calculated using the expression.

$$g_{tensors} = \frac{\chi_{max} * T_{max} * K_B}{0.064085 * 0.146926 * \mu_B * \mu_B * N_A} \tag{4.4}$$

(Bonner and Fisher, 1964)

From the figures above (figures 4.1(a) -(d)) the g tensors for $\beta - VOSO_4$ ranges from 1.9750 to 2.0508 as is shown in the table 4.1 below. The exchange interaction $|J|$ is given by (Bonner and Fisher, 1964):

$$|J| = \frac{T_{max} * K_B}{0.640851} \tag{4.5}$$

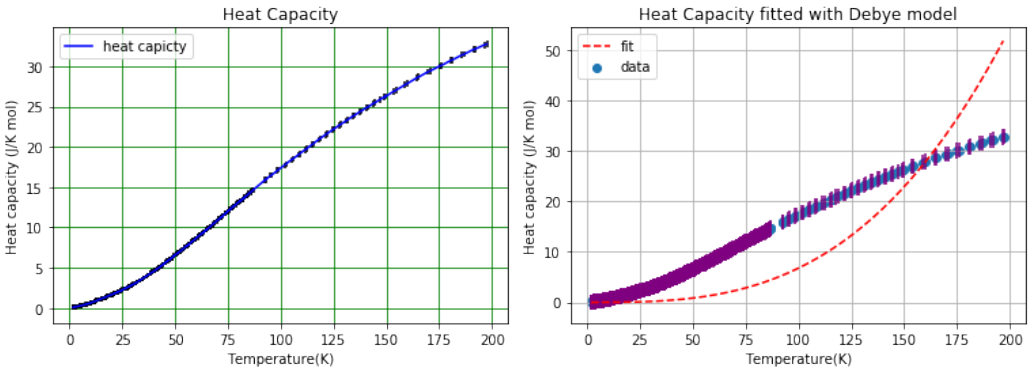
field //	χ $(cm^3 mol^{-1})$	$T\chi max$ (K)	g_{tensor}	$\|J\|$(meV)	$\|J\|$ (K)
a	0.00481(2)	29.10(2)	2.0180(14)	3.913(25)	45.4(3)
b	0.00477 (2)	28.11(4)	1.9540(92)	3.780(12)	43.9(5)
c	0.00485(2)	29.12(3)	2.0299(70)	2.0508(21)	45.4(3)

Table 4.2: $|J|$, g, maximum χ and T_χ

direction	Curie constant $(cm^3 K mol^{-}1)$	Curie Weise Temp (K)
a	0.40377(44)	-34.7592(30)
b	0.40919(27)	-38.4826(19)
c	0.40523(27)	-34.68684(19)

Table 4.3: the Curie constant and Curie Weiss temperature for each axis

4.2 Specific Heat Capacity:



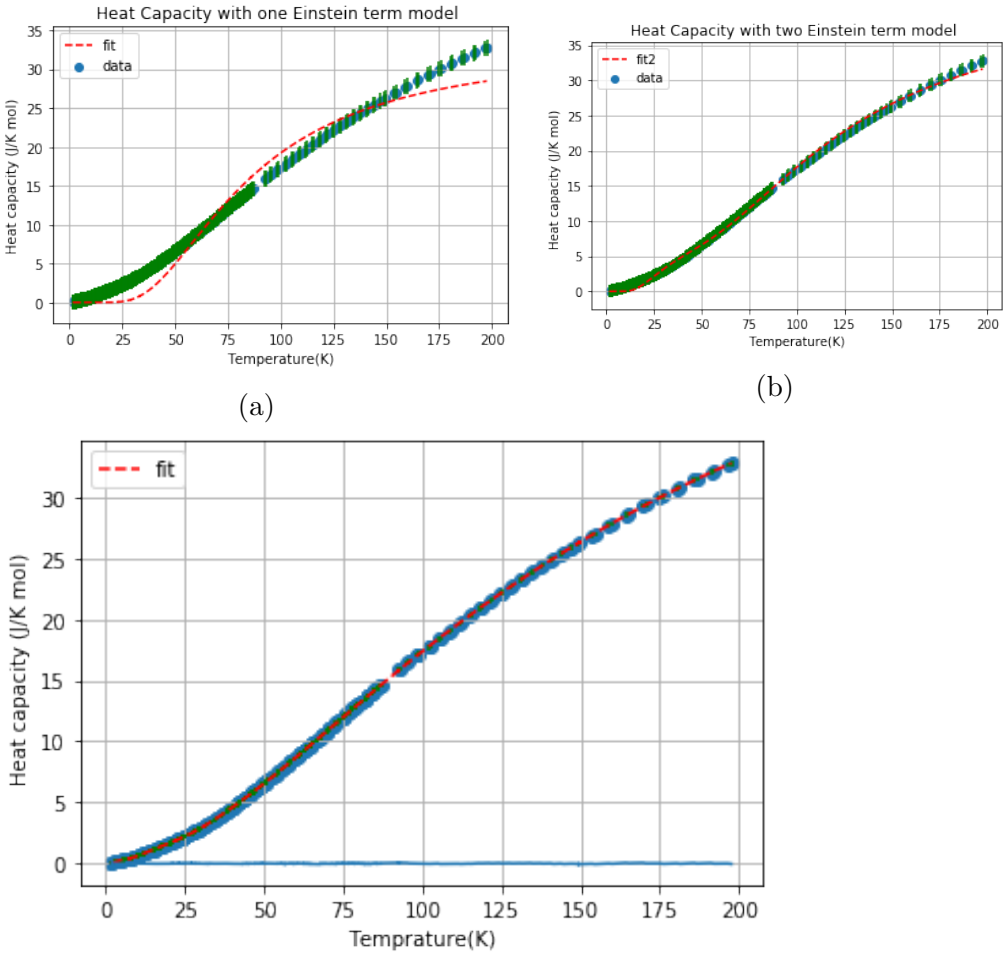
(a) (b)

Figure 4.4: (a) Heat capacity of $\beta - VOSO_4$ against temperature, (b) heat capacity of $\beta - VOSO_4$ modeled with one Debye model.

Fig 4.4(a)shows the measured heat capacity as a function of temperature in $\beta - VOSO_4$. The heat capacity curve plotted as blue solid line, shows a slow increase in heat capacity with increase in temperature up to around 50K, above 50K the heat capacity starts increasing significantly with increase in temperature, this slow increment in temperature is a characteristic feature of hard materials (Byung Shin 2017). The heat capacity has been initially modeled using the Debye model given by equation 4.6 below. In Fig 4.4(b), the doted red line shows the specific heat capacity of a model containing one Debye term given by the equation

$$C = 3R\frac{4\pi^2}{5}(\frac{T}{\theta})^3 \tag{4.6}$$

(Debye as in Blundell and Blundell, 2010) where C is the Specific heat capacity , θ is the Debye Temperature, T is the thermodynamic temperature and R is molar gas constant. From fig 4.4(b) the Debye model for the heat capacity is significantly off both in shape and value, it has an estimated Debye temperature θ_D of 8.98(89)K the Debye model only agrees with the experimental result at very low temperatures below 3K not shown here. above 2K, the Debye model predicts very low specific heat capacity compared with what was measured experimentally between 2K up to 150K above which the debye model is still off but has higher value of heat capacity than what was measured. Upon the addition of more Debye terms the models deviate even more from the experimental result.



(a)

(b)

(c) heat capacity fitted with 3 Einstein terms

Figure 4.5: einstein model improvement

The red doted line in fig4.5a is the Einstein model of the specific heat capacity of $\beta - VOSO_4$ given by the equation, in the model in fig4.5a only one Einstein term. **(A Einstein.)**.

$$C = 3 * 7 * RS(\frac{\theta_E}{T})^2 \frac{e^{(\frac{\theta_E}{T})}}{(e^{(\frac{\theta_E}{T})} - 1)^2} \tag{4.7}$$

where S is the scaling term and R is gass constant. The model has a visible deviation from the experimental result, but the model and experimental result has similar curves.

The model predicts lower values of specific heat capacity at low temperatures between 4K to 50K and predicts higher heat capacity between 75K to 125K after which the model predicts lower temperatures and tend to saturate. The variation in the results predicted by the model and the experimentally measured results can be improved by adding more Einstein terms to equation 4.7 above, and the deviation can be attributed to the Einstein assumption of a common frequency for all modes. On addition of one more Einstein term given by

$$C = 3 * 7 * RS(\frac{\theta_E}{T})^2 \frac{e^{(\frac{\theta_E}{T})}}{(e^{(\frac{\theta_E}{T})} - 1)^2} + S1(\frac{\theta_{1E}}{T})^2 \frac{e^{(\frac{\theta_{1E}}{T})}}{(e^{(\frac{\theta_{1E}}{T})} - 1)^2} \tag{4.8}$$

The model improved significantly as is shown by the red doted lines in fig 4.5b, this shows that there are other modes of vibration with different frequency hence different Einstein temperatures given by θ_{1E} in equation 4.8. The model needs further improvement from observation, to do this more Einstein terms are added, to account for all the possible modes. Fig 4.5c show a fit results to a model with three terms given by

$$C = 3*7*RS(\frac{\theta_E}{T})^2 \frac{e^{(\frac{\theta_E}{T})}}{(e^{(\frac{\theta_E}{T})} - 1)^2} + S1(\frac{\theta_{1E}}{T})^2 \frac{e^{(\frac{\theta_{1E}}{T})}}{(e^{(\frac{\theta_{1E}}{T})} - 1)^2} + S2(\frac{\theta_{2E}}{T})^2 \frac{e^{(\frac{\theta_{2E}}{T})}}{(e^{(\frac{\theta_{2E}}{T})} - 1)^2} \tag{4.9}$$

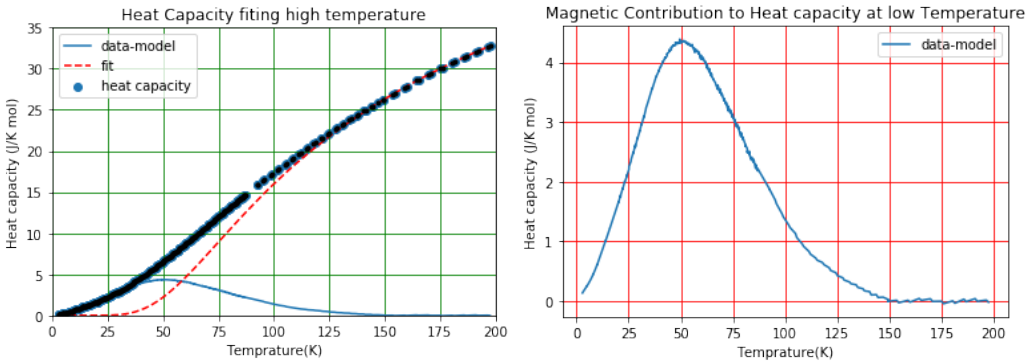
The model in fig 4.5(c) has small error, and the model fits with the experimental result with three Einstein temperatures as θ_E,θ_{1E} ,θ_{2E} and scaling terms S, S1, S2, but when a Debye term is added to the equation the model deviates largely from the experimental results and the shape of the model curve looks different. This is a clear suggestion that $\beta - VOSO_4$ is an Einstein type material.

Heat capacity of a material results from phonon vibrations and magnetic excitations. mathematically the heat capacity is given by

$$(C_m) = (C_p) + C_\chi \tag{4.10}$$

where (C_m) is measured Heat capacity, (C_p) is phonon Heat capacity and C_χ is Magnetic Heat Capacity

At lower temperatures magnetic excitations contribute more to the heat capacity of the material than the phonon vibration because at low temperature the atoms in the lattice have less thermal energy while at higher temperature phonon vibrations contribute more to the heat capacity of the material.



(a) heat capcit modeled at high temperature

(b) magentic contribution to heat capacity

Figure 4.6: magnetic contribution to heat capacity .

In order to obtain the phonon contributions to the heat capacity of $\beta - VOSO_4$, the model with three Einstein terms is used and fitted to temperatures above 150K as shown in fig 4.6(a), since phonon contribution is more pronouced at higher temperatures ($C_p >> C_\chi$). Then fitting to higher temperatures will better describe phonon contributions to heat capacity. The fit to high temperature shows three einstein temperatures θ_E,θ_{1E} ,θ_{2E} with values 999.937(12)K, 622.493(41)K, 326,37(13)K respectively. Extending the model obtained from the higher temperatures fit to lower temperature will predict the phonon contribution at lower temperatures. From fig 4.6(a). the phonon model is shown as red dotted lines showing a deviation in the measured values of heat capacity from the estimated value from the Einstein model at low temperatures. Recall that this same model have described this material with a good precision as is seen in fig 4.5(c) where the difference between the measured value and the model appears as a constant zero line in blue. From equation 4.10, it follows that the difference between the measured value (C_m) and the phonon model C_p is the magnetic contribution to heat capacity C_χ this difference is plotted as a light-blue line in fig 4.6a and b, this difference has a hill top shape with its peak at around 50K, and a contribution of $4.5(2)JK^{-1}mol^{-1}$. This is not a normal difference because it show a rapide increase between 1.8K to its peak at 50K the a rapid decrease as the temperature increases.

Chapter 5

Conclusions

The $\beta - VOSO_4$ crystal is a green needle like single crystal. A From the x-ray and neutron diffraction result, we got the lattice parameters as follows $a = 7.36022(11)$,$b = 6.27603(12)$ and $c = 7.06650(12)$. These results are in agreement with the result of Paufler et al. (2014), up to the second place of decimal. The Raman spectroscopy result using Ar 514nm laser identified 23 Raman active modes. The spectrum we got is the same visually as that obtained by Boghosian et al. (1995). The TGA analysis confirm that $\beta - VOSO_4$ has no residual water of crystallization which agrees with is in agreement with the result of Paufler et al., 2014. Drawing conclusions from the results above we confirmed that our sample is indeed the same $\beta - VOSO_4$ as in the literature. Moving forward analyzing the result from the magnetic susceptibility of experiment performed on 'the sample $\beta VOSO_4$ a key feature of low dimensional magnetism like broad peak at low thermodynamic temperatures, was identified. The susceptibility profile of the $\beta - VOSO_4$ was modeled with good precision with the expression

$$\chi = \frac{(N(g\mu_B)^2)}{(K_B T)}\left(\frac{(0.25 + 0.14995\frac{J}{T} + 0.30094(\frac{J}{T})^2)}{(1 + 1.982\frac{J}{T} + 0.68854(\frac{J}{T})^2 + 6.0626(\frac{J}{T})^3)} + \frac{C}{(T - \theta_{cw})}\right)$$

which is a combination of the peak fit from Bonner and Fisher Bonner and Fisher (1964) and the Curie Weiss law. From the susceptibility peak we got the exchange interaction as 45.4(3)K, but from our fit of the peak the exchange interaction is approximately 25.05(99)K, for all the axial directions. The magnetic susceptibility of $\beta - VOSO_4$ shows no magnetic transitions. The low values of J indicates weak exchange interaction and magnetic correlation between neighboring spins, this couple to the axial isotropy observed in the magnetic susceptibility curve leads to the conclusion that it is a spin 1/2 Heisenberg chain. The bulk analysis of the crystal reveals that at lower tem-

perature the spin1/2 magnetic excitations contribute up to $4.5JK^{-1}mol^{-1}$ to the internal energy of the crystal or heat capacity of the crystal. The specific heat capacity of the material suggest that $\beta - VOSO_4$ is a hard Einstein type material.

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Appendix:A Pcr-file

appendix A

pcrfile.pdf

```
       ***********************************************************
       ** PROGRAM FullProf.2k (Version 6.00 - Mar2017-ILL JRC) **
       ***********************************************************
                     M U L T I -- P A T T E R N
           Rietveld, Profile Matching & Integrated Intensity
                Refinement of X-ray and/or Neutron Data


   Date: 10/06/2021  Time: 17:15:19.747

=> PCR file code: VOSO4_test-working_beforerefinement (1) (1)
=> DAT file code: hrp77265_abscor_b1_T -> Relative contribution: 0.3333
=> DAT file code: hrp77265_abscor_b2_T -> Relative contribution: 0.3333
=> DAT file code: PK752.dat            -> Relative contribution: 0.3333

==> CONDITIONS OF THIS RUN FOR PATTERN No.:  1

=> Global Refinement of neutron powder data
=> Neutron Time-Of-Flight data
=> Abcisa variable is T.O.F. in microsecs
=> Title:Multi-pattern b-VOSO4 hrpd

=> Number of phases:    1
=> Number of excluded regions:    2
=> Number of scattering factors supplied:    0
=> Maximum Likelihood weighting scheme ( w=1/(calculated variance) )
=> Asymmetry correction as in J.Appl.Cryst. 26,128(1993)
=> Background linearly interpolated between the   60 points given
=> The    9th default profile function was selected
=> T.O.F Profile Function #1
   Decay double Exponential convoluted with pseudo-Voigt:
   Omega(DT) = (1-eta)N {Exp(u).Erfc(y)+ Exp(v).Erfc(z)} +
               2N eta/pi{-Im[Exp(p)E1(p)]-Im[Exp(q)E1(q)]}

==> CONDITIONS OF THIS RUN FOR PATTERN No.:  2

=> Global Refinement of neutron powder data
=> Neutron Time-Of-Flight data
=> Abcisa variable is T.O.F. in microsecs
=> Title:Multi-pattern b-VOSO4 hrpd

=> Number of phases:    1
=> Number of excluded regions:    2
=> Number of scattering factors supplied:    0
=> Maximum Likelihood weighting scheme ( w=1/(calculated variance) )
=> Asymmetry correction as in J.Appl.Cryst. 26,128(1993)
=> Background linearly interpolated between the   20 points given
=> The    9th default profile function was selected
=> T.O.F Profile Function #1
   Decay double Exponential convoluted with pseudo-Voigt:
   Omega(DT) = (1-eta)N {Exp(u).Erfc(y)+ Exp(v).Erfc(z)} +
               2N eta/pi{-Im[Exp(p)E1(p)]-Im[Exp(q)E1(q)]}

==> CONDITIONS OF THIS RUN FOR PATTERN No.:  3

=> Global Refinement of X-ray powder diffraction data
=> Global Refinement of X-ray powder diffraction data
   Bragg-Brentano(X-rays) or Debye-Scherrer geometry(Neutrons)
=> Title:Multi-pattern b-VOSO4 hrpd
```

```
=> Number of phases:    1
=> Number of excluded regions:    2
=> Number of scattering factors supplied:    0
=> Conventional weights: w=1.0/Variance(yobs)
=> Asymmetry correction as in J.Appl.Cryst. 26,128(1993)
=> Background linearly interpolated between the   76 points given
=> The    7th default profile function was selected
=> T-C-H Pseudo-Voigt function
   This function is convoluted with asymmetry due to axial
   divergence as formulated by:
   van Laar and Yelon, J. Appl. Cryst. 17, 47(1984).
   and using the method of:
   Finger, Cox and Jephcoat, J. Appl. Cryst. 27, 892 (1994).
   Fortran 90 module adapted from function PROFVAL (in F77) :
   L.W. Finger, J. Appl. Cryst. 31, 111 (1998).


==> INPUT/OUTPUT OPTIONS:

=> Generate bacground file *.bac
=> Generate file *.PRF for plot
=> Output Integrated Intensities
=> Generate bacground file *.bac
=> Generate file *.PRF for plot
=> Output Integrated Intensities
=> Generate file *.PRF for plot
=> Output Integrated Intensities
=> Generate new input file *.PCR

=> X-Y type of data: 2theta/TOF/E(Kev) Intens sigma for pattern:  1
=> Plot pattern at each cycle
=> Absorption correction type: 2
=> Base of peaks: 2.0*HW*    6.00

=> X-Y type of data: 2theta/TOF/E(Kev) Intens sigma for pattern:  2
=> Plot pattern at each cycle
=> Absorption correction type: 2
=> Base of peaks: 2.0*HW*    2.00

=> X-Y type of data: 2theta/TOF/E(Kev) Intens sigma for pattern:  3
=> Wavelengths:  1.54397 0.00000
=> Alpha2/Alpha1 ratio:   0.0000
=> Cos(Monochromator angle)=   0.9100
=> Asymmetry correction for angles lower than    0.000 degrees
=> Absorption correction (AC), muR-eff =   0.0000  0.0000
=> Base of peaks: 2.0*HW*    8.00

=> Number of cycles:   40
=> Relaxation factors ==>    for coordinates:  0.20
=> for anisotropic temperature factors:  0.20
=> for halfwidth/strain/size parameters:  0.20
=> for lattice constants and propagation vectors:  0.20
=> EPS-value for convergence:    0.1
=> Background ==>
   Position   Intensity
   31417.23        1.56        0.00
   33050.90        1.51        0.00
   35443.45        1.64        0.00
   35710.23        1.62        0.00
   37522.09        1.77        0.00
   39461.37        1.77        0.00
   39782.26        1.80        0.00
   41563.17        1.82        0.00
   42905.91        1.91        0.00
   44212.39        1.91        0.00
   46553.28        2.05        0.00
   47398.70        2.00        0.00
   48506.18        2.04        0.00
   49938.23        2.08        0.00
   52079.98        2.12        0.00
   52393.35        2.12        0.00
   55532.64        2.21        0.00
   57896.95        2.31        0.00
   58630.96        2.33        0.00
   60597.76        2.35        0.00

   60725.13        2.36        0.00
   62442.95        2.38        0.00
   64673.28        2.42        0.00
   66184.39        2.42        0.00
   66363.30        2.46        0.00
   70276.38        2.56        0.00
```

```
   70784.12        2.50        0.00
   71918.41        2.60        0.00
   73620.88        2.60        0.00
   77101.43        2.69        0.00
   77495.59        2.71        0.00
   80215.43        2.74        0.00
   80311.73        2.71        0.00
   83430.16        2.83        0.00
   85841.77        2.89        0.00
   86384.20        2.85        0.00
   87479.36        2.95        0.00
   89121.45        3.01        0.00
   91258.53        3.04        0.00
   91807.65        3.05        0.00

   94830.47        3.06        0.00
   96148.00        3.17        0.00
   97806.02        3.28        0.00
  100241.52        3.23        0.00
  101725.73        3.37        0.00
  104040.15        3.30        0.00
  104352.69        3.26        0.00
  107369.06        3.33        0.00
  108828.16        3.51        0.00
  110937.52        3.42        0.00
  111170.70        3.42        0.00
  112816.73        3.53        0.00
  115037.91        3.40        0.00
  116008.16        3.37        0.00
  117373.22        3.37        0.00
  119254.08        3.34        0.00
  120259.88        3.37        0.00
  121930.72        3.24        0.00
  123254.51        3.21        0.00
  124704.84        3.28        0.00


=> Excluded regions for Pattern#  1
   From     to
   100.0000  31360.0000
115000.0000 300000.0000

=> Background ==>
   Position   Intensity
   29924.81        1.10        0.00
   32293.23        1.20        0.00
   39060.15        1.41        0.00
   46729.32        1.50        0.00
   56090.23        1.61        0.00
   63195.49        1.71        0.00
   72443.61        1.80        0.00
   79436.09        1.89        0.00
   83834.59        1.90        0.00
   87105.26        1.90        0.00
   91954.89        2.00        0.00
   95225.57        2.00        0.00
  100187.98        2.00        0.00
  105263.16        2.10        0.00
  112030.08        2.10        0.00
  116541.36        2.10        0.00
  120601.51        2.09        0.00
  127142.86        2.00        0.00
  133909.78        1.90        0.00
  135150.38        1.90        0.00


=> Excluded regions for Pattern#  2
   From     to
   100.0000  29000.0000
135000.0000 300000.0000

=> Background ==>
   Position   Intensity
      13.66    12101.32        0.00
      14.24    12213.08        0.00
      14.82    12101.32        0.00
      15.31    12078.97        0.00
      15.98    12324.83        0.00
      16.70    12324.83        0.00
      17.54    11944.87        0.00
      18.17    11654.31        0.00
```

```
     19.06    11028.50        0.00
     19.51    10782.64        0.00
     20.13    10670.89        0.00
     20.62    10916.75        0.00
     21.70    11028.50        0.00
     22.05    10872.04        0.00
     22.72    10804.99        0.00
     23.39    10804.99        0.00
     23.88    10492.08        0.00
     24.06    10156.83        0.00
     24.38     9754.52        0.00
     24.60     9285.16        0.00

     24.73     9151.05        0.00
     25.13     8435.84        0.00
     25.54     8055.88        0.00
     25.76     7698.27        0.00
     25.98     7385.36        0.00
     26.07     7072.45        0.00
     26.34     6692.49        0.00
     26.61     6468.99        0.00
     26.74     6089.03        0.00
     27.59     5843.17        0.00
     28.08     5910.23        0.00
     28.62     5284.41        0.00
     29.15     4993.85        0.00
     29.78     4882.10        0.00
     30.40     4815.05        0.00
     31.07     4680.95        0.00
     31.79     4591.54        0.00
     32.37     4412.74        0.00
     33.08     4435.09        0.00
     33.79     4211.58        0.00

     34.33     4211.58        0.00
     35.09     4211.58        0.00
     35.98     4122.18        0.00
     36.43     4278.64        0.00
     36.70     4569.19        0.00
     37.01     4815.05        0.00
     38.04     4904.45        0.00
     38.21     4658.60        0.00
     38.39     4435.09        0.00
     39.02     4390.39        0.00
     40.00     4300.99        0.00
     40.49     4368.04        0.00
     41.16     4233.94        0.00
     42.01     4166.88        0.00
     43.08     4166.88        0.00
     43.75     4055.13        0.00
     44.38     3853.98        0.00
     45.36     3563.42        0.00
     46.12     3496.37        0.00
     46.74     3451.67        0.00

     47.59     3272.86        0.00
     48.35     3272.86        0.00
     49.02     3138.76        0.00
     49.82     3138.76        0.00
     50.58     3004.66        0.00
     51.03     3049.36        0.00
     52.14     2892.90        0.00
     52.86     2870.55        0.00
     53.57     2803.50        0.00
     54.38     2781.15        0.00
     54.96     2758.80        0.00
     55.58     2647.05        0.00
     56.52     2736.45        0.00
     57.37     2669.40        0.00
     58.44     2624.70        0.00
     59.20     2647.05        0.00


=> Excluded regions for Pattern#  3
   From     to
     0.0000     13.6500
    60.0000    120.0000

=> Number of Least-Squares parameters varied:    23

=>--------------------------->
=>------->  PATTERN number:  1
```

```
=>--------------------------->
=> Global parameters and codes ==>
=> Zero-point:    -1.9860   31.0000
=> D-spacing to T.O.F. coefficient dtt1 and code:  48329.055    61.000
=> D-spacing to T.O.F. coefficient dtt2 and code:     -3.264    91.000
=> T.O.F. 2theta average detector angle      :    168.330

=> Reading Intensity data  =>>

-> No recognizable heading in input data file X,Y,sigma
   First 6 lines are considered as COMMENTS (except for TSAMP keyword)
-> COMMENT:     31370.14550        1.78958093        0.07817861
-> COMMENT:     31379.55654        1.70332124        0.07721400
-> COMMENT:     31388.97041        1.52623027        0.07186282
-> COMMENT:     31398.38710        1.66464591        0.07488378
-> COMMENT:     31407.80662        1.64923724        0.07479645
-> COMMENT:     31417.22896        1.51009650        0.07020225
==> T.O.F. range, and number of points:
   TOFmin:   31426.654297  TOFmax:  125005.390625
   No. of points:   4604

=>--------------------------->
=>------->  PATTERN number:  2
=>--------------------------->
=> Global parameters and codes ==>
=> Zero-point:    -5.4160  121.0000
=> D-spacing to T.O.F. coefficient dtt1 and code:  34808.883   151.000
=> D-spacing to T.O.F. coefficient dtt2 and code:     -3.173   201.000
=> T.O.F. 2theta average detector angle      :     89.580

=> Reading Intensity data  =>>

-> No recognizable heading in input data file X,Y,sigma
   First 6 lines are considered as COMMENTS (except for TSAMP keyword)
-> COMMENT:     29421.77496        1.50198738        0.09937595
-> COMMENT:     29442.37020        1.61397357        0.09610834
-> COMMENT:     29462.97986        1.40734600        0.08841921
-> COMMENT:     29483.60395        1.48815299        0.09451091
-> COMMENT:     29504.24247        1.35736807        0.08246329
-> COMMENT:     29524.89544        1.44424067        0.08349656
==> T.O.F. range, and number of points:
   TOFmin:   29545.562500  TOFmax:  135554.000000
   No. of points:   2178

=>--------------------------->
=>------->  PATTERN number:  3
=>--------------------------->
=> Global parameters and codes ==>
=> Zero-point:    -0.1171    0.0000
=> Displacement peak-shift parameter and code:     0.00    0.00
=> Transparency peak-shift parameter and code:     0.00    0.00

=> Reading Intensity data  =>>

-> No recognizable heading in input data file X,Y,sigma
   First 6 lines are considered as COMMENTS (except for TSAMP keyword)
-> COMMENT: 4.000 1790
-> COMMENT: 4.005 1766
-> COMMENT: 4.010 1802
-> COMMENT: 4.015 1842
-> COMMENT: 4.020 1853
-> COMMENT: 4.025 1878
==> Angular range, step and number of points:
    2Thmin:       4.030000  2Thmax:     100.000000  Step:       0.005000  No. of points:  19195
------------------------------------------------------------------------------
=> Phase  No. 1
     VOSO4 Nuclear
------------------------------------------------------------------------------
=>-------> Pattern#  1
=> Crystal Structure Refinement
=> Preferred orientation vector:   1.0000  0.0000  0.0000
=>-------> Pattern#  2
=> Crystal Structure Refinement
=> Preferred orientation vector:   1.0000  0.0000  0.0000
=>-------> Pattern#  3
=> Crystal Structure Refinement
=> The    2th profile function was selected for phase no.  1
=> Preferred orientation vector:   0.0000  0.0000  1.0000

=>-------> Data for PHASE: 1
=> Number of atoms:    6
=> Number of distance  constraints:    0
=> Number of angle     constraints:    0
```

```
=> Symmetry information on space group: P n m a
-> The multiplicity of the general position is:   8
-> The space group is Centric (-1 at origin)
-> Lattice type  P: { 000 }
-> Reduced set of symmetry operators:

 No.  IT   Symmetry symbol    Rotation part     Associated Translation
  1: ( 1)   1            -->     ( x, y, z) + {  0.0000  0.0000  0.0000}
  2: ( 4)   2 ( x, 0, 0) -->     ( x,-y,-z) + {  0.5000  0.5000  0.5000}
  3: ( 3)   2 ( 0, y, 0) -->     (-x, y,-z) + {  0.0000  0.5000  0.0000}
  4: ( 2)   2 ( 0, 0, z) -->     (-x,-y, z) + {  0.5000  0.0000  0.5000}


       Information on Space Group:
       ---------------------------

=>   Number of Space group:  62
=>  Hermann-Mauguin Symbol: P n m a
=>             Hall Symbol: -P 2ac 2n
=>            Setting Type: IT (Generated from Hermann-Mauguin symbol)
=>          Crystal System: Orthorhombic
=>              Laue Class: mmm
=>             Point Group: mmm
=>         Bravais Lattice: P
=>          Lattice Symbol: oP
=>  Reduced Number of S.O.:   4
=>    General multiplicity:   8
=>          Centrosymmetry: Centric (-1 at origin)
=>  Generators (exc. -1&L):   2
=>         Asymmetric unit:  0.000 <= x <=  0.500
                            0.000 <= y <=  0.250
                            0.000 <= z <=  1.000

=> List of S.O. without inversion and lattice centring translations
=> SYMM(  1): x,y,z                              => SYMM(  2): x+1/2,-y+1/2,-z+1/2
=> SYMM(  3): -x,y+1/2,-z                        => SYMM(  4): -x+1/2,-y,z+1/2


=> Initial parameters ==>
Atom    Ntyp                 X         Y         Z         B         occ.         in  fin  Spc  Mult
                          B11       B22       B33       B12       B13       B23
V1     V                0.16364   0.25000   0.23748   0.05000   0.50000           0    0    0    4
                Codes:   21.00000   0.00000  41.00000   0.00000   0.00000
S1     S                 0.87406   0.25000   0.87408   0.05000   0.50000           0    0    0    4
                Codes:   51.00000   0.00000  71.00000   0.00000   0.00000
O1     O                 0.71441   0.25000   0.98821   0.05000   0.50000           0    0    0    4
                Codes:   81.00000   0.00000 101.00000   0.00000   0.00000
O2     O                 0.04463   0.25000   0.97938   0.05000   0.50000           0    0    0    4
                Codes:  111.00000   0.00000 131.00000   0.00000   0.00000
O3     O                 0.37423   0.25000   0.16946   0.05000   0.50000           0    0    0    4
                Codes:  141.00000   0.00000 161.00000   0.00000   0.00000
O4     O                 0.11908   0.56241   0.25824   0.05000   1.00000           0    0    0    8
                Codes:  171.00000 181.00000 191.00000   0.00000   0.00000

=> IT IS ASSUMED THAT THE FIRST GIVEN SITE IS FULLY OCCUPIED
   OR THE FIRST AND SECOND ATOMS ARE IN THE SAME SITE WITH TOTAL FULL OCCUPATION
 (If this is not the case, change the order of atoms to obtain correct values for the content of the unit cell)
   The given occupation factors have been obtained mutiplying m/M by   1.0000
     -> Atom: V   ,  Chemical element: V   Atomic Mass:    50.9414
     -> Atom: S   ,  Chemical element: S   Atomic Mass:    32.0600
     -> Atom: O   ,  Chemical element: O   Atomic Mass:    15.9994
     -> Atom: O   ,  Chemical element: O   Atomic Mass:    15.9994
     -> Atom: O   ,  Chemical element: O   Atomic Mass:    15.9994
     -> Atom: O   ,  Chemical element: O   Atomic Mass:    15.9994
=> The given value of ATZ is        651.99 the program has calculated:         651.99
   The value of ATZ given in the input PCR file will be used for quantitative analysis
=> The chemical content of the unit cell is:
      4.0000 V    +   4.0000 S    +   4.0000 O    +   4.0000 O    +   4.0000 O    +   8.0000 O
=> The normalized site occupation numbers in % are:
    100.0000 V1     :      100.0000 S1     :      100.0000 O1     :      100.0000 O2     :      100.0000 O3     :      100.0000 O4
=> The density (volumic mass) of the compound is:    3.325 g/cm3

=>-------> PROFILE PARAMETERS FOR PATTERN:  1

=> Overall scale factor:    1.12500
=> T.O.F. Extinction parameter:   0.0000
=> Overall temperature factor:      0.00000
=> T.O.F. Gaussian variances Sig-2, Sig-1, Sig-0:     -2.64100   166.84900     0.00000
=> T.O.F. <Unused> Xt,Yt parameters:       0.0000      0.0000
=> T.O.F. Gaussian and <unused> Size parameters Z1,Z0  :      0.00000     0.00000
=> T.O.F. Lorentzian FWHM Gam-2, Gam-1, Gam-0:      0.00000     5.49800     0.00000
=> T.O.F. Lorentzian strain and size parameters (LStr,LSiz):      0.00000     0.00000
```

```
=> Direct cell parameters:    7.3540   6.2706   7.0604  90.0000  90.0000  90.0000
=> Preferred orientation parameters:   0.0000  0.0000
=> T.O.F. Peak shape parameter alpha0,beta0,alpha1,beta1/kappa:      0.00000     0.02518     2.83057     0.00908
=> Strain parameters s2,s1,s0:      0.00000     0.00000     0.00000


==> CODEWORDS FOR PROFILE PARAMETERS of PATTERN#  1

=> Codeword - Overall scale factor:   211.000
=> Codeword  - T.O.F. Extinction parameter:   0.0000
=> Codeword  - Overall temperature factor:      0.00000
=> Codewords - T.O.F. Gaussian variances Sig-2, Sig-1, Sig-0:      0.00000     0.00000     0.00000
=> Codewords - T.O.F. <Unused> Xt,Yt parameters:       0.0000      0.0000
=> Codewords - T.O.F. Gaussian and <unused> Size parameters Z1,Z0  :      0.00000     0.00000
=> Codewords - T.O.F. Lorentzian FWHM Gam-2, Gam-1, Gam-0:      0.00000     0.00000     0.00000
=> Codewords - T.O.F. Lorentzian strain and size parameters (LStr,LSiz):      0.00000     0.00000
=> Codewords - Direct cell parameters:   11.0000 221.0000 231.0000   0.0000   0.0000   0.0000
=> Codewords - Preferred orientation parameters:   0.0000  0.0000
=> Codewords - T.O.F. Peak shape parameter alpha0,beta0,alpha1,beta1/kappa:      0.00000     0.00000     0.00000     0.00000
=> Codewords - Strain parameters s2,s1,s0:      0.00000     0.00000     0.00000


=> Cell constraints according to Laue symmetry: mmm

       Metric information:
       -------------------

=> Direct cell parameters:

        a =       7.3540      b =       6.2706      c =       7.0604
    alpha =      90.000   beta =      90.000  gamma =      90.000
                     Direct Cell Volume =     325.5859

=> Reciprocal cell parameters:

        a*=     0.135981      b*=     0.159473      c*=     0.141634
    alpha*=      90.000   beta*=      90.000  gamma*=      90.000
                  Reciprocal Cell Volume =   0.00307139

=> Direct and Reciprocal Metric Tensors:

                 GD                                      GR
    54.0809      0.0000      0.0000          0.018491    0.000000    0.000000
     0.0000     39.3210      0.0000          0.000000    0.025432    0.000000
     0.0000      0.0000     49.8498          0.000000    0.000000    0.020060

=>  Cartesian frame: x // a; y is in the ab-plane; z is x ^ y

    Crystal_to_Orthonormal_Matrix             Orthonormal_to_Crystal Matrix
            Cr_Orth_cel                               Orth_Cr_cel
     7.3540      0.0000      0.0000          0.135981   -0.000000   -0.000000
     0.0000      6.2706      0.0000          0.000000    0.159473   -0.000000
     0.0000      0.0000      7.0604          0.000000    0.000000    0.141634

    Busing-Levy B-matrix: Hc=B.H            Inverse of the Busing-Levy B-matrix
              BL_M                                      BL_Minv
   0.135981    0.000000    0.000000            7.3540     -0.0000     -0.0000
   0.000000    0.159473   -0.000000            0.0000      6.2706      0.0000
   0.000000    0.000000    0.141634            0.0000      0.0000      7.0604

=>-------> PROFILE PARAMETERS FOR PATTERN:  2

=> Overall scale factor:    1.26420
=> T.O.F. Extinction parameter:   0.0000
=> Overall temperature factor:      0.00000
=> T.O.F. Gaussian variances Sig-2, Sig-1, Sig-0:    252.28700  3568.98804     0.00000
=> T.O.F. <Unused> Xt,Yt parameters:       0.0000      0.0000
=> T.O.F. Gaussian and <unused> Size parameters Z1,Z0  :      0.00000     0.00000
=> T.O.F. Lorentzian FWHM Gam-2, Gam-1, Gam-0:      0.00000     6.07100     0.00000
=> T.O.F. Lorentzian strain and size parameters (LStr,LSiz):      0.00000     0.00000
=> Direct cell parameters:    7.3615   6.2762   7.0672  90.0000  90.0000  90.0000
=> Preferred orientation parameters:   0.0000  0.0000
=> T.O.F. Peak shape parameter alpha0,beta0,alpha1,beta1/kappa:      0.00000     0.02518     2.83057     0.00908
=> Strain parameters s2,s1,s0:      0.00000     0.00000     0.00000


==> CODEWORDS FOR PROFILE PARAMETERS of PATTERN#  2

=> Codeword - Overall scale factor:   0.00000
=> Codeword  - T.O.F. Extinction parameter:   0.0000
=> Codeword  - Overall temperature factor:      0.00000
=> Codewords - T.O.F. Gaussian variances Sig-2, Sig-1, Sig-0:      0.00000     0.00000     0.00000
=> Codewords - T.O.F. <Unused> Xt,Yt parameters:       0.0000      0.0000
```

```
=> Codewords - T.O.F. Gaussian and <unused> Size parameters Z1,Z0  :      0.00000     0.00000
=> Codewords - T.O.F. Lorentzian FWHM Gam-2, Gam-1, Gam-0:      0.00000     0.00000     0.00000
=> Codewords - T.O.F. Lorentzian strain and size parameters (LStr,LSiz):      0.00000     0.00000
=> Codewords - Direct cell parameters:    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
=> Codewords - Preferred orientation parameters:   0.0000  0.0000
=> Codewords - T.O.F. Peak shape parameter alpha0,beta0,alpha1,beta1/kappa:      0.00000     0.00000     0.00000     0.00000
=> Codewords - Strain parameters s2,s1,s0:      0.00000     0.00000     0.00000


=> Cell constraints according to Laue symmetry: mmm

=>-------> PROFILE PARAMETERS FOR PATTERN:  3

=> Overall scale factor:   0.223100E-02
=> ETA (p-Voigt) OR M (Pearson VII):   0.0000
=> Overall temperature factor:      0.00000
=> Halfwidth U,V,W:      0.37277    -0.14637     0.23141
=> X and Y parameters:       0.0000      0.0000
=> Direct cell parameters:    7.3615   6.2762   7.0672  90.0000  90.0000  90.0000
=> Preferred orientation parameters:   0.0000  0.0000
=> Asymmetry parameters     :      0.00000     0.00000     0.00000     0.00000
=> Strain parameters        :      0.00000     0.00000     0.00000
=> Size   parameters        :     -0.19498     0.00000

==> CODEWORDS FOR PROFILE PARAMETERS of PATTERN#  3

=> Overall scale factor:    0.000
=> ETA (p-Voigt) OR M (Pearson VII):    0.000
=> Overall temperature factor:    0.000
=> Halfwidth U,V,W:    0.000   0.000   0.000
=> X and Y parameters:    0.000   0.000
=> Direct cell parameters:    0.000   0.000   0.000   0.000   0.000   0.000
=> Preferred orientation parameters:    0.000   0.000
=> Asymmetry parameters     :    0.000   0.000   0.000   0.000
=> Strain parameters        :    0.000   0.000   0.000
=> Size   parameters        :    0.000   0.000

=> Cell constraints according to Laue symmetry: mmm

=> Laue symmetry mmm   will be used to generate HKL for pattern#   1
=> Reflections generated between S(1/d)min:  0.3866 A-1 and S(1/d)max:  1.8173 A-1
=>                                  dmax:  2.5865 A   and      dmin:  0.5503 A
=> The number of reflections generated is:   1090
=> The max. scatt. variable (gen.ref.) is:    125005.3906
=> Scattering coefficients from internal table

=> Scattering lengths:

V     -0.0382
S      0.2847
O      0.5803

=> Laue symmetry mmm   will be used to generate HKL for pattern#   2
=> Reflections generated between S(1/d)min:  0.2568 A-1 and S(1/d)max:  1.4310 A-1
=>                                  dmax:  3.8942 A   and      dmin:  0.6988 A
=> The number of reflections generated is:    541
=> The max. scatt. variable (gen.ref.) is:    135554.0000
=> Scattering coefficients from internal table

=> Scattering lengths:

V     -0.0382
S      0.2847
O      0.5803

=> Laue symmetry mmm   will be used to generate HKL for pattern#   3
=> Reflections generated between S(1/d)min:  0.0455 A-1 and S(1/d)max:  1.0019 A-1
=>                                  dmax: 21.9556 A   and      dmin:  0.9982 A
=> The number of reflections generated is:    190
=> The max. scatt. variable (gen.ref.) is:       101.3230
=> Scattering coefficients from internal table


=> X-ray scattering coeff. (A1, B1, A2,...C, f(0), Z, Dfp,Dfpp)

V      10.2971   6.8657   7.3511   0.4385   2.0703  26.8938   2.0571 102.4780   1.2199  22.9955  23.0000   0.0350   2.1100
S       6.9053   1.4679   5.2034  22.2151   1.4379   0.2536   1.5863  56.1720   0.8669  15.9998  16.0000   0.3190   0.5570
O       3.0485  13.2771   2.2868   5.7011   1.5463   0.3239   0.8670  32.9089   0.2508   7.9994   8.0000   0.0470   0.0320

    ---------------------------------------------------------------
     SYMBOLIC NAMES AND INITIAL VALUES OF PARAMETERS TO BE VARIED:
    ---------------------------------------------------------------
```

```
     ->  Parameter number    1   -> Symbolic Name:      Cell_A_ph1_pat1     7.3539691
     ->  Parameter number    2   -> Symbolic Name:             X_V1_ph1    0.16364001
     ->  Parameter number    3   -> Symbolic Name:            Zero_pat1    -1.9859999
     ->  Parameter number    4   -> Symbolic Name:             Z_V1_ph1    0.23748000
     ->  Parameter number    5   -> Symbolic Name:             X_S1_ph1    0.87405998
     ->  Parameter number    6   -> Symbolic Name:            Dtt1_pat1     48329.055
     ->  Parameter number    7   -> Symbolic Name:             Z_S1_ph1    0.87408000
     ->  Parameter number    8   -> Symbolic Name:             X_O1_ph1    0.71441001
     ->  Parameter number    9   -> Symbolic Name:            Dtt2_pat1    -3.2639999
     ->  Parameter number   10   -> Symbolic Name:             Z_O1_ph1    0.98821002
     ->  Parameter number   11   -> Symbolic Name:             X_O2_ph1    0.44629999E-01
     ->  Parameter number   12   -> Symbolic Name:            Zero_pat2    -5.4159999
     ->  Parameter number   13   -> Symbolic Name:             Z_O2_ph1    0.97938001
     ->  Parameter number   14   -> Symbolic Name:             X_O3_ph1    0.37423000
     ->  Parameter number   15   -> Symbolic Name:            Dtt1_pat2     34808.883
     ->  Parameter number   16   -> Symbolic Name:             Z_O3_ph1    0.16946000
     ->  Parameter number   17   -> Symbolic Name:             X_O4_ph1    0.11908000
     ->  Parameter number   18   -> Symbolic Name:             Y_O4_ph1    0.56241000
     ->  Parameter number   19   -> Symbolic Name:             Z_O4_ph1    0.25824001
     ->  Parameter number   20   -> Symbolic Name:            Dtt2_pat2    -3.1730001
     ->  Parameter number   21   -> Symbolic Name:       Scale_ph1_pat1     1.1250000
     ->  Parameter number   22   -> Symbolic Name:      Cell_B_ph1_pat1     6.2706432
     ->  Parameter number   23   -> Symbolic Name:      Cell_C_ph1_pat1     7.0604382


=> No optimization for routine tasks
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

=> CYCLE No.:    1
------------------------------------------------------------------------------
=> Phase  1 Name: VOSO4 Nuclear
------------------------------------------------------------------------------
=> New parameters, shifts, and standard deviations

Atom        x       dx      sx       y       dy      sy       z       dz      sz       B       dB      sB      occ.    docc.   socc.

V1       0.16364 0.00000 0.00127  0.25000 0.00000 0.00000  0.23748-0.00000 0.00140  0.05000 0.00000 0.00000  0.50000 0.00000 0.00000
S1       0.87406-0.00000 0.00126  0.25000 0.00000 0.00000  0.87408-0.00000 0.00092  0.05000 0.00000 0.00000  0.50000 0.00000 0.00000
O1       0.71441 0.00000 0.00053  0.25000 0.00000 0.00000  0.98821-0.00000 0.00070  0.05000 0.00000 0.00000  0.50000 0.00000 0.00000
O2       0.04463-0.00000 0.00054  0.25000 0.00000 0.00000  0.97938 0.00000 0.00067  0.05000 0.00000 0.00000  0.50000 0.00000 0.00000
O3       0.37423-0.00000 0.00079  0.25000 0.00000 0.00000  0.16946-0.00000 0.00049  0.05000 0.00000 0.00000  0.50000 0.00000 0.00000
O4       0.11908 0.00000 0.00086  0.56241 0.00000 0.00036  0.25824-0.00000 0.00040  0.05000 0.00000 0.00000  1.00000 0.00000 0.00000

==> PROFILE PARAMETERS FOR PATTERN#  1

=> Overall scale factor:      1.125015855     0.000015825     0.008038120
=> T.O.F. extinct. parameter :     0.000000    0.000000    0.000000
=> Overall tem. factor:     0.000000    0.000000    0.000000
=> T.O.F. FWHM: sig2,sig1,sig0:
       -2.641000    0.000000    0.000000
      166.848999    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Cell parameters:
        7.353978    0.000009    0.039002
        6.270650    0.000007    0.033257
        7.060446    0.000008    0.037445
       90.000000    0.000000    0.000000
       90.000000    0.000000    0.000000
       90.000000    0.000000    0.000000
=> Preferred orientation:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> T.O.F. shape a0,b0,a1,b1/kappa:
        0.000000    0.000000    0.000000
        0.025178    0.000000    0.000000
        2.830569    0.000000    0.000000
        0.009083    0.000000    0.000000
=> Xtof and Ytof parameters:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Strain parameters s2,s1,s0:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Size   parameters z1,z0:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000

=> T.O.F. FWHM: GAM2,GAM1,GAM0:
        0.000000    0.000000    0.000000
        5.498000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> STRAIN PARAMETER  LSTR :
```

```
        0.000000    0.000000    0.000000

=> Absorption parameters:
      0.021680  0.000000  0.000000
      0.000000  0.000000  0.000000

==> PROFILE PARAMETERS FOR PATTERN#  2

=> Overall scale factor:      1.264199972     0.000000000     0.000000000
=> T.O.F. extinct. parameter :     0.000000    0.000000    0.000000
=> Overall tem. factor:     0.000000    0.000000    0.000000
=> T.O.F. FWHM: sig2,sig1,sig0:
      252.287003    0.000000    0.000000
     3568.988037    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Cell parameters:
       7.361516    0.000000    0.000000
       6.276170    0.000000    0.000000
       7.067196    0.000000    0.000000
      90.000000    0.000000    0.000000
      90.000000    0.000000    0.000000
      90.000000    0.000000    0.000000
=> Preferred orientation:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> T.O.F. shape a0,b0,a1,b1/kappa:
        0.000000    0.000000    0.000000
        0.025178    0.000000    0.000000
        2.830569    0.000000    0.000000
        0.009083    0.000000    0.000000
=> Xtof and Ytof parameters:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Strain parameters s2,s1,s0:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Size   parameters z1,z0:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000

=> T.O.F. FWHM: GAM2,GAM1,GAM0:
        0.000000    0.000000    0.000000
        6.071000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> STRAIN PARAMETER  LSTR :
        0.000000    0.000000    0.000000

=> Absorption parameters:
      0.029020  0.000000  0.000000
      0.000000  0.000000  0.000000

==> PROFILE PARAMETERS FOR PATTERN#  3

=> Overall scale factor:      0.002231000     0.000000000     0.000000000
=> Eta(p-Voigt) or m(Pearson VII):   0.000000  0.000000  0.000000
=> Overall tem. factor:     0.000000    0.000000    0.000000
=> Halfwidth parameters:
        0.372771    0.000000    0.000000
       -0.146366    0.000000    0.000000
        0.231411    0.000000    0.000000
=> Cell parameters:
       7.361516    0.000000    0.000000
       6.276170    0.000000    0.000000
       7.067196    0.000000    0.000000
      90.000000    0.000000    0.000000
      90.000000    0.000000    0.000000
      90.000000    0.000000    0.000000
=> Preferred orientation:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Asymmetry parameters:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> X and Y parameters:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Strain parameters:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
```

```
=> Size   parameters (G,L):
       -0.194981    0.000000    0.000000
        0.000000    0.000000    0.000000

==> GLOBAL PARAMETERS FOR PATTERN#  1


=> Zero-point:    -1.9953   -0.0093    2.1816

=> T.O.F.- dtt1 (    TOFo=dtt1*dsp    ):  48329.04     -0.01    256.28
=> T.O.F.- dtt2 (TOF=TOFo+dtt2*dsp*dsp):     -3.27     -0.01      1.07

==> RELIABILITY FACTORS WITH ALL NON-EXCLUDED POINTS FOR PATTERN:  1

=> R-Factors:   5.04      8.25     Chi2:  41.1     DW-Stat.:  0.5884   Patt#:  1
=> Expected :             1.29                                1.9088
=> Deviance :  89.1         Dev*:  0.1941E-01
=> GoF-index:  6.4         Sqrt(Residual/N)
=> N-P+C:  4317

=>    SumYdif       SumYobs      SumYcal      SumwYobsSQ     Residual    Condition
     673.2        0.1336E+05    0.1317E+05    0.2611E+08    0.1776E+06    0.9488E+18


=> Conventional Rietveld Rp,Rwp,Re and Chi2:   22.2      23.2      3.61      41.15
=> (Values obtained using Ynet, but true sigma(y))
=>  SumYnet, Sum(w Ynet**2):      3031.        0.3309E+07


==> RELIABILITY FACTORS FOR POINTS WITH BRAGG CONTRIBUTIONS FOR PATTERN:  1

=> R-Factors:   5.33      8.57     Chi2:  45.0     DW-Stat.:  0.5968   Patt#:
=> Expected :             1.28                                1.9041
=> Deviance :  86.2         Dev*:  0.2082E-01
=> GoF-index:  6.7         Sqrt(Residual/N)
=> N-P+C:  3890

=>    SumYdif       SumYobs      SumYcal      SumwYobsSQ     Residual    Condition
     640.8        0.1202E+05    0.1186E+05    0.2386E+08    0.1751E+06    0.9488E+18


=> Conventional Rietveld Rp,Rwp,Re and Chi2:   21.3      23.0      3.43      45.01
=> (Values obtained using Ynet, but true sigma(y))
=>  SumYnet, Sum(w Ynet**2):      3004.        0.3306E+07


==> GLOBAL PARAMETERS FOR PATTERN#  2


=> Zero-point:    -5.3568    0.0592    8.9366

=> T.O.F.- dtt1 (    TOFo=dtt1*dsp    ):  34808.74     -0.14     11.00
=> T.O.F.- dtt2 (TOF=TOFo+dtt2*dsp*dsp):     -3.15      0.03      3.02

==> RELIABILITY FACTORS WITH ALL NON-EXCLUDED POINTS FOR PATTERN:  2

=> R-Factors:   5.33      6.97     Chi2:  73.0     DW-Stat.:  0.1314   Patt#:  2
=> Expected :           0.816                                 1.8730
=> Deviance :  26.9         Dev*:  0.1149E-01
=> GoF-index:  8.5         Sqrt(Residual/N)
=> N-P+C:  2164

=>    SumYdif       SumYobs      SumYcal      SumwYobsSQ     Residual    Condition
     270.6         5073.         4936.        0.3248E+08    0.1579E+06    0.9488E+18


=> Conventional Rietveld Rp,Rwp,Re and Chi2:   19.2      19.3      2.25      72.99
=> (Values obtained using Ynet, but true sigma(y))
=>  SumYnet, Sum(w Ynet**2):      1411.        0.4260E+07


==> RELIABILITY FACTORS FOR POINTS WITH BRAGG CONTRIBUTIONS FOR PATTERN:  2

=> R-Factors:   5.99      7.93     Chi2:  88.9     DW-Stat.:  0.1375   Patt#:
=> Expected :           0.841                                 1.8575
=> Deviance :  25.9         Dev*:  0.1410E-01
=> GoF-index:  9.4         Sqrt(Residual/N)
=> N-P+C:  1699

=>    SumYdif       SumYobs      SumYcal      SumwYobsSQ     Residual    Condition
     247.6         4133.         4018.        0.2400E+08    0.1510E+06    0.9488E+18
```

```
=> Conventional Rietveld Rp,Rwp,Re and Chi2:   17.8      18.8      2.00      88.85
=> (Values obtained using Ynet, but true sigma(y))
=>  SumYnet, Sum(w Ynet**2):      1389.        0.4253E+07


==> GLOBAL PARAMETERS FOR PATTERN#  3


=> Zero-point:    -0.1171    0.0000    0.0000

=> Cos( theta)-shift parameter :   0.0000  0.0000  0.0000
=> Sin(2theta)-shift parameter :   0.0000  0.0000  0.0000

==> RELIABILITY FACTORS WITH ALL NON-EXCLUDED POINTS FOR PATTERN:  3

=> R-Factors:   2.46      4.50     Chi2:  12.4     DW-Stat.:  0.0358   Patt#:  3
=> Expected :            1.28                                1.9371
=> Deviance : 0.126E+06     Dev*:   13.59
=> GoF-index:  3.5         Sqrt(Residual/N)
=> N-P+C:  9262

=>    SumYdif       SumYobs      SumYcal      SumwYobsSQ     Residual    Condition
    0.1398E+07    0.5689E+08    0.5622E+08    0.5689E+08    0.1150E+06    0.9488E+18


=> Conventional Rietveld Rp,Rwp,Re and Chi2:   44.1      33.7      9.56      12.41
=> (Values obtained using Ynet, but true sigma(y))
=>  SumYnet, Sum(w Ynet**2):     0.3169E+07    0.1013E+07


==> RELIABILITY FACTORS FOR POINTS WITH BRAGG CONTRIBUTIONS FOR PATTERN:  3

=> R-Factors:   2.90      5.08     Chi2:  14.7     DW-Stat.:  0.0367   Patt#:
=> Expected :            1.33                                1.9309
=> Deviance : 0.123E+06     Dev*:   16.10
=> GoF-index:  3.8         Sqrt(Residual/N)
=> N-P+C:  7643

=>    SumYdif       SumYobs      SumYcal      SumwYobsSQ     Residual    Condition
    0.1261E+07    0.4347E+08    0.4287E+08    0.4347E+08    0.1122E+06    0.9488E+18


=> Conventional Rietveld Rp,Rwp,Re and Chi2:   40.6      33.3      8.70      14.68
=> (Values obtained using Ynet, but true sigma(y))
=>  SumYnet, Sum(w Ynet**2):     0.3103E+07    0.1010E+07


=> Global user-weigthed Chi2 (Bragg contrib.):   51.2

=> ---------> Pattern#  1
=> Phase:  1
=>    Bragg R-factor:  11.4
=>    RF-factor     :  10.5

=> ---------> Pattern#  2
=> Phase:  1
=>    Bragg R-factor:  14.0
=>    RF-factor     :  8.28

=> ---------> Pattern#  3
=> Phase:  1
=>    Bragg R-factor:  25.4
=>    RF-factor     :  17.7


  Standard deviations have to be multiplied by: 2.5620
  (correlated residuals) See references:
 -J.F.Berar & P.Lelann, J. Appl. Cryst. 24, 1-5 (1991)
 -J.F.Berar, Acc. in Pow. Diff. II,NIST Sp.Pub. 846, 63(1992)



  Standard deviations have to be multiplied by: 5.0247
  (correlated residuals) See references:
 -J.F.Berar & P.Lelann, J. Appl. Cryst. 24, 1-5 (1991)
 -J.F.Berar, Acc. in Pow. Diff. II,NIST Sp.Pub. 846, 63(1992)



  Standard deviations have to be multiplied by: 5.8240
  (correlated residuals) See references:
 -J.F.Berar & P.Lelann, J. Appl. Cryst. 24, 1-5 (1991)
 -J.F.Berar, Acc. in Pow. Diff. II,NIST Sp.Pub. 846, 63(1992)
```

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

=> CYCLE No.:    1
=>  Convergence reached at this CYCLE !!!!
=>  Parameter shifts set to zero
-------------------------------------------------------------------------------
=> Phase  1 Name: VOSO4 Nuclear
-------------------------------------------------------------------------------
=> New parameters, shifts, and standard deviations

Atom        x       dx      sx       y       dy      sy       z       dz      sz       B       dB      sB      occ.    docc.   socc.

V1       0.16364 0.00000 0.00127  0.25000 0.00000 0.00000  0.23748 0.00000 0.00140  0.05000 0.00000 0.00000  0.50000 0.00000 0.00000
S1       0.87406 0.00000 0.00126  0.25000 0.00000 0.00000  0.87408 0.00000 0.00092  0.05000 0.00000 0.00000  0.50000 0.00000 0.00000
O1       0.71441 0.00000 0.00053  0.25000 0.00000 0.00000  0.98821 0.00000 0.00070  0.05000 0.00000 0.00000  0.50000 0.00000 0.00000
O2       0.04463 0.00000 0.00054  0.25000 0.00000 0.00000  0.97938 0.00000 0.00067  0.05000 0.00000 0.00000  0.50000 0.00000 0.00000
O3       0.37423 0.00000 0.00079  0.25000 0.00000 0.00000  0.16946 0.00000 0.00049  0.05000 0.00000 0.00000  0.50000 0.00000 0.00000
O4       0.11908 0.00000 0.00086  0.56241 0.00000 0.00036  0.25824 0.00000 0.00040  0.05000 0.00000 0.00000  1.00000 0.00000 0.00000

==> PROFILE PARAMETERS FOR PATTERN#  1

=> Overall scale factor:      1.125015855     0.000000000     0.008038120
=> T.O.F. extinct. parameter :     0.000000    0.000000    0.000000
=> Overall tem. factor:     0.000000    0.000000    0.000000
=> T.O.F. FWHM: sig2,sig1,sig0:
       -2.641000    0.000000    0.000000
      166.848999    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Cell parameters:
        7.353978    0.000000    0.039002
        6.270650    0.000000    0.033257
        7.060446    0.000000    0.037445
       90.000000    0.000000    0.000000
       90.000000    0.000000    0.000000
       90.000000    0.000000    0.000000
=> Preferred orientation:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> T.O.F. shape a0,b0,a1,b1/kappa:
        0.000000    0.000000    0.000000
        0.025178    0.000000    0.000000
        2.830569    0.000000    0.000000
        0.009083    0.000000    0.000000
=> Xtof and Ytof parameters:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Strain parameters s2,s1,s0:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Size   parameters z1,z0:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000

=> T.O.F. FWHM: GAM2,GAM1,GAM0:
        0.000000    0.000000    0.000000
        5.498000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> STRAIN PARAMETER  LSTR :
        0.000000    0.000000    0.000000

=> Absorption parameters:
      0.021680  0.000000  0.000000
      0.000000  0.000000  0.000000

==> PROFILE PARAMETERS FOR PATTERN#  2

=> Overall scale factor:      1.264199972     0.000000000     0.000000000
=> T.O.F. extinct. parameter :     0.000000    0.000000    0.000000
=> Overall tem. factor:     0.000000    0.000000    0.000000
=> T.O.F. FWHM: sig2,sig1,sig0:
      252.287003    0.000000    0.000000
     3568.988037    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Cell parameters:
        7.361516    0.000000    0.000000
        6.276170    0.000000    0.000000
        7.067196    0.000000    0.000000
       90.000000    0.000000    0.000000
       90.000000    0.000000    0.000000
       90.000000    0.000000    0.000000
=> Preferred orientation:
```

```
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> T.O.F. shape a0,b0,a1,b1/kappa:
        0.000000    0.000000    0.000000
        0.025178    0.000000    0.000000
        2.830569    0.000000    0.000000
        0.009083    0.000000    0.000000
=> Xtof and Ytof parameters:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Strain parameters s2,s1,s0:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Size   parameters z1,z0:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000

=> T.O.F. FWHM: GAM2,GAM1,GAM0:
        0.000000    0.000000    0.000000
        6.071000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> STRAIN PARAMETER  LSTR :
        0.000000    0.000000    0.000000

=> Absorption parameters:
      0.029020  0.000000  0.000000
      0.000000  0.000000  0.000000

==> PROFILE PARAMETERS FOR PATTERN#  3

=> Overall scale factor:      0.002231000     0.000000000     0.000000000
=> Eta(p-Voigt) or m(Pearson VII):   0.000000  0.000000  0.000000
=> Overall tem. factor:     0.000000    0.000000    0.000000
=> Halfwidth parameters:
        0.372771    0.000000    0.000000
       -0.146366    0.000000    0.000000
        0.231411    0.000000    0.000000
=> Cell parameters:
       7.361516    0.000000    0.000000
       6.276170    0.000000    0.000000
       7.067196    0.000000    0.000000
      90.000000    0.000000    0.000000
      90.000000    0.000000    0.000000
      90.000000    0.000000    0.000000
=> Preferred orientation:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Asymmetry parameters:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> X and Y parameters:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Strain parameters:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Size   parameters (G,L):
       -0.194981    0.000000    0.000000
        0.000000    0.000000    0.000000

==> GLOBAL PARAMETERS FOR PATTERN#  1


=> Zero-point:    -1.9953    0.0000    2.1816

=> T.O.F.- dtt1 (    TOFo=dtt1*dsp    ):  48329.04      0.00    256.28
=> T.O.F.- dtt2 (TOF=TOFo+dtt2*dsp*dsp):     -3.27      0.00      1.07

==> RELIABILITY FACTORS WITH ALL NON-EXCLUDED POINTS FOR PATTERN:  1

=> R-Factors:   5.04      8.25     Chi2:  41.1     DW-Stat.:  0.5884   Patt#:  1
=> Expected :            1.29                                1.9088
=> Deviance :  89.1         Dev*:  0.1941E-01
=> GoF-index:  6.4          Sqrt(Residual/N)
=> N-P+C:  4317

=>    SumYdif       SumYobs      SumYcal      SumwYobsSQ     Residual    Condition
     673.2        0.1336E+05    0.1317E+05    0.2611E+08    0.1776E+06    0.9488E+18
```

```
=> Conventional Rietveld Rp,Rwp,Re and Chi2:   22.2      23.2      3.61      41.15
=> (Values obtained using Ynet, but true sigma(y))
=>  SumYnet, Sum(w Ynet**2):      3031.        0.3309E+07

=> N-sigma of the GoF: 1865.181

==> RELIABILITY FACTORS FOR POINTS WITH BRAGG CONTRIBUTIONS FOR PATTERN:  1

=> R-Factors:   5.33      8.57     Chi2:  45.0     DW-Stat.:  0.5968   Patt#:
=> Expected :            1.28                                1.9041
=> Deviance :  86.2         Dev*:  0.2082E-01
=> GoF-index:  6.7         Sqrt(Residual/N)
=> N-P+C:  3890

=>    SumYdif       SumYobs      SumYcal      SumwYobsSQ     Residual    Condition
     640.8        0.1202E+05    0.1186E+05    0.2386E+08    0.1751E+06    0.9488E+18


=> Conventional Rietveld Rp,Rwp,Re and Chi2:   21.3      23.0      3.43      45.01
=> (Values obtained using Ynet, but true sigma(y))
=>  SumYnet, Sum(w Ynet**2):      3004.        0.3306E+07

=> N-sigma of the GoF:     1941.074

==> GLOBAL PARAMETERS FOR PATTERN#  2


=> Zero-point:    -5.3568    0.0000    8.9366

=> T.O.F.- dtt1 (    TOFo=dtt1*dsp    ):  34808.74      0.00     11.00
=> T.O.F.- dtt2 (TOF=TOFo+dtt2*dsp*dsp):     -3.15      0.00      3.02

==> RELIABILITY FACTORS WITH ALL NON-EXCLUDED POINTS FOR PATTERN:  2

=> R-Factors:   5.33      6.97     Chi2:  73.0     DW-Stat.:  0.1314   Patt#:  2
=> Expected :          0.816                                1.8730
=> Deviance :  26.9         Dev*:  0.1149E-01
=> GoF-index:  8.5         Sqrt(Residual/N)
=> N-P+C:  2164

=>    SumYdif       SumYobs      SumYcal      SumwYobsSQ     Residual    Condition
     270.6         5073.         4936.        0.3248E+08    0.1579E+06    0.9488E+18


=> Conventional Rietveld Rp,Rwp,Re and Chi2:   19.2      19.3      2.25      72.99
=> (Values obtained using Ynet, but true sigma(y))
=>  SumYnet, Sum(w Ynet**2):      1411.        0.4260E+07

=> N-sigma of the GoF: 2367.961

==> RELIABILITY FACTORS FOR POINTS WITH BRAGG CONTRIBUTIONS FOR PATTERN:  2

=> R-Factors:   5.99      7.93     Chi2:  88.9     DW-Stat.:  0.1375   Patt#:
=> Expected :          0.841                                1.8575
=> Deviance :  25.9         Dev*:  0.1410E-01
=> GoF-index:  9.4         Sqrt(Residual/N)
=> N-P+C:  1699

=>    SumYdif       SumYobs      SumYcal      SumwYobsSQ     Residual    Condition
     247.6         4133.         4018.        0.2400E+08    0.1510E+06    0.9488E+18


=> Conventional Rietveld Rp,Rwp,Re and Chi2:   17.8      18.8      2.00      88.85
=> (Values obtained using Ynet, but true sigma(y))
=>  SumYnet, Sum(w Ynet**2):      1389.        0.4253E+07

=> N-sigma of the GoF:     2560.634

==> GLOBAL PARAMETERS FOR PATTERN#  3


=> Zero-point:    -0.1171    0.0000    0.0000

=> Cos( theta)-shift parameter :   0.0000  0.0000  0.0000
=> Sin(2theta)-shift parameter :   0.0000  0.0000  0.0000

==> RELIABILITY FACTORS WITH ALL NON-EXCLUDED POINTS FOR PATTERN:  3

=> R-Factors:   2.46      4.50     Chi2:  12.4     DW-Stat.:  0.0358   Patt#:  3
=> Expected :            1.28                                1.9371
=> Deviance : 0.126E+06     Dev*:   13.59
=> GoF-index:  3.5         Sqrt(Residual/N)
```

```
=> N-P+C:  9262

=>    SumYdif       SumYobs      SumYcal      SumwYobsSQ     Residual    Condition
    0.1398E+07    0.5689E+08    0.5622E+08    0.5689E+08    0.1150E+06    0.9488E+18


=> Conventional Rietveld Rp,Rwp,Re and Chi2:   44.1      33.7      9.56      12.41
=> (Values obtained using Ynet, but true sigma(y))
=>  SumYnet, Sum(w Ynet**2):     0.3169E+07    0.1013E+07

=> N-sigma of the GoF:  776.663

==> RELIABILITY FACTORS FOR POINTS WITH BRAGG CONTRIBUTIONS FOR PATTERN:  3

=> R-Factors:   2.90      5.08     Chi2:  14.7     DW-Stat.:  0.0367   Patt#:
=> Expected :            1.33                                1.9309
=> Deviance : 0.123E+06     Dev*:   16.10
=> GoF-index:  3.8         Sqrt(Residual/N)
=> N-P+C:  7643

=>    SumYdif       SumYobs      SumYcal      SumwYobsSQ     Residual    Condition
    0.1261E+07    0.4347E+08    0.4287E+08    0.4347E+08    0.1122E+06    0.9488E+18


=> Conventional Rietveld Rp,Rwp,Re and Chi2:   40.6      33.3      8.70      14.68
=> (Values obtained using Ynet, but true sigma(y))
=>  SumYnet, Sum(w Ynet**2):     0.3103E+07    0.1010E+07

=> N-sigma of the GoF:      845.557

=> Global user-weigthed Chi2 (Bragg contrib.):   51.2

=> ---------> Pattern#  1
=> Phase:  1
=>    Bragg R-factor:  11.4
=>    RF-factor     :  10.5

=> ---------> Pattern#  2
=> Phase:  1
=>    Bragg R-factor:  14.0
=>    RF-factor     :  8.28

=> ---------> Pattern#  3
=> Phase:  1
=>    Bragg R-factor:  25.4
=>    RF-factor     :  17.7

-------------------------------------------------------------------------------------------------------------------
Pattern#  1 Phase No:   1 Phase name: VOSO4 Nuclear
-------------------------------------------------------------------------------------------------------------------

  No.  Code     H   K   L  Mult     Hw     2theta/TOF      Icalc       Iobs      Sigma    HwG     HwL     ETA     d-hkl  TOF_alpha  TOF_beta     CORR

    1   1      6   8   2     8    21.604   31369.666        0.1        0.0      0.001  19.677   3.569   0.213  0.649085  4.360860  0.076349
    2   1      1   8   6     8    21.628   31404.418        0.2        0.0      0.021  19.699   3.573   0.213  0.649804  4.356034  0.076123
    3   1      3   6   8     8    21.639   31420.838        0.0        0.0      0.005  19.709   3.574   0.213  0.650144  4.353758  0.076016
    4   1      5   6   7     8    21.662   31454.432        8.3        2.9      1.896  19.730   3.578   0.213  0.650839  4.349108  0.075800
    5   1     11   2   1     8    21.669   31465.020        0.6        0.3      0.157  19.737   3.580   0.213  0.651058  4.347645  0.075731
    6   1      6   4   8     8    21.682   31483.328        0.7        0.4      0.171  19.748   3.582   0.213  0.651437  4.345116  0.075614
    7   1      4   9   0     4    21.684   31487.416        0.4        0.2      0.092  19.751   3.582   0.213  0.651521  4.344553  0.075588
    8   1     10   0   5     4    21.708   31522.447       12.7       10.1      2.038  19.773   3.586   0.213  0.652246  4.339724  0.075364
    9   1      0   8   6     4    21.712   31527.738       80.6       63.6     13.106  19.776   3.587   0.213  0.652356  4.338996  0.075330
   10   1     11   1   2     8    21.743   31573.037        9.8       12.0      2.561  19.804   3.592   0.213  0.653293  4.332770  0.075043
   11   1     10   4   2     8    21.775   31619.164        0.8        0.5      0.187  19.833   3.597   0.213  0.654248  4.326450  0.074753
   12   1      2   5   9     8    21.782   31629.949        0.8        0.4      0.192  19.840   3.598   0.213  0.654471  4.324975  0.074685
   13   1      7   7   3     8    21.791   31642.766       11.4        5.6      2.838  19.848   3.600   0.213  0.654736  4.323223  0.074605
   14   1      4   4   9     8    21.814   31677.445        0.8        0.1      0.146  19.869   3.604   0.213  0.655453  4.318490  0.074389
   15   1      4   1  10     8    21.816   31679.695        0.6        0.1      0.117  19.871   3.604   0.213  0.655500  4.318183  0.074375
   16   1      7   6   5     8    21.836   31708.406        0.4        0.2      0.105  19.888   3.607   0.213  0.656094  4.314273  0.074197
   17   1      9   2   6     8    21.842   31718.279        3.8        2.0      0.928  19.895   3.608   0.213  0.656298  4.312930  0.074136
   18   1      8   5   5     8    21.847   31724.707       22.6       13.3      5.346  19.899   3.609   0.213  0.656431  4.312057  0.074096
   19   1     11   0   2     4    21.861   31745.791        2.6        1.8      0.510  19.912   3.611   0.213  0.656868  4.309193  0.073967
   20   1      5   3   9     8    21.869   31756.705       17.9       13.2      3.370  19.919   3.613   0.213  0.657093  4.307711  0.073900
   21   1      6   1   9     8    21.869   31757.084        0.8        0.6      0.158  19.919   3.613   0.213  0.657101  4.307660  0.073897
   22   1      2   9   3     8    21.876   31767.426        0.3        0.3      0.054  19.925   3.614   0.213  0.657315  4.306258  0.073834
   23   1      9   5   3     8    21.878   31770.053        1.0        0.8      0.158  19.927   3.614   0.213  0.657370  4.305902  0.073818
   24   1      6   8   1     8    21.881   31775.078       41.1       34.3      5.616  19.930   3.615   0.213  0.657474  4.305221  0.073787
   25   1      8   4   6     8    21.885   31781.059        0.9        0.8      0.101  19.934   3.615   0.213  0.657597  4.304410  0.073750
   26   1      2   3  10     8    21.902   31805.924        4.2        4.4      0.227  19.949   3.618   0.213  0.658112  4.301045  0.073599
   27   1      3   9   2     8    21.913   31821.420        4.6        4.9      0.364  19.959   3.620   0.213  0.658432  4.298951  0.073504
   28   1      6   6   6     8    21.928   31843.836        0.1        0.1      0.010  19.973   3.623   0.213  0.658896  4.295925  0.073368
   29   1      2   7   7     8    21.930   31845.982        0.8        0.6      0.112  19.974   3.623   0.213  0.658941  4.295635  0.073355
   30   1      4   0  10     4    21.935   31854.219       27.9       21.6      4.808  19.979   3.624   0.213  0.659111  4.294525  0.073306
```

31	1	7	4	7	8	21.964	31895.600	3.2	2.4	0.617	20.005	3.629	0.213	0.659967	4.288953	0.073056
32	1	3	8	5	8	21.965	31898.076	17.4	12.8	3.327	20.007	3.629	0.213	0.660019	4.288620	0.073042
33	1	6	8	0	4	21.976	31913.750	0.0	0.0	0.006	20.016	3.631	0.213	0.660343	4.286513	0.072948
34	1	7	2	8	8	21.984	31925.348	5.5	3.9	1.112	20.024	3.632	0.213	0.660583	4.284956	0.072878
35	1	6	0	9	4	21.989	31932.895	57.5	40.6	11.635	20.028	3.633	0.213	0.660739	4.283944	0.072833
36	1	6	5	7	8	22.019	31975.746	0.1	0.1	0.006	20.055	3.638	0.213	0.661626	4.278203	0.072578
37	1	11	1	1	8	22.026	31986.488	2.7	2.4	0.329	20.062	3.639	0.213	0.661848	4.276766	0.072515
38	1	8	6	3	8	22.042	32010.225	1.3	0.7	0.328	20.076	3.642	0.213	0.662339	4.273595	0.072374
39	1	1	5	9	8	22.044	32012.555	9.2	4.8	2.275	20.078	3.642	0.213	0.662387	4.273283	0.072361
40	1	10	4	1	8	22.059	32034.457	2.7	1.2	0.649	20.092	3.644	0.213	0.662841	4.270362	0.072232
41	1	3	2	10	8	22.068	32047.691	8.5	3.2	1.952	20.100	3.646	0.213	0.663114	4.268599	0.072154
42	1	2	6	8	8	22.072	32053.389	0.3	0.1	0.071	20.103	3.646	0.213	0.663232	4.267840	0.072121
43	1	10	2	4	8	22.079	32064.598	3.4	1.2	0.763	20.110	3.648	0.213	0.663464	4.266348	0.072055
44	1	5	8	3	8	22.086	32073.988	6.8	2.6	1.578	20.116	3.649	0.213	0.663658	4.265099	0.072000
45	1	8	2	7	8	22.097	32090.604	2.2	1.0	0.554	20.127	3.651	0.213	0.664002	4.262890	0.071903
46	1	4	7	6	8	22.116	32118.342	0.3	0.2	0.063	20.144	3.654	0.213	0.664576	4.259209	0.071742
47	1	7	5	6	8	22.117	32119.502	1.2	0.9	0.236	20.145	3.654	0.213	0.664600	4.259055	0.071735
48	1	0	5	9	4	22.133	32143.209	58.7	38.4	12.969	20.159	3.657	0.213	0.665091	4.255914	0.071598
49	1	1	9	3	8	22.141	32155.104	9.3	6.3	2.017	20.167	3.658	0.213	0.665337	4.254340	0.071529
50	1	10	3	3	8	22.144	32158.607	1.8	1.2	0.375	20.169	3.658	0.213	0.665409	4.253876	0.071509
51	1	11	0	1	4	22.149	32166.160	0.2	0.1	0.043	20.174	3.659	0.213	0.665566	4.252877	0.071466
52	1	10	4	0	4	22.156	32176.564	0.5	0.4	0.106	20.180	3.660	0.213	0.665781	4.251502	0.071406
53	1	1	3	10	8	22.169	32195.033	11.1	9.1	1.619	20.192	3.663	0.213	0.666163	4.249063	0.071300
54	1	1	7	7	8	22.197	32236.580	1.6	1.7	0.110	20.217	3.667	0.213	0.667023	4.243587	0.071063
55	1	3	9	1	8	22.203	32244.836	21.2	20.6	0.608	20.223	3.668	0.213	0.667194	4.242500	0.071016
56	1	9	1	6	8	22.208	32252.654	17.8	16.4	1.318	20.227	3.669	0.213	0.667355	4.241472	0.070971
57	1	4	8	4	8	22.212	32259.195	126.3	115.2	9.945	20.231	3.670	0.213	0.667491	4.240612	0.070934
58	1	0	9	3	4	22.232	32287.518	11.9	13.4	1.762	20.249	3.673	0.213	0.668077	4.236892	0.070774
59	1	6	7	4	8	22.270	32343.312	0.2	0.2	0.006	20.284	3.679	0.213	0.669231	4.229583	0.070460
60	1	7	7	2	8	22.272	32345.797	9.9	9.6	0.461	20.285	3.680	0.213	0.669283	4.229259	0.070446

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
61	1	0	7	7	4	22.288	32370.008	2.1	1.5	0.415	20.300	3.682	0.213	0.669784	4.226095	0.070311	
62	1	9	3	5	8	22.293	32376.967	15.0	10.0	3.262	20.305	3.683	0.213	0.669928	4.225187	0.070272	
63	1	9	4	4	8	22.306	32395.295	10.0	6.3	2.275	20.316	3.685	0.213	0.670307	4.222796	0.070170	
64	1	9	0	6	4	22.334	32436.873	5.7	4.0	1.181	20.342	3.690	0.213	0.671167	4.217383	0.069940	
65	1	1	6	8	8	22.344	32451.764	14.6	10.4	2.962	20.351	3.692	0.213	0.671475	4.215448	0.069858	
66	1	4	5	8	8	22.356	32469.236	1.4	0.9	0.288	20.362	3.694	0.213	0.671837	4.213180	0.069761	
67	1	7	1	8	8	22.357	32470.438	7.8	5.3	1.680	20.363	3.694	0.213	0.671862	4.213024	0.069755	
68	1	2	9	2	8	22.363	32478.984	5.3	3.4	1.208	20.368	3.695	0.213	0.672038	4.211915	0.069708	
69	1	9	5	2	8	22.365	32481.791	1.2	0.8	0.282	20.370	3.695	0.213	0.672097	4.211551	0.069693	
70	1	5	7	5	8	22.384	32510.143	0.2	0.1	0.045	20.388	3.698	0.213	0.672683	4.207879	0.069538	
71	1	2	8	5	8	22.419	32560.508	34.9	33.1	1.776	20.419	3.704	0.213	0.673725	4.201369	0.069264	
72	1	0	6	8	4	22.437	32587.893	26.3	20.3	4.543	20.436	3.707	0.213	0.674292	4.197839	0.069116	
73	1	3	4	9	8	22.443	32596.729	0.2	0.1	0.037	20.442	3.708	0.213	0.674475	4.196701	0.069068	
74	1	3	1	10	8	22.445	32599.184	21.7	15.9	4.173	20.443	3.709	0.213	0.674526	4.196385	0.069055	
75	1	10	1	4	8	22.457	32616.977	15.3	11.1	2.955	20.454	3.711	0.213	0.674894	4.194096	0.068959	
76	1	4	6	7	8	22.463	32625.377	2.6	1.8	0.512	20.459	3.712	0.213	0.675068	4.193016	0.068914	
77	1	8	1	7	8	22.476	32644.354	55.8	36.0	12.486	20.471	3.714	0.213	0.675460	4.190578	0.068813	
78	1	7	0	8	4	22.486	32658.438	18.0	11.1	4.146	20.480	3.715	0.213	0.675752	4.188771	0.068737	
79	1	5	2	9	8	22.491	32666.109	38.7	24.6	8.771	20.485	3.716	0.213	0.675910	4.187788	0.068696	
80	1	2	2	10	8	22.527	32719.682	1.2	1.1	0.034	20.518	3.722	0.213	0.677019	4.180931	0.068412	
81	1	8	6	2	8	22.540	32738.605	65.9	52.6	10.364	20.530	3.724	0.213	0.677410	4.178514	0.068312	
82	1	6	3	8	8	22.544	32744.490	1.8	1.5	0.302	20.534	3.725	0.213	0.677532	4.177763	0.068281	
83	1	3	0	10	4	22.575	32789.441	24.5	17.9	4.752	20.562	3.730	0.213	0.678462	4.172036	0.068045	
84	1	7	7	1	8	22.576	32790.793	6.6	4.7	1.298	20.562	3.730	0.213	0.678490	4.171864	0.068038	
85	1	5	8	2	8	22.587	32806.828	14.4	9.9	3.069	20.572	3.732	0.213	0.678822	4.169825	0.067955	
86	1	10	0	4	4	22.588	32807.543	1.5	1.0	0.314	20.573	3.732	0.213	0.678837	4.169734	0.067951	
87	1	8	0	7	4	22.607	32835.406	0.8	0.6	0.166	20.590	3.735	0.213	0.679413	4.166196	0.067806	
88	1	1	9	2	8	22.646	32893.648	13.5	10.4	2.417	20.626	3.742	0.213	0.680618	4.158819	0.067505	
89	1	10	3	2	8	22.649	32897.398	0.1	0.1	0.026	20.629	3.742	0.213	0.680696	4.158345	0.067485	
90	1	2	9	1	8	22.671	32929.574	0.0	0.0	0.003	20.649	3.746	0.213	0.681362	4.154282	0.067320	
91	1	9	5	1	8	22.673	32932.500	12.0	8.0	2.590	20.651	3.746	0.213	0.681422	4.153912	0.067305	
92	1	5	4	8	8	22.676	32936.898	13.8	8.9	3.090	20.653	3.747	0.213	0.681513	4.153358	0.067283	
93	1	4	3	9	8	22.694	32963.051	32.1	16.4	7.850	20.670	3.750	0.213	0.682055	4.150063	0.067149	
94	1	1	8	5	8	22.704	32978.340	0.7	0.3	0.179	20.679	3.752	0.213	0.682371	4.148139	0.067072	
95	1	7	6	4	8	22.731	33017.344	0.0	0.0	0.012	20.703	3.756	0.213	0.683178	4.143239	0.066874	
96	1	8	5	4	8	22.744	33035.746	0.6	0.0	0.155	20.715	3.758	0.213	0.683559	4.140930	0.066781	
97	1	3	7	6	8	22.772	33077.727	6.5	3.0	1.627	20.741	3.763	0.213	0.684427	4.135675	0.066570	
98	1	8	3	6	8	22.774	33079.844	0.4	0.2	0.100	20.742	3.763	0.213	0.684471	4.135410	0.066560	
99	1	2	9	0	4	22.777	33083.992	0.1	0.1	0.033	20.745	3.764	0.213	0.684557	4.134892	0.066539	
100	1	10	2	3	8	22.790	33104.020	17.0	7.6	4.147	20.757	3.766	0.213	0.684971	4.132390	0.066439	
101	1	1	2	10	8	22.817	33143.754	2.4	0.7	0.565	20.782	3.770	0.213	0.685794	4.127436	0.066241	
102	1	8	6	1	8	22.856	33200.242	2.6	0.6	0.517	20.817	3.777	0.213	0.686962	4.120414	0.065963	
103	1	7	3	7	8	22.862	33209.066	0.0	0.0	0.000	20.823	3.778	0.213	0.687145	4.119318	0.065919	
104	1	3	8	4	8	22.878	33231.645	22.9	13.9	5.366	20.837	3.780	0.213	0.687612	4.116519	0.065809	
105	1	5	1	9	8	22.891	33250.738	6.8	4.5	1.498	20.849	3.783	0.213	0.688007	4.114156	0.065716	
106	1	5	8	1	8	22.905	33271.398	4.9	3.4	1.057	20.862	3.785	0.213	0.688435	4.111601	0.065615	
107	1	0	2	10	4	22.917	33288.820	17.6	12.1	3.689	20.872	3.787	0.213	0.688795	4.109450	0.065530	
108	1	2	4	9	8	22.927	33304.629	0.7	0.5	0.140	20.882	3.789	0.213	0.689122	4.107499	0.065454	
109	1	2	1	10	8	22.929	33307.250	22.6	16.7	4.285	20.884	3.789	0.213	0.689176	4.107176	0.065441	
110	1	4	8	3	8	22.937	33318.293	0.0	0.0	0.006	20.891	3.790	0.213	0.689405	4.105814	0.065388	

111	1	9	2	5	8	22.953	33342.355	29.6	23.5	4.762	20.906	3.793	0.213	0.689903	4.102851	0.065272
112	1	5	6	6	8	22.959	33350.355	0.0	0.0	0.004	20.911	3.794	0.213	0.690068	4.101867	0.065233
113	1	8	6	0	4	22.964	33358.520	19.7	15.7	3.161	20.916	3.795	0.213	0.690237	4.100863	0.065194
114	1	1	9	1	8	22.967	33361.965	3.8	3.0	0.611	20.918	3.795	0.213	0.690309	4.100440	0.065178
115	1	10	3	1	8	22.969	33365.883	5.7	4.6	0.899	20.920	3.796	0.213	0.690390	4.099958	0.065159
116	1	6	7	3	8	23.000	33410.996	0.9	0.8	0.156	20.948	3.801	0.213	0.691323	4.094422	0.064943
117	1	8	4	5	8	23.003	33415.301	0.3	0.2	0.043	20.951	3.801	0.213	0.691412	4.093894	0.064923
118	1	5	0	9	4	23.029	33452.699	3.3	2.9	0.367	20.974	3.806	0.213	0.692186	4.089318	0.064745
119	1	3	5	8	8	23.035	33461.398	0.1	0.1	0.008	20.980	3.807	0.213	0.692366	4.088255	0.064704
120	1	9	4	3	8	23.039	33468.305	14.4	12.1	1.873	20.984	3.807	0.213	0.692509	4.087411	0.064672

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
121	1	6	6	5	8	23.053	33488.293	73.4	56.4	12.772	20.997	3.810	0.213	0.692923	4.084971	0.064577	
122	1	5	5	7	8	23.062	33501.980	2.9	2.3	0.458	21.005	3.811	0.213	0.693206	4.083302	0.064513	
123	1	0	9	1	4	23.068	33509.926	5.0	4.2	0.681	21.010	3.812	0.213	0.693370	4.082334	0.064476	
124	1	2	0	10	4	23.068	33510.250	1.7	1.4	0.224	21.010	3.812	0.213	0.693377	4.082295	0.064474	
125	1	10	3	0	4	23.079	33526.547	9.6	8.8	0.793	21.020	3.814	0.213	0.693714	4.080310	0.064398	
126	1	3	6	7	8	23.151	33632.367	3.9	0.0	0.628	21.086	3.826	0.213	0.695904	4.067472	0.063907	
127	1	6	4	7	8	23.204	33709.035	0.0	0.0	0.000	21.134	3.835	0.213	0.697490	4.058221	0.063556	
128	1	10	1	3	8	23.207	33712.922	2.3	0.0	0.389	21.136	3.835	0.213	0.697571	4.057754	0.063538	
129	1	6	2	8	8	23.228	33744.156	0.0	0.0	0.000	21.156	3.839	0.213	0.698217	4.053997	0.063396	
130	1	1	4	9	8	23.233	33752.172	12.4	7.0	2.996	21.161	3.840	0.213	0.698383	4.053035	0.063360	
131	1	1	1	10	8	23.235	33754.891	0.4	0.2	0.102	21.162	3.840	0.213	0.698439	4.052708	0.063347	
132	1	9	3	4	8	23.248	33774.195	26.1	17.3	5.736	21.174	3.842	0.213	0.698838	4.050392	0.063260	
133	1	4	7	5	8	23.272	33807.996	5.4	4.5	0.786	21.195	3.846	0.213	0.699538	4.046342	0.063108	
134	1	7	5	5	8	23.272	33809.355	1.0	0.8	0.137	21.196	3.846	0.213	0.699566	4.046180	0.063102	
135	1	2	7	6	8	23.278	33818.152	8.7	7.5	1.097	21.202	3.847	0.213	0.699748	4.045127	0.063063	
136	1	7	4	6	8	23.319	33877.590	1.7	0.9	0.501	21.239	3.854	0.213	0.700978	4.038030	0.062797	
137	1	10	2	2	8	23.342	33911.570	0.4	0.2	0.091	21.260	3.858	0.213	0.701681	4.033984	0.062647	
138	1	10	0	3	4	23.350	33923.480	16.6	11.6	3.464	21.267	3.859	0.213	0.701927	4.032568	0.062594	
139	1	5	7	4	8	23.352	33925.449	3.4	2.4	0.694	21.268	3.859	0.213	0.701968	4.032334	0.062586	
140	1	9	1	5	8	23.379	33964.750	27.1	18.4	5.770	21.293	3.864	0.213	0.702781	4.027668	0.062413	
141	1	1	0	10	4	23.380	33966.246	2.1	1.4	0.458	21.294	3.864	0.213	0.702812	4.027490	0.062406	
142	1	6	5	6	8	23.385	33973.672	7.9	5.3	1.731	21.298	3.865	0.213	0.702966	4.026610	0.062374	
143	1	2	8	4	8	23.391	33982.691	0.6	0.4	0.121	21.304	3.866	0.213	0.703152	4.025541	0.062334	
144	1	4	2	9	8	23.391	33983.500	2.6	1.8	0.564	21.305	3.866	0.213	0.703169	4.025445	0.062331	
145	1	3	3	9	8	23.405	34002.648	4.5	3.4	0.867	21.316	3.868	0.213	0.703565	4.023179	0.062247	
146	1	8	2	6	8	23.479	34111.523	28.4	25.4	2.666	21.384	3.881	0.213	0.705818	4.010337	0.061776	
147	1	0	0	10	2	23.486	34122.430	2.9	2.7	0.217	21.391	3.882	0.213	0.706044	4.009056	0.061729	
148	1	4	8	2	8	23.500	34142.027	2.0	1.9	0.049	21.403	3.884	0.213	0.706449	4.006754	0.061645	
149	1	7	6	3	8	23.509	34155.574	15.5	14.3	1.166	21.412	3.886	0.213	0.706730	4.005165	0.061588	
150	1	8	5	3	8	23.523	34175.949	27.7	22.9	3.926	21.424	3.888	0.213	0.707151	4.002777	0.061501	
151	1	9	0	5	4	23.526	34180.098	34.4	28.4	4.850	21.427	3.888	0.213	0.707237	4.002292	0.061483	
152	1	2	5	8	8	23.559	34228.496	10.3	9.4	0.787	21.457	3.894	0.213	0.708238	3.996633	0.061278	
153	1	6	7	2	8	23.568	34241.793	48.7	42.8	5.095	21.465	3.895	0.213	0.708514	3.995080	0.061222	
154	1	7	2	7	8	23.576	34253.270	1.6	1.4	0.133	21.472	3.897	0.213	0.708751	3.993742	0.061174	
155	1	1	7	6	8	23.599	34287.008	2.7	2.6	0.100	21.493	3.901	0.213	0.709449	3.989812	0.061033	
156	1	4	4	8	8	23.600	34288.707	8.6	8.4	0.333	21.494	3.901	0.213	0.709484	3.989614	0.061025	
157	1	9	4	2	8	23.610	34303.496	6.5	6.5	0.272	21.504	3.902	0.213	0.709790	3.987895	0.060964	
158	1	5	3	8	8	23.669	34389.297	1.1	1.0	0.071	21.557	3.912	0.213	0.711566	3.977945	0.060608	
159	1	6	1	8	8	23.669	34389.773	38.4	35.6	2.611	21.557	3.912	0.213	0.711576	3.977890	0.060606	
160	1	3	8	3	8	23.671	34392.977	9.6	8.7	0.856	21.559	3.913	0.213	0.711642	3.977519	0.060593	
161	1	2	6	7	8	23.684	34411.562	108.6	92.2	13.665	21.571	3.915	0.213	0.712026	3.975371	0.060516	
162	1	10	2	1	8	23.693	34425.426	39.3	35.8	3.147	21.579	3.916	0.213	0.712313	3.973770	0.060459	
163	1	1	8	4	8	23.716	34458.527	6.4	8.5	2.690	21.600	3.920	0.213	0.712998	3.969953	0.060324	
164	1	10	1	2	8	23.790	34567.027	58.5	49.3	7.680	21.667	3.932	0.213	0.715243	3.957491	0.059885	
165	1	10	2	0	4	23.814	34601.973	4.3	4.1	0.196	21.689	3.936	0.213	0.715966	3.953495	0.059745	
166	1	6	0	8	4	23.822	34613.355	2.8	2.8	0.113	21.696	3.938	0.213	0.716202	3.952195	0.059699	
167	1	0	8	4	4	23.827	34621.633	7.1	7.5	0.515	21.701	3.939	0.213	0.716373	3.951250	0.059666	
168	1	4	1	9	8	23.842	34643.223	2.2	2.5	0.436	21.715	3.941	0.213	0.716820	3.948787	0.059580	
169	1	4	8	1	8	23.858	34666.590	1.0	1.1	0.228	21.729	3.944	0.213	0.717303	3.946126	0.059488	
170	1	1	5	8	8	23.891	34714.875	36.7	28.7	6.176	21.759	3.949	0.213	0.718302	3.940637	0.059297	
171	1	4	6	6	8	23.919	34755.930	15.3	10.7	3.146	21.785	3.954	0.213	0.719152	3.935982	0.059136	
172	1	6	7	1	8	23.930	34771.043	0.4	0.3	0.094	21.794	3.956	0.213	0.719465	3.934272	0.059077	
173	1	8	1	6	8	23.935	34778.875	3.1	2.0	0.709	21.799	3.957	0.213	0.719627	3.933385	0.059047	
174	1	10	0	2	4	23.945	34794.109	6.2	4.2	1.335	21.809	3.958	0.213	0.719942	3.931663	0.058988	
175	1	2	3	9	8	23.955	34808.488	0.1	0.0	0.010	21.818	3.960	0.213	0.720239	3.930040	0.058932	
176	1	9	4	1	8	23.974	34835.656	37.3	31.5	4.852	21.834	3.963	0.213	0.720802	3.926974	0.058827	
177	1	4	8	0	4	23.981	34846.895	14.5	13.1	1.215	21.841	3.964	0.213	0.721034	3.925708	0.058783	
178	1	4	0	9	4	23.998	34871.816	0.0	0.0	0.001	21.857	3.967	0.213	0.721550	3.922902	0.058687	
179	1	9	2	4	8	24.000	34874.426	16.8	18.1	1.367	21.859	3.967	0.213	0.721604	3.922609	0.058677	
180	1	1	6	7	8	24.022	34905.902	6.7	7.3	0.540	21.878	3.971	0.213	0.722255	3.919072	0.058557	

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
181	1	4	5	7	8	24.037	34927.648	154.7	131.7	19.167	21.892	3.973	0.213	0.722705	3.916631	0.058473	
182	1	7	1	7	8	24.038	34929.145	7.7	6.5	0.976	21.893	3.974	0.213	0.722736	3.916464	0.058468	
183	1	3	7	5	8	24.040	34932.398	37.8	31.8	4.884	21.895	3.974	0.213	0.722803	3.916099	0.058455	
184	1	8	3	5	8	24.041	34934.898	34.5	29.1	4.421	21.896	3.974	0.213	0.722855	3.915819	0.058446	
185	1	6	7	0	4	24.054	34952.988	42.8	39.7	2.849	21.907	3.976	0.213	0.723229	3.913792	0.058377	
186	1	8	4	4	8	24.057	34957.922	31.7	30.4	1.241	21.910	3.977	0.213	0.723331	3.913239	0.058358	
187	1	9	3	3	8	24.083	34995.477	4.3	4.8	0.486	21.934	3.981	0.213	0.724108	3.909040	0.058216	

188	1	8	0	6	4	24.093	35010.188	12.7	13.2	0.600	21.943	3.983	0.213	0.724413	3.907398	0.058161
189	1	6	6	4	8	24.114	35041.520	6.0	5.0	0.814	21.962	3.986	0.213	0.725061	3.903904	0.058043
190	1	7	6	2	8	24.116	35044.672	12.5	10.2	1.880	21.964	3.987	0.213	0.725126	3.903553	0.058031
191	1	8	5	2	8	24.131	35066.684	5.3	3.7	1.110	21.978	3.989	0.213	0.725582	3.901103	0.057949
192	1	10	1	1	8	24.162	35111.746	0.4	0.2	0.100	22.006	3.994	0.213	0.726514	3.896096	0.057781
193	1	3	2	9	8	24.172	35126.105	3.6	1.5	0.912	22.015	3.996	0.213	0.726811	3.894503	0.057727
194	1	7	0	7	4	24.198	35163.484	5.9	4.1	1.213	22.038	4.000	0.213	0.727585	3.890363	0.057589
195	1	5	7	3	8	24.198	35163.816	9.0	6.4	1.868	22.038	4.000	0.213	0.727592	3.890326	0.057588
196	1	2	8	3	8	24.241	35227.578	54.3	55.9	1.799	22.078	4.008	0.213	0.728911	3.883285	0.057354
197	1	5	6	5	8	24.259	35253.965	0.5	0.5	0.014	22.094	4.011	0.213	0.729457	3.880378	0.057258
198	1	6	3	7	8	24.271	35270.969	5.5	5.3	0.307	22.105	4.012	0.213	0.729809	3.878508	0.057196
199	1	10	1	0	4	24.290	35299.121	6.5	5.4	0.869	22.122	4.016	0.213	0.730391	3.875414	0.057094
200	1	3	8	2	8	24.292	35301.246	7.5	6.1	1.084	22.124	4.016	0.213	0.730435	3.875181	0.057086
201	1	1	3	9	8	24.305	35320.383	58.5	41.0	12.010	22.136	4.018	0.213	0.730831	3.873081	0.057017
202	1	10	0	1	4	24.325	35349.809	10.1	7.4	1.948	22.154	4.021	0.213	0.731440	3.869858	0.056911
203	1	4	7	4	8	24.365	35408.305	0.4	0.2	0.109	22.190	4.028	0.213	0.732650	3.863465	0.056702
204	1	7	5	4	8	24.366	35409.867	1.8	0.6	0.489	22.191	4.028	0.213	0.732683	3.863294	0.056696
205	1	3	4	8	8	24.402	35463.453	3.2	0.8	0.726	22.225	4.034	0.213	0.733792	3.857456	0.056506
206	1	7	3	6	8	24.403	35464.188	0.4	0.1	0.090	22.225	4.034	0.213	0.733807	3.857377	0.056504
207	1	0	3	9	4	24.425	35496.102	1.3	0.5	0.335	22.245	4.038	0.213	0.734467	3.853908	0.056391
208	1	5	4	7	8	24.435	35511.777	5.1	2.5	1.318	22.255	4.040	0.213	0.734791	3.852207	0.056336
209	1	10	0	0	2	24.455	35541.039	0.4	0.3	0.093	22.273	4.043	0.213	0.735397	3.849035	0.056234
210	1	5	2	8	8	24.463	35552.848	10.2	7.4	2.062	22.280	4.045	0.213	0.735641	3.847757	0.056193
211	1	9	1	4	8	24.488	35588.516	15.8	12.2	2.737	22.302	4.049	0.213	0.736379	3.843901	0.056068
212	1	7	6	1	8	24.504	35612.656	2.9	2.4	0.413	22.317	4.051	0.213	0.736879	3.841295	0.055985
213	1	8	5	1	8	24.520	35635.758	15.8	12.4	2.756	22.332	4.054	0.213	0.737357	3.838805	0.055905
214	1	1	8	3	8	24.604	35758.477	10.6	6.4	2.574	22.408	4.068	0.213	0.739896	3.825631	0.055485
215	1	2	7	5	8	24.638	35807.902	0.1	0.1	0.023	22.439	4.074	0.213	0.740919	3.820350	0.055318
216	1	5	5	6	8	24.647	35821.582	2.9	2.2	0.561	22.447	4.075	0.213	0.741202	3.818891	0.055272
217	1	8	5	0	4	24.654	35831.695	0.3	0.2	0.062	22.453	4.076	0.213	0.741411	3.817813	0.055238
218	1	9	0	4	4	24.657	35836.469	5.2	4.1	0.933	22.456	4.077	0.213	0.741510	3.817305	0.055222
219	1	3	1	9	8	24.670	35856.098	0.9	0.8	0.089	22.468	4.079	0.213	0.741916	3.815215	0.055157
220	1	7	4	5	8	24.686	35878.480	0.0	0.0	0.005	22.482	4.082	0.213	0.742379	3.812835	0.055082
221	1	3	8	1	8	24.688	35882.008	22.6	19.7	2.581	22.485	4.082	0.213	0.742452	3.812460	0.055070
222	1	4	3	8	8	24.725	35936.645	0.1	0.1	0.017	22.519	4.088	0.213	0.743583	3.806664	0.054889
223	1	9	3	2	8	24.737	35953.668	6.8	5.5	1.043	22.529	4.090	0.213	0.743935	3.804861	0.054832
224	1	3	6	6	8	24.756	35981.105	28.2	19.8	5.750	22.546	4.093	0.213	0.744503	3.801960	0.054742
225	1	6	5	5	8	24.764	35992.676	2.9	2.0	0.642	22.553	4.095	0.213	0.744742	3.800738	0.054704
226	1	2	2	9	8	24.780	36016.633	31.2	19.8	7.103	22.568	4.097	0.213	0.745238	3.798210	0.054626
227	1	6	4	6	8	24.820	36075.031	0.5	0.5	0.078	22.604	4.104	0.213	0.746446	3.792061	0.054435
228	1	3	0	9	4	24.844	36109.727	1.1	1.1	0.143	22.626	4.108	0.213	0.747164	3.788417	0.054323
229	1	5	7	2	8	24.862	36136.297	15.3	13.3	1.877	22.643	4.111	0.213	0.747714	3.785632	0.054237
230	1	8	2	5	8	24.876	36156.715	0.8	0.6	0.121	22.655	4.113	0.213	0.748136	3.783494	0.054172
231	1	3	5	7	8	24.886	36171.727	5.7	4.6	0.915	22.665	4.115	0.213	0.748447	3.781924	0.054124
232	1	2	8	2	8	24.909	36205.504	0.0	0.0	0.005	22.685	4.119	0.213	0.749146	3.778396	0.054016
233	1	9	2	3	8	24.921	36223.895	26.8	20.8	4.626	22.697	4.121	0.213	0.749526	3.776478	0.053957
234	1	5	1	8	8	24.980	36310.352	19.1	15.6	2.973	22.751	4.131	0.213	0.751315	3.767486	0.053684
235	1	8	4	3	8	24.985	36317.492	0.0	0.0	0.000	22.755	4.132	0.213	0.751463	3.766745	0.053662
236	1	1	7	5	8	25.018	36365.895	0.5	0.4	0.142	22.785	4.137	0.213	0.752464	3.761731	0.053511
237	1	2	4	8	8	25.028	36380.562	1.2	0.6	0.365	22.794	4.139	0.213	0.752768	3.760215	0.053465
238	1	6	6	3	8	25.049	36411.254	1.8	0.9	0.652	22.813	4.142	0.213	0.753403	3.757045	0.053370
239	1	6	2	7	8	25.130	36529.680	23.9	20.7	2.859	22.887	4.156	0.213	0.755853	3.744865	0.053006
240	1	0	7	5	4	25.149	36557.766	3.8	3.1	0.559	22.904	4.159	0.213	0.756435	3.741988	0.052920

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
241	1	9	3	1	8	25.156	36567.797	15.7	12.2	2.681	22.910	4.160	0.213	0.756642	3.740962	0.052890	
242	1	5	0	8	4	25.160	36573.816	19.8	15.0	3.538	22.914	4.161	0.213	0.756767	3.740346	0.052872	
243	1	1	2	9	8	25.168	36584.590	34.8	26.7	6.100	22.921	4.162	0.213	0.756990	3.739244	0.052839	
244	1	3	7	4	8	25.251	36706.406	23.5	17.5	4.379	22.996	4.176	0.213	0.759510	3.726835	0.052474	
245	1	8	3	4	8	25.253	36709.301	9.2	6.8	1.722	22.998	4.176	0.213	0.759570	3.726542	0.052465	
246	1	7	2	6	8	25.277	36744.465	8.9	7.2	1.371	23.020	4.180	0.213	0.760298	3.722975	0.052361	
247	1	5	7	1	8	25.287	36759.992	3.1	2.8	0.300	23.030	4.182	0.213	0.760619	3.721402	0.052315	
248	1	1	8	2	8	25.303	36782.594	19.2	20.6	1.565	23.044	4.184	0.213	0.761087	3.719116	0.052248	
249	1	2	1	9	8	25.318	36804.832	0.8	1.0	0.142	23.058	4.187	0.213	0.761547	3.716869	0.052183	
250	1	4	7	3	8	25.330	36823.270	9.4	10.3	0.904	23.069	4.189	0.213	0.761928	3.715008	0.052129	
251	1	7	5	3	8	25.332	36825.023	35.2	38.3	3.347	23.070	4.189	0.213	0.761964	3.714831	0.052124	
252	1	2	8	1	8	25.337	36832.855	103.2	114.4	12.194	23.075	4.190	0.213	0.762127	3.714041	0.052101	
253	1	4	6	5	8	25.401	36926.828	0.0	0.0	0.003	23.133	4.201	0.213	0.764071	3.704589	0.051828	
254	1	2	6	6	8	25.410	36940.062	1.8	2.4	0.809	23.141	4.202	0.213	0.764345	3.703262	0.051790	
255	1	8	1	5	8	25.420	36954.355	7.0	8.3	1.584	23.150	4.204	0.213	0.764641	3.701829	0.051749	
256	1	1	4	8	8	25.428	36966.199	12.3	13.7	1.519	23.158	4.205	0.213	0.764886	3.700643	0.051714	
257	1	0	8	2	4	25.438	36981.176	88.4	96.6	8.876	23.167	4.207	0.213	0.765195	3.699145	0.051672	
258	1	9	1	3	8	25.469	37026.082	2.7	3.6	1.073	23.195	4.212	0.213	0.766125	3.694659	0.051543	
259	1	2	8	0	4	25.485	37049.332	0.3	0.3	0.095	23.209	4.215	0.213	0.766606	3.692340	0.051477	
260	1	2	0	9	4	25.505	37079.289	16.7	16.2	0.920	23.228	4.218	0.213	0.767226	3.689357	0.051392	
261	1	5	6	4	8	25.505	37080.031	0.2	0.2	0.012	23.228	4.218	0.213	0.767241	3.689283	0.051390	
262	1	2	5	7	8	25.551	37146.430	0.3	0.2	0.033	23.270	4.226	0.213	0.768615	3.682688	0.051203	
263	1	0	4	8	4	25.565	37167.789	10.1	6.6	2.333	23.283	4.228	0.213	0.769057	3.680572	0.051143	
264	1	4	4	7	8	25.603	37223.426	1.8	1.1	0.423	23.317	4.235	0.213	0.770208	3.675071	0.050989	
265	1	8	0	5	4	25.609	37232.199	4.0	2.8	0.827	23.323	4.236	0.213	0.770390	3.674205	0.050964	
266	1	4	2	8	8	25.635	37270.734	71.7	55.8	12.130	23.347	4.240	0.213	0.771187	3.670406	0.050858	
267	1	9	2	2	8	25.648	37289.727	10.7	9.1	1.331	23.358	4.242	0.213	0.771580	3.668537	0.050805	

268	1	3	3	8	8	25.653	37296.000	10.8	9.6	1.047	23.362	4.243	0.213	0.771710	3.667919	0.050788
269	1	9	0	3	4	25.659	37305.562	6.6	6.4	0.291	23.368	4.244	0.213	0.771908	3.666979	0.050762
270	1	5	3	7	8	25.691	37352.223	0.6	0.7	0.150	23.397	4.249	0.213	0.772873	3.662399	0.050634
271	1	6	1	7	8	25.691	37352.824	0.3	0.3	0.074	23.398	4.249	0.213	0.772886	3.662339	0.050633
272	1	8	4	2	8	25.718	37391.859	29.1	23.1	4.711	23.422	4.254	0.213	0.773693	3.658516	0.050527
273	1	1	1	9	8	25.732	37411.543	29.9	22.6	5.443	23.434	4.256	0.213	0.774100	3.656592	0.050473
274	1	1	8	1	8	25.752	37440.977	7.7	6.5	1.027	23.452	4.259	0.213	0.774709	3.653717	0.050394
275	1	6	6	2	8	25.788	37494.215	0.0	0.0	0.004	23.485	4.265	0.213	0.775811	3.648529	0.050251
276	1	1	6	6	8	25.828	37553.602	2.1	0.9	0.628	23.522	4.272	0.213	0.777040	3.642759	0.050093
277	1	4	5	6	8	25.847	37580.688	0.5	0.3	0.093	23.539	4.275	0.213	0.777600	3.640134	0.050021
278	1	7	1	6	8	25.848	37582.551	0.8	0.6	0.148	23.540	4.275	0.213	0.777639	3.639953	0.050016
279	1	0	1	9	4	25.874	37620.543	61.2	45.6	11.420	23.564	4.280	0.213	0.778425	3.636277	0.049916
280	1	6	0	7	4	25.887	37639.828	25.6	20.3	4.116	23.576	4.282	0.213	0.778824	3.634414	0.049865
281	1	1	0	9	4	25.928	37699.906	1.6	1.9	0.303	23.613	4.289	0.213	0.780067	3.628622	0.049708
282	1	2	7	4	8	25.946	37726.207	99.5	98.8	1.218	23.629	4.292	0.213	0.780611	3.626093	0.049640
283	1	0	6	6	4	25.972	37765.008	14.4	15.6	1.314	23.653	4.296	0.213	0.781414	3.622367	0.049540
284	1	1	5	7	8	25.976	37770.480	18.4	20.2	2.076	23.657	4.297	0.213	0.781527	3.621842	0.049525
285	1	7	3	5	8	25.982	37779.648	4.2	4.8	0.686	23.662	4.298	0.213	0.781717	3.620964	0.049502
286	1	7	4	4	8	26.002	37808.773	0.5	0.7	0.236	23.680	4.301	0.213	0.782320	3.618174	0.049427
287	1	7	0	6	4	26.047	37874.922	0.1	0.1	0.008	23.721	4.309	0.213	0.783688	3.611855	0.049258
288	1	0	8	0	2	26.052	37881.781	8.2	8.5	0.541	23.726	4.309	0.213	0.783830	3.611201	0.049241
289	1	6	5	4	8	26.093	37942.480	113.2	103.6	8.560	23.763	4.316	0.213	0.785086	3.605424	0.049087
290	1	4	7	2	8	26.095	37944.562	0.1	0.1	0.008	23.765	4.317	0.213	0.785129	3.605226	0.049082
291	1	7	5	2	8	26.096	37946.480	14.4	13.1	1.129	23.766	4.317	0.213	0.785169	3.605044	0.049077
292	1	9	2	1	8	26.116	37976.234	49.1	47.3	1.736	23.784	4.320	0.213	0.785785	3.602219	0.049002
293	1	0	5	7	4	26.123	37985.594	25.2	23.9	1.172	23.790	4.321	0.213	0.785978	3.601332	0.048979
294	1	6	3	6	8	26.139	38009.332	303.5	282.0	19.642	23.805	4.324	0.213	0.786470	3.599083	0.048919
295	1	8	4	1	8	26.190	38084.129	0.2	0.3	0.165	23.851	4.333	0.213	0.788017	3.592014	0.048733
296	1	8	2	4	8	26.225	38134.801	147.1	131.8	13.409	23.883	4.338	0.213	0.789066	3.587241	0.048608
297	1	4	1	8	8	26.232	38146.227	1.0	0.9	0.075	23.890	4.340	0.213	0.789302	3.586167	0.048580
298	1	9	1	2	8	26.246	38166.586	3.8	4.0	0.235	23.902	4.342	0.213	0.789723	3.584254	0.048530
299	1	6	6	1	8	26.264	38192.293	18.0	21.6	4.209	23.918	4.345	0.213	0.790255	3.581841	0.048467
300	1	5	5	5	8	26.278	38212.602	4.6	6.0	1.679	23.931	4.347	0.213	0.790676	3.579937	0.048418

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
301	1	3	7	3	8	26.330	38289.953	20.3	19.4	0.830	23.979	4.356	0.213	0.792276	3.572706	0.048231	
302	1	8	3	3	8	26.332	38293.238	59.4	56.4	2.845	23.981	4.356	0.213	0.792344	3.572399	0.048223	
303	1	5	4	6	8	26.345	38311.195	0.6	0.6	0.011	23.992	4.358	0.213	0.792716	3.570724	0.048180	
304	1	8	4	0	4	26.353	38323.570	3.9	4.2	0.324	24.000	4.360	0.213	0.792972	3.569571	0.048150	
305	1	2	3	8	8	26.383	38367.199	97.4	86.5	9.477	24.027	4.365	0.213	0.793874	3.565512	0.048046	
306	1	1	7	4	8	26.392	38380.457	2.2	1.9	0.205	24.035	4.366	0.213	0.794149	3.564281	0.048014	
307	1	3	6	5	8	26.410	38406.426	69.3	64.5	4.409	24.051	4.369	0.213	0.794686	3.561871	0.047952	
308	1	6	6	0	4	26.428	38433.793	3.8	3.8	0.072	24.068	4.372	0.213	0.795252	3.559335	0.047888	
309	1	4	0	8	4	26.441	38452.055	7.2	7.2	0.210	24.079	4.374	0.213	0.795630	3.557644	0.047844	
310	1	9	0	2	4	26.455	38472.914	4.0	4.0	0.161	24.092	4.377	0.213	0.796062	3.555715	0.047795	
311	1	6	4	5	8	26.487	38520.715	34.4	25.2	6.656	24.122	4.382	0.213	0.797051	3.551303	0.047683	
312	1	4	7	1	8	26.588	38668.590	32.1	29.8	2.207	24.214	4.399	0.213	0.800111	3.537722	0.047341	
313	1	7	5	1	8	26.590	38670.617	9.5	8.8	0.694	24.215	4.399	0.213	0.800153	3.537536	0.047336	
314	1	5	6	3	8	26.620	38714.625	31.7	26.3	4.463	24.242	4.404	0.213	0.801063	3.533516	0.047236	
315	1	3	4	7	8	26.637	38740.453	15.5	12.3	2.495	24.258	4.407	0.213	0.801598	3.531160	0.047177	
316	1	3	2	8	8	26.673	38793.793	16.3	10.4	3.744	24.291	4.413	0.213	0.802701	3.526304	0.047056	
317	1	5	2	7	8	26.717	38857.074	0.9	1.2	0.331	24.330	4.420	0.213	0.804011	3.520562	0.046914	
318	1	9	1	1	8	26.748	38903.645	22.4	25.7	3.815	24.359	4.426	0.213	0.804974	3.516347	0.046810	
319	1	4	7	0	4	26.759	38919.297	0.9	1.2	0.426	24.369	4.428	0.213	0.805298	3.514933	0.046775	
320	1	4	6	4	8	26.842	39041.629	6.0	9.7	5.708	24.445	4.441	0.213	0.807829	3.503919	0.046506	
321	1	1	3	8	8	26.852	39055.984	9.2	12.6	4.620	24.454	4.443	0.213	0.808126	3.502632	0.046475	
322	1	8	1	4	8	26.864	39074.164	0.1	0.1	0.035	24.465	4.445	0.213	0.808503	3.501002	0.046435	
323	1	3	5	6	8	26.912	39143.684	32.8	31.4	1.685	24.508	4.453	0.213	0.809941	3.494784	0.046284	
324	1	9	0	1	4	26.969	39228.219	33.3	27.5	4.855	24.560	4.463	0.213	0.811690	3.487253	0.046103	
325	1	7	2	5	8	27.045	39338.957	0.3	0.1	0.157	24.629	4.475	0.213	0.813981	3.477437	0.045869	
326	1	4	3	7	8	27.059	39359.719	1.0	0.1	0.464	24.642	4.478	0.213	0.814411	3.475602	0.045825	
327	1	8	0	4	4	27.088	39403.059	0.5	0.0	0.295	24.669	4.483	0.213	0.815308	3.471779	0.045734	
328	1	2	7	3	8	27.122	39451.828	0.8	0.2	0.451	24.699	4.488	0.213	0.816317	3.467488	0.045633	
329	1	7	4	3	8	27.186	39546.277	23.3	21.0	2.099	24.757	4.499	0.213	0.818271	3.459206	0.045438	
330	1	3	7	2	8	27.192	39555.379	11.1	9.6	1.262	24.763	4.500	0.213	0.818460	3.458410	0.045419	
331	1	8	3	2	8	27.195	39559.008	3.2	2.8	0.382	24.765	4.500	0.213	0.818535	3.458093	0.045412	
332	1	2	6	5	8	27.208	39579.262	32.0	27.5	3.848	24.778	4.503	0.213	0.818954	3.456323	0.045371	
333	1	6	2	6	8	27.221	39598.465	4.7	4.2	0.476	24.790	4.505	0.213	0.819351	3.454647	0.045331	
334	1	6	5	3	8	27.290	39699.348	1.3	0.0	0.568	24.852	4.516	0.214	0.821439	3.445868	0.045127	
335	1	3	1	8	8	27.348	39783.992	0.7	0.5	0.495	24.904	4.526	0.214	0.823190	3.438537	0.044958	
336	1	5	1	7	8	27.394	39852.246	2.1	4.6	5.055	24.947	4.534	0.214	0.824602	3.432648	0.044823	
337	1	8	2	3	8	27.440	39919.801	3.4	4.4	1.194	24.989	4.541	0.214	0.826000	3.426839	0.044690	
338	1	2	4	7	8	27.457	39945.133	67.7	53.9	10.801	25.004	4.544	0.214	0.826524	3.424666	0.044641	
339	1	2	2	8	8	27.497	40003.613	3.0	2.9	0.173	25.040	4.551	0.214	0.827734	3.419659	0.044527	
340	1	5	6	2	8	27.511	40024.094	22.9	22.2	0.911	25.053	4.553	0.214	0.828158	3.417909	0.044488	
341	1	7	3	4	8	27.531	40053.684	11.8	12.8	1.196	25.071	4.557	0.214	0.828770	3.415384	0.044431	
342	1	3	0	8	4	27.584	40131.297	0.1	0.2	0.059	25.120	4.565	0.214	0.830376	3.408779	0.044282	
343	1	5	0	7	4	27.632	40201.355	15.4	14.3	1.125	25.163	4.573	0.214	0.831826	3.402838	0.044149	
344	1	1	7	3	8	27.632	40201.859	23.0	21.3	1.658	25.163	4.573	0.214	0.831836	3.402796	0.044148	
345	1	1	6	5	8	27.724	40336.730	2.7	3.6	1.204	25.247	4.589	0.214	0.834627	3.391418	0.043896	
346	1	4	5	5	8	27.747	40370.305	65.8	65.9	0.476	25.267	4.593	0.214	0.835322	3.388598	0.043834	
347	1	7	1	5	8	27.748	40372.617	0.1	0.1	0.001	25.269	4.593	0.214	0.835369	3.388404	0.043830	

348	1	3	7	1	8	27.752	40377.637	52.5	51.6	0.909	25.272	4.593	0.214	0.835473	3.387982	0.043820
349	1	8	3	1	8	27.754	40381.496	121.2	119.6	1.703	25.274	4.594	0.214	0.835553	3.387659	0.043813
350	1	2	5	6	8	27.758	40387.598	51.2	51.4	0.361	25.278	4.595	0.214	0.835679	3.387147	0.043802
351	1	0	7	3	4	27.809	40461.543	30.1	40.8	14.119	25.324	4.603	0.214	0.837209	3.380957	0.043666
352	1	4	4	6	8	27.826	40486.613	0.6	0.9	0.505	25.339	4.606	0.214	0.837728	3.378863	0.043620
353	1	5	5	4	8	27.883	40570.730	0.3	0.8	1.003	25.391	4.615	0.214	0.839469	3.371858	0.043468
354	1	5	3	6	8	27.939	40652.492	4.5	4.6	0.090	25.442	4.625	0.214	0.841160	3.365076	0.043321
355	1	6	1	6	8	27.939	40653.277	76.0	76.7	1.358	25.443	4.625	0.214	0.841177	3.365011	0.043320
356	1	8	3	0	4	27.949	40667.277	7.9	8.1	0.249	25.451	4.626	0.214	0.841466	3.363853	0.043295
357	1	1	4	7	8	27.987	40724.223	3.4	5.1	2.569	25.486	4.633	0.214	0.842645	3.359149	0.043194
358	1	7	0	5	4	27.995	40735.707	1.1	1.7	1.047	25.494	4.634	0.214	0.842882	3.358202	0.043173
359	1	1	2	8	8	28.030	40786.191	6.1	8.5	3.293	25.525	4.640	0.214	0.843927	3.354045	0.043084
360	1	3	6	4	8	28.041	40802.922	22.0	28.4	8.102	25.535	4.642	0.214	0.844273	3.352670	0.043055

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
361	1	2	7	2	8	28.066	40840.270	12.9	17.8	6.557	25.558	4.646	0.214	0.845046	3.349604	0.042990	
362	1	5	6	1	8	28.091	40876.566	7.2	10.0	3.743	25.581	4.650	0.214	0.845797	3.346630	0.042927	
363	1	6	3	5	8	28.109	40903.078	2.2	2.9	0.975	25.597	4.653	0.214	0.846345	3.344460	0.042881	
364	1	6	4	4	8	28.134	40940.047	3.7	3.9	0.246	25.620	4.657	0.214	0.847110	3.341440	0.042817	
365	1	7	4	2	8	28.138	40945.078	29.5	31.0	1.687	25.623	4.658	0.214	0.847215	3.341030	0.042808	
366	1	4	6	3	8	28.150	40963.629	4.2	4.7	0.470	25.635	4.660	0.214	0.847598	3.339517	0.042776	
367	1	8	1	3	8	28.176	41001.211	7.7	9.9	2.738	25.658	4.664	0.214	0.848376	3.336456	0.042712	
368	1	6	0	6	4	28.191	41024.066	0.6	0.8	0.385	25.672	4.667	0.214	0.848849	3.334597	0.042673	
369	1	0	2	8	4	28.214	41057.441	0.2	0.4	0.345	25.693	4.671	0.214	0.849540	3.331886	0.042616	
370	1	2	1	8	8	28.238	41092.031	0.0	0.0	0.005	25.714	4.675	0.214	0.850255	3.329082	0.042557	
371	1	6	5	2	8	28.253	41115.047	3.8	6.6	4.777	25.728	4.677	0.214	0.850731	3.327218	0.042518	
372	1	4	2	7	8	28.265	41132.477	0.5	0.7	0.286	25.739	4.679	0.214	0.851092	3.325808	0.042489	
373	1	3	3	7	8	28.288	41166.441	63.2	59.0	4.152	25.760	4.683	0.214	0.851795	3.323064	0.042432	
374	1	1	5	6	8	28.306	41193.387	0.2	0.2	0.033	25.777	4.686	0.214	0.852352	3.320890	0.042387	
375	1	5	4	5	8	28.365	41279.980	0.2	0.6	1.196	25.830	4.696	0.214	0.854144	3.313924	0.042243	
376	1	8	2	2	8	28.420	41360.082	0.0	0.0	0.021	25.880	4.705	0.214	0.855802	3.307506	0.042111	
377	1	8	0	3	4	28.434	41381.691	3.8	3.2	1.181	25.893	4.708	0.214	0.856249	3.305779	0.042076	
378	1	2	0	8	4	28.498	41475.070	0.3	1.0	2.495	25.951	4.718	0.214	0.858181	3.298336	0.041924	
379	1	1	7	2	8	28.633	41674.027	35.2	46.5	14.629	26.074	4.741	0.214	0.862298	3.282589	0.041607	
380	1	2	7	1	8	28.683	41747.168	0.0	0.1	0.082	26.119	4.749	0.214	0.863811	3.276838	0.041492	
381	1	7	4	1	8	28.759	41859.133	6.4	7.4	1.372	26.188	4.762	0.214	0.866128	3.268074	0.041318	
382	1	7	2	4	8	28.805	41926.441	4.5	4.9	0.449	26.230	4.770	0.214	0.867520	3.262827	0.041215	
383	1	1	1	8	8	28.815	41941.629	53.1	53.0	1.209	26.239	4.771	0.214	0.867835	3.261646	0.041191	
384	1	6	5	1	8	28.882	42040.793	3.7	5.2	2.107	26.301	4.783	0.214	0.869887	3.253952	0.041041	
385	1	2	7	0	4	28.898	42063.164	0.4	0.8	0.620	26.314	4.785	0.214	0.870349	3.252221	0.041007	
386	1	7	3	3	8	28.948	42137.273	28.3	35.8	9.362	26.360	4.794	0.214	0.871883	3.246502	0.040896	
387	1	2	6	4	8	29.003	42217.723	0.0	0.0	0.006	26.410	4.803	0.214	0.873547	3.240315	0.040777	
388	1	8	2	1	8	29.060	42302.863	2.4	2.5	0.158	26.463	4.812	0.214	0.875309	3.233794	0.040651	
389	1	4	1	7	8	29.071	42318.465	176.1	163.6	11.349	26.472	4.814	0.214	0.875632	3.232601	0.040629	
390	1	3	5	5	8	29.077	42326.914	136.6	126.5	9.143	26.477	4.815	0.214	0.875807	3.231956	0.040616	
391	1	1	0	8	4	29.092	42349.160	27.0	26.6	0.386	26.491	4.818	0.214	0.876267	3.230258	0.040584	
392	1	6	5	0	4	29.102	42363.555	350.9	362.7	12.021	26.500	4.819	0.214	0.876565	3.229161	0.040563	
393	1	3	4	6	8	29.168	42461.027	32.6	43.2	13.734	26.560	4.830	0.214	0.878582	3.221748	0.040422	
394	1	4	6	2	8	29.211	42524.395	219.5	268.3	58.236	26.599	4.838	0.214	0.879893	3.216947	0.040331	
395	1	8	1	2	8	29.239	42566.449	3.2	4.4	1.624	26.625	4.842	0.214	0.880763	3.213769	0.040272	
396	1	5	2	6	8	29.272	42614.715	5.0	6.1	1.253	26.655	4.848	0.214	0.881762	3.210129	0.040203	
397	1	2	3	7	8	29.276	42620.770	3.9	4.5	0.676	26.659	4.849	0.214	0.881887	3.209673	0.040195	
398	1	8	2	0	4	29.284	42631.746	6.0	6.3	0.341	26.666	4.850	0.214	0.882114	3.208846	0.040179	
399	1	1	7	1	8	29.289	42638.945	10.3	10.4	0.157	26.670	4.851	0.214	0.882263	3.208304	0.040169	
400	1	0	0	8	2	29.298	42653.039	58.1	56.1	2.046	26.679	4.852	0.214	0.882555	3.207245	0.040149	
401	1	4	0	7	4	29.355	42737.188	5.1	4.9	0.204	26.731	4.862	0.214	0.884296	3.200930	0.040032	
402	1	5	5	3	8	29.358	42740.527	31.7	30.6	1.439	26.733	4.862	0.214	0.884365	3.200679	0.040027	
403	1	6	2	5	8	29.468	42903.633	0.1	0.0	0.055	26.834	4.881	0.214	0.887740	3.188512	0.039803	
404	1	0	7	1	4	29.499	42949.152	14.1	15.4	1.451	26.862	4.886	0.214	0.888682	3.185132	0.039741	
405	1	8	0	2	4	29.529	42992.648	144.2	135.4	8.167	26.889	4.891	0.214	0.889582	3.181910	0.039682	
406	1	3	6	3	8	29.542	43012.262	10.0	10.0	0.160	26.901	4.893	0.214	0.889988	3.180459	0.039655	
407	1	1	6	4	8	29.629	43140.676	2.2	2.6	0.537	26.980	4.908	0.214	0.892645	3.170992	0.039484	
408	1	6	4	3	8	29.651	43172.980	26.6	24.7	1.830	27.000	4.911	0.214	0.893313	3.168619	0.039441	
409	1	4	5	4	8	29.657	43181.750	1.1	1.0	0.106	27.005	4.912	0.214	0.893495	3.167975	0.039430	
410	1	7	1	4	8	29.659	43184.578	6.7	5.9	0.700	27.007	4.913	0.214	0.893553	3.167768	0.039426	
411	1	3	2	7	8	29.675	43207.855	42.7	35.9	5.671	27.021	4.915	0.214	0.894035	3.166061	0.039395	
412	1	4	3	6	8	29.724	43280.375	3.4	2.2	0.860	27.066	4.924	0.214	0.895535	3.160757	0.039300	
413	1	0	6	4	4	29.848	43462.039	68.7	81.6	15.119	27.178	4.944	0.214	0.899294	3.147545	0.039065	
414	1	4	6	1	8	29.908	43551.074	1.3	1.3	0.213	27.233	4.954	0.214	0.901137	3.141110	0.038952	
415	1	1	3	7	8	29.921	43571.008	0.9	0.8	0.256	27.246	4.957	0.214	0.901549	3.139673	0.038927	
416	1	8	1	1	8	29.939	43596.254	0.2	0.1	0.093	27.261	4.960	0.214	0.902071	3.137855	0.038895	
417	1	7	0	4	4	29.961	43629.816	0.4	0.2	0.352	27.282	4.963	0.214	0.902766	3.135441	0.038853	
418	1	6	3	4	8	30.101	43835.637	22.9	23.9	1.177	27.409	4.987	0.214	0.907025	3.120719	0.038598	
419	1	7	3	2	8	30.105	43841.812	37.2	39.2	2.149	27.413	4.988	0.214	0.907152	3.120280	0.038590	
420	1	0	3	7	4	30.146	43902.164	42.1	50.4	9.664	27.450	4.994	0.214	0.908401	3.115991	0.038517	

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
421	1	4	6	0	4	30.152	43910.195	46.6	56.7	12.104	27.455	4.995	0.214	0.908567	3.115421	0.038507	
422	1	2	5	5	8	30.153	43912.590	2.4	2.9	0.651	27.456	4.996	0.214	0.908617	3.115251	0.038504	
423	1	5	1	6	8	30.170	43937.828	1.2	1.6	0.621	27.472	4.998	0.214	0.909139	3.113461	0.038474	
424	1	8	1	0	4	30.183	43956.496	0.1	0.2	0.097	27.484	5.001	0.214	0.909525	3.112139	0.038451	

425	1	4	4	5	8	30.240	44039.949	1.4	1.4	0.152	27.535	5.010	0.214	0.911252	3.106242	0.038351
426	1	8	0	1	4	30.249	44054.480	7.1	6.3	1.054	27.544	5.012	0.214	0.911553	3.105217	0.038333
427	1	2	4	6	8	30.255	44062.402	1.8	1.6	0.294	27.549	5.013	0.214	0.911717	3.104659	0.038324
428	1	5	3	5	8	30.385	44253.688	0.0	0.0	0.001	27.667	5.034	0.214	0.915675	3.091239	0.038098
429	1	6	1	5	8	30.385	44254.703	1.8	1.5	0.642	27.667	5.034	0.214	0.915696	3.091168	0.038097
430	1	5	4	4	8	30.416	44300.520	2.4	2.6	0.422	27.696	5.040	0.214	0.916644	3.087971	0.038044
431	1	7	2	3	8	30.439	44334.480	29.8	28.6	1.557	27.717	5.044	0.214	0.917346	3.085606	0.038004
432	1	5	0	6	4	30.489	44407.023	0.3	0.4	0.028	27.761	5.052	0.214	0.918847	3.080565	0.037921
433	1	8	0	0	2	30.502	44426.301	51.1	51.3	1.173	27.773	5.054	0.214	0.919246	3.079228	0.037898
434	1	5	5	2	8	30.567	44522.492	22.2	25.3	3.565	27.833	5.065	0.214	0.921237	3.072576	0.037789
435	1	3	1	7	8	30.612	44588.812	28.1	27.7	0.961	27.874	5.073	0.214	0.922609	3.068006	0.037714
436	1	2	6	3	8	30.673	44679.316	47.8	59.7	14.647	27.929	5.083	0.214	0.924481	3.061791	0.037613
437	1	6	0	5	4	30.710	44734.238	170.5	153.4	15.113	27.963	5.089	0.214	0.925618	3.058032	0.037552
438	1	3	6	2	8	30.775	44829.898	8.3	9.6	1.554	28.022	5.100	0.214	0.927597	3.051507	0.037446
439	1	2	2	7	8	30.822	44898.668	8.5	7.2	1.241	28.065	5.108	0.214	0.929020	3.046833	0.037372
440	1	1	5	5	8	30.859	44954.039	2.2	1.9	0.211	28.099	5.114	0.214	0.930166	3.043080	0.037312
441	1	7	3	1	8	30.870	44969.488	26.2	23.0	2.895	28.108	5.116	0.214	0.930486	3.042034	0.037295
442	1	6	4	2	8	30.899	45011.949	2.6	2.2	0.384	28.134	5.121	0.214	0.931364	3.039165	0.037249
443	1	3	0	7	4	30.944	45079.410	4.0	1.2	1.106	28.176	5.128	0.214	0.932760	3.034616	0.037177
444	1	1	4	6	8	30.968	45114.805	0.2	0.0	0.072	28.198	5.132	0.214	0.933492	3.032236	0.037140
445	1	0	5	5	4	31.106	45318.008	177.7	184.8	7.560	28.323	5.155	0.214	0.937697	3.018639	0.036926
446	1	0	4	6	4	31.218	45482.723	120.7	136.4	17.443	28.424	5.174	0.214	0.941105	3.007707	0.036757
447	1	3	5	4	8	31.299	45602.078	30.5	35.0	5.124	28.498	5.188	0.214	0.943575	2.999835	0.036636
448	1	4	2	6	8	31.346	45671.762	77.1	76.6	1.201	28.541	5.196	0.214	0.945017	2.995258	0.036567
449	1	5	5	1	8	31.368	45704.953	5.3	5.3	0.097	28.561	5.199	0.214	0.945703	2.993083	0.036534
450	1	3	3	6	8	31.377	45718.277	13.6	13.9	0.392	28.570	5.201	0.214	0.945979	2.992211	0.036520
451	1	1	6	3	8	31.418	45777.656	57.9	64.4	7.109	28.606	5.208	0.214	0.947208	2.988329	0.036462
452	1	4	5	3	8	31.451	45826.750	106.3	114.4	8.636	28.636	5.213	0.214	0.948224	2.985128	0.036413
453	1	7	1	3	8	31.453	45830.129	69.7	75.3	5.961	28.638	5.214	0.214	0.948294	2.984908	0.036410
454	1	1	2	7	8	31.577	46013.676	0.0	0.0	0.019	28.751	5.235	0.214	0.952091	2.973001	0.036232
455	1	3	6	1	8	31.594	46037.699	72.2	95.4	30.004	28.766	5.237	0.214	0.952588	2.971450	0.036209
456	1	6	4	1	8	31.727	46234.934	3.9	5.5	2.426	28.888	5.260	0.214	0.956670	2.958774	0.036022
457	1	6	2	4	8	31.789	46325.684	0.4	0.4	0.020	28.944	5.270	0.214	0.958547	2.952978	0.035937
458	1	7	2	2	8	31.794	46332.969	59.6	60.1	1.251	28.948	5.271	0.214	0.958698	2.952514	0.035930
459	1	7	0	3	4	31.814	46363.359	28.6	28.3	0.817	28.967	5.274	0.214	0.959327	2.950578	0.035902
460	1	2	1	7	8	31.876	46454.180	1.6	0.6	0.464	29.023	5.285	0.214	0.961206	2.944810	0.035819
461	1	6	3	3	8	31.981	46610.562	11.0	9.0	1.625	29.119	5.303	0.214	0.964442	2.934930	0.035676
462	1	3	4	5	8	31.985	46616.328	118.8	96.7	17.671	29.122	5.303	0.214	0.964561	2.934567	0.035671
463	1	6	4	0	4	32.018	46665.293	2.4	2.2	0.184	29.153	5.309	0.214	0.965574	2.931488	0.035627
464	1	2	6	2	8	32.060	46726.996	1.5	0.8	0.448	29.191	5.316	0.214	0.966851	2.927617	0.035572
465	1	5	2	5	8	32.123	46819.926	5.7	1.4	1.378	29.248	5.326	0.214	0.968774	2.921806	0.035490
466	1	2	0	7	4	32.252	47009.754	262.4	211.9	39.941	29.364	5.348	0.214	0.972702	2.910007	0.035324
467	1	5	4	3	8	32.360	47170.602	52.5	46.5	5.470	29.463	5.366	0.214	0.976030	2.900084	0.035187
468	1	4	1	6	8	32.456	47312.020	0.0	0.0	0.013	29.550	5.382	0.214	0.978956	2.891416	0.035068
469	1	2	5	4	8	32.653	47603.383	0.1	0.2	0.108	29.730	5.415	0.214	0.984985	2.873719	0.034828
470	1	7	2	1	8	32.698	47670.094	12.3	16.3	5.217	29.771	5.423	0.214	0.986365	2.869697	0.034774
471	1	1	1	7	8	32.713	47692.422	26.6	30.7	4.581	29.784	5.426	0.214	0.986827	2.868353	0.034756
472	1	4	3	5	8	32.723	47707.059	125.5	138.6	14.180	29.793	5.427	0.214	0.987130	2.867473	0.034744
473	1	2	3	6	8	32.743	47735.605	153.7	169.5	16.983	29.811	5.430	0.214	0.987721	2.865759	0.034721
474	1	4	4	4	8	32.763	47765.754	153.0	177.4	27.671	29.829	5.434	0.214	0.988344	2.863950	0.034697
475	1	4	0	6	4	32.853	47899.340	60.6	55.8	4.494	29.911	5.449	0.214	0.991109	2.855963	0.034591
476	1	1	6	2	8	32.913	47987.781	34.9	39.8	5.457	29.966	5.459	0.214	0.992939	2.850699	0.034522
477	1	5	3	4	8	32.948	48038.805	23.7	23.5	0.329	29.997	5.465	0.214	0.993994	2.847671	0.034483
478	1	6	1	4	8	32.948	48040.102	107.4	106.2	1.525	29.998	5.465	0.214	0.994021	2.847594	0.034482
479	1	4	5	2	8	32.951	48044.340	4.0	3.9	0.049	30.001	5.466	0.214	0.994109	2.847343	0.034478
480	1	7	1	2	8	32.954	48048.234	41.5	41.4	0.382	30.003	5.466	0.214	0.994189	2.847113	0.034475

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
481	1	2	6	1	8	32.989	48099.547	21.7	26.0	4.979	30.035	5.472	0.214	0.995251	2.844075	0.034436	
482	1	0	1	7	4	33.008	48127.703	11.6	14.1	3.078	30.052	5.475	0.214	0.995834	2.842411	0.034414	
483	1	1	0	7	4	33.120	48294.203	17.9	17.6	1.488	30.154	5.494	0.214	0.999279	2.832612	0.034287	
484	1	0	6	2	4	33.213	48431.270	0.1	0.0	0.164	30.238	5.510	0.214	1.002115	2.824595	0.034185	
485	1	3	2	6	8	33.303	48564.828	27.3	25.1	2.293	30.320	5.525	0.214	1.004879	2.816827	0.034086	
486	1	2	6	0	4	33.316	48584.664	0.1	0.1	0.009	30.333	5.527	0.214	1.005289	2.815677	0.034071	
487	1	5	1	5	8	33.321	48591.941	6.0	5.4	0.586	30.337	5.528	0.214	1.005440	2.815255	0.034066	
488	1	6	0	4	4	33.364	48655.309	15.5	13.2	1.953	30.376	5.535	0.214	1.006751	2.811589	0.034020	
489	1	7	0	2	4	33.370	48663.754	21.0	18.5	2.319	30.381	5.536	0.214	1.006925	2.811101	0.034014	
490	1	3	5	3	8	33.429	48751.293	27.0	33.9	8.534	30.435	5.546	0.214	1.008737	2.806053	0.033950	
491	1	2	4	5	8	33.435	48760.602	0.2	0.2	0.064	30.441	5.547	0.214	1.008929	2.805517	0.033944	
492	1	1	5	4	8	33.555	48938.504	0.1	0.1	0.005	30.550	5.567	0.214	1.012610	2.795319	0.033817	
493	1	6	3	2	8	33.563	48949.848	452.7	457.7	5.562	30.557	5.569	0.214	1.012845	2.794671	0.033809	
494	1	1	3	6	8	33.652	49082.207	24.7	24.4	1.056	30.638	5.584	0.214	1.015584	2.787135	0.033716	
495	1	5	0	5	4	33.752	49228.879	2.6	1.1	1.033	30.728	5.600	0.214	1.018619	2.778831	0.033615	
496	1	1	6	1	8	33.920	49478.090	15.6	21.6	8.097	30.881	5.629	0.214	1.023775	2.764835	0.033446	
497	1	4	5	1	8	33.962	49540.086	72.1	91.4	23.979	30.919	5.636	0.214	1.025058	2.761374	0.033405	
498	1	7	1	1	8	33.964	49544.355	29.2	36.8	9.366	30.922	5.636	0.214	1.025146	2.761136	0.033402	
499	1	5	4	2	8	34.002	49599.719	62.6	69.9	7.994	30.956	5.643	0.214	1.026292	2.758054	0.033365	
500	1	6	2	3	8	34.028	49638.438	264.2	258.7	5.689	30.979	5.647	0.214	1.027093	2.755903	0.033340	
501	1	4	5	0	4	34.320	50070.594	0.1	2.1	34.246	31.244	5.696	0.214	1.036035	2.732117	0.033062	
502	1	1	4	5	8	34.406	50198.496	0.4	0.5	0.288	31.323	5.711	0.214	1.038682	2.725156	0.032982	
503	1	7	0	1	4	34.420	50220.016	5.3	4.7	1.490	31.336	5.713	0.214	1.039127	2.723988	0.032968	
504	1	0	6	0	2	34.615	50509.039	298.0	345.4	53.773	31.513	5.746	0.214	1.045107	2.708401	0.032792	

505	1	6	3	1	8	34.633	50534.621	9.4	10.7	1.437	31.529	5.749	0.214	1.045636	2.707030	0.032776
506	1	3	1	6	8	34.644	50551.113	65.1	74.1	10.045	31.539	5.751	0.214	1.045978	2.706146	0.032766
507	1	4	2	5	8	34.926	50969.164	9.4	9.5	0.724	31.795	5.798	0.214	1.054628	2.683951	0.032520
508	1	2	2	6	8	34.949	51003.980	1.2	1.2	0.086	31.817	5.802	0.214	1.055348	2.682119	0.032500
509	1	3	3	5	8	34.969	51033.832	133.8	133.1	1.626	31.835	5.806	0.214	1.055966	2.680550	0.032483
510	1	6	3	0	4	35.012	51098.094	73.9	81.2	7.931	31.874	5.813	0.214	1.057296	2.677179	0.032446
511	1	3	4	4	8	35.018	51105.695	80.9	90.1	10.125	31.879	5.814	0.214	1.057453	2.676780	0.032442
512	1	2	5	3	8	35.095	51220.094	0.0	0.0	0.003	31.949	5.827	0.214	1.059820	2.670802	0.032377
513	1	5	4	1	8	35.115	51250.625	21.7	22.2	0.602	31.968	5.830	0.214	1.060452	2.669211	0.032360
514	1	3	0	6	4	35.128	51269.406	69.9	66.4	3.418	31.979	5.832	0.214	1.060840	2.668233	0.032350
515	1	5	2	4	8	35.199	51374.312	10.8	13.5	3.486	32.043	5.844	0.214	1.063011	2.662785	0.032291
516	1	4	4	3	8	35.231	51422.523	2.9	4.1	1.538	32.073	5.850	0.214	1.064008	2.660288	0.032265
517	1	3	5	2	8	35.248	51447.332	19.1	28.8	14.386	32.088	5.853	0.214	1.064522	2.659005	0.032251
518	1	5	3	3	8	35.461	51763.676	33.9	35.6	2.809	32.282	5.889	0.214	1.071067	2.642755	0.032080
519	1	6	1	3	8	35.462	51765.301	0.0	0.0	0.003	32.283	5.889	0.214	1.071101	2.642672	0.032079
520	1	6	2	2	8	35.952	52493.215	21.0	14.2	4.728	32.728	5.972	0.214	1.086163	2.606027	0.031704
521	1	6	0	3	4	35.982	52537.410	26.1	21.3	3.957	32.755	5.977	0.214	1.087077	2.603835	0.031682
522	1	4	3	4	8	35.993	52553.219	6.7	5.9	0.780	32.765	5.979	0.214	1.087404	2.603051	0.031674
523	1	1	2	6	8	36.062	52656.547	2.9	4.8	3.239	32.828	5.990	0.214	1.089542	2.597943	0.031623
524	1	1	5	3	8	36.222	52894.461	109.2	134.2	30.131	32.973	6.017	0.214	1.094465	2.586258	0.031508
525	1	0	2	6	4	36.457	53244.156	511.0	539.4	29.402	33.187	6.057	0.214	1.101701	2.569272	0.031344
526	1	4	1	5	8	36.481	53279.895	34.4	37.9	3.806	33.209	6.061	0.214	1.102440	2.567549	0.031327
527	1	3	5	1	8	36.493	53296.762	180.9	205.4	27.147	33.219	6.063	0.214	1.102789	2.566736	0.031319
528	1	2	1	6	8	36.508	53319.664	18.1	21.5	3.845	33.233	6.066	0.214	1.103263	2.565634	0.031309
529	1	0	5	3	4	36.623	53490.164	25.9	45.1	32.775	33.338	6.085	0.214	1.106791	2.557456	0.031231
530	1	5	1	4	8	36.793	53743.199	6.3	16.6	26.564	33.492	6.114	0.214	1.112027	2.545415	0.031118
531	1	2	3	5	8	36.890	53887.035	0.0	0.5	10.339	33.580	6.130	0.214	1.115003	2.538620	0.031055
532	1	2	4	4	8	36.946	53971.656	0.5	6.0	64.005	33.632	6.140	0.214	1.116754	2.534640	0.031018
533	1	4	0	5	4	37.048	54122.906	0.2	1.4	10.917	33.724	6.157	0.214	1.119883	2.527557	0.030953
534	1	2	0	6	4	37.076	54164.594	5.1	8.4	5.331	33.749	6.162	0.214	1.120746	2.525611	0.030935
535	1	2	5	2	8	37.217	54374.520	776.2	1019.9	313.276	33.878	6.186	0.214	1.125090	2.515861	0.030847
536	1	6	2	1	8	37.276	54462.164	201.3	235.3	38.914	33.931	6.196	0.214	1.126903	2.511812	0.030810
537	1	5	0	4	4	37.374	54608.754	0.1	0.1	0.023	34.020	6.212	0.214	1.129936	2.505069	0.030750
538	1	4	4	2	8	37.380	54616.883	165.3	203.2	45.596	34.025	6.213	0.214	1.130105	2.504697	0.030747
539	1	5	3	2	8	37.655	55026.164	97.0	100.8	4.069	34.275	6.260	0.214	1.138573	2.486067	0.030583
540	1	6	1	2	8	37.656	55028.117	29.3	30.3	1.076	34.276	6.260	0.214	1.138614	2.485979	0.030582

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
541	1	3	2	5	8	37.697	55088.555	175.9	168.9	6.821	34.313	6.267	0.214	1.139864	2.483251	0.030558	
542	1	6	2	0	4	37.751	55169.414	0.1	0.1	0.028	34.362	6.276	0.214	1.141537	2.479612	0.030527	
543	1	1	1	6	8	37.782	55216.363	1.7	2.6	1.385	34.391	6.282	0.214	1.142509	2.477503	0.030509	
544	1	3	4	3	8	38.082	55662.254	41.6	50.7	11.120	34.663	6.332	0.214	1.151735	2.457657	0.030340	
545	1	1	3	5	8	38.206	55847.188	11.2	18.6	12.050	34.776	6.353	0.214	1.155561	2.449519	0.030272	
546	1	1	4	4	8	38.269	55941.402	17.7	24.9	10.052	34.833	6.364	0.214	1.157511	2.445393	0.030238	
547	1	6	0	2	4	38.280	55958.344	0.9	1.2	0.389	34.843	6.366	0.214	1.157861	2.444653	0.030232	
548	1	5	2	3	8	38.315	56009.832	73.9	73.4	1.794	34.875	6.372	0.214	1.158927	2.442405	0.030213	
549	1	1	0	6	4	38.413	56156.332	9.3	11.0	2.299	34.964	6.388	0.214	1.161958	2.436034	0.030161	
550	1	1	5	2	8	38.570	56390.375	82.1	113.7	42.940	35.106	6.415	0.215	1.166801	2.425923	0.030079	
551	1	0	3	5	4	38.677	56549.691	3.5	6.0	4.219	35.203	6.433	0.215	1.170097	2.419089	0.030024	
552	1	2	5	1	8	38.692	56571.984	1.9	3.1	1.906	35.217	6.436	0.215	1.170558	2.418136	0.030016	
553	1	0	4	4	4	38.742	56647.516	28.2	36.0	9.884	35.263	6.444	0.215	1.172121	2.414912	0.029990	
554	1	4	4	1	8	38.875	56845.078	0.0	0.0	0.002	35.383	6.467	0.215	1.176209	2.406518	0.029924	
555	1	0	0	6	2	38.892	56870.719	12.4	18.4	8.708	35.399	6.470	0.215	1.176740	2.405434	0.029915	
556	1	4	2	4	8	38.988	57014.000	902.9	921.7	19.034	35.486	6.486	0.215	1.179704	2.399388	0.029868	
557	1	3	3	4	8	39.048	57104.555	167.7	187.9	22.277	35.541	6.496	0.215	1.181578	2.395583	0.029838	
558	1	5	3	1	8	39.184	57306.961	21.0	29.5	11.582	35.664	6.519	0.215	1.185766	2.387122	0.029772	
559	1	6	1	1	8	39.185	57309.172	1.8	2.6	1.037	35.665	6.520	0.215	1.185812	2.387030	0.029772	
560	1	2	5	0	4	39.223	57365.875	249.0	349.5	137.909	35.700	6.526	0.215	1.186985	2.384671	0.029754	
561	1	4	3	3	8	39.345	57547.590	295.5	318.5	24.451	35.810	6.547	0.215	1.190745	2.377141	0.029696	
562	1	4	4	0	4	39.414	57650.691	6.8	7.5	0.824	35.873	6.558	0.215	1.192878	2.372890	0.029664	
563	1	3	1	5	8	39.675	58040.375	393.4	371.6	20.311	36.110	6.603	0.215	1.200942	2.356958	0.029545	
564	1	6	1	0	4	39.738	58134.965	788.2	765.0	22.237	36.167	6.614	0.215	1.202899	2.353123	0.029516	
565	1	6	0	1	4	39.890	58362.207	117.8	110.1	7.362	36.305	6.639	0.215	1.207601	2.343961	0.029449	
566	1	2	2	5	8	40.135	58728.762	190.4	211.6	23.171	36.528	6.681	0.215	1.215185	2.329331	0.029343	
567	1	1	5	1	8	40.218	58852.848	27.0	28.6	2.051	36.603	6.695	0.215	1.217753	2.324420	0.029308	
568	1	5	1	3	8	40.397	59120.828	95.9	91.5	4.225	36.766	6.726	0.215	1.223298	2.313884	0.029234	
569	1	3	0	5	4	40.407	59135.020	211.7	193.5	16.398	36.775	6.727	0.215	1.223591	2.313329	0.029230	
570	1	6	0	0	2	40.474	59235.066	15.3	12.6	2.305	36.835	6.739	0.215	1.225662	2.309421	0.029203	
571	1	2	4	3	8	40.601	59425.363	2.1	16.6	109.187	36.951	6.760	0.215	1.229599	2.302026	0.029152	
572	1	0	5	1	4	40.769	59676.715	124.8	300.0	411.781	37.103	6.789	0.215	1.234800	2.292330	0.029085	
573	1	3	4	2	8	40.838	59781.047	38.7	89.1	113.677	37.166	6.801	0.215	1.236959	2.288329	0.029058	
574	1	5	2	2	8	41.126	60212.254	155.0	160.7	6.086	37.428	6.850	0.215	1.245881	2.271941	0.028948	
575	1	5	0	3	4	41.171	60278.988	103.1	98.0	5.077	37.468	6.857	0.215	1.247262	2.269426	0.028931	
576	1	4	1	4	8	41.188	60305.445	0.2	0.2	0.008	37.484	6.860	0.215	1.247809	2.268431	0.028925	
577	1	2	3	4	8	41.778	61190.086	1372.1	1497.2	133.404	38.020	6.961	0.215	1.266114	2.235636	0.028713	
578	1	1	2	5	8	41.847	61292.781	3.2	3.7	0.560	38.082	6.973	0.215	1.268239	2.231890	0.028689	
579	1	4	0	4	4	42.009	61536.102	0.0	0.0	0.001	38.229	7.000	0.215	1.273273	2.223065	0.028634	
580	1	1	4	3	8	42.375	62085.930	148.9	154.1	6.266	38.562	7.063	0.215	1.284650	2.203377	0.028513	
581	1	4	3	2	8	42.408	62135.223	6.5	6.5	0.265	38.592	7.069	0.215	1.285670	2.201629	0.028502	
582	1	2	1	5	8	42.548	62345.711	5.0	0.0	1.550	38.719	7.093	0.215	1.290025	2.194196	0.028458	
583	1	3	4	1	8	42.810	62739.332	230.8	293.0	77.240	38.957	7.137	0.215	1.298170	2.180430	0.028376	
584	1	3	2	4	8	42.961	62966.656	259.4	269.8	10.985	39.094	7.163	0.215	1.302874	2.172558	0.028330	

585	1	5	2	1	8	43.142	63238.328	59.9	66.1	7.109	39.258	7.194	0.215	1.308495	2.163225	0.028276
586	1	4	2	3	8	43.357	63562.117	0.1	0.2	0.510	39.453	7.231	0.215	1.315195	2.152205	0.028214
587	1	3	3	3	8	43.441	63687.672	192.0	212.7	22.499	39.529	7.245	0.215	1.317793	2.147962	0.028190
588	1	2	0	5	4	43.455	63708.438	220.5	232.3	12.302	39.541	7.248	0.215	1.318222	2.147262	0.028186
589	1	1	3	4	8	43.719	64106.777	35.1	46.2	14.272	39.782	7.293	0.215	1.326465	2.133920	0.028112
590	1	5	1	2	8	43.734	64129.195	116.2	142.3	31.423	39.795	7.295	0.215	1.326928	2.133174	0.028108
591	1	2	4	2	8	43.993	64518.391	1.3	5.1	14.864	40.030	7.340	0.215	1.334981	2.120306	0.028038
592	1	1	1	5	8	44.604	65439.363	0.7	1.1	0.683	40.584	7.444	0.215	1.354038	2.090465	0.027880
593	1	4	3	1	8	44.629	65477.211	828.4	966.7	157.757	40.607	7.449	0.215	1.354821	2.089257	0.027874
594	1	5	0	2	4	44.720	65615.086	76.4	80.2	4.243	40.690	7.464	0.215	1.357674	2.084867	0.027851
595	1	0	1	5	4	45.358	66577.641	376.1	339.7	32.331	41.268	7.574	0.215	1.377590	2.054725	0.027700
596	1	4	3	0	4	45.450	66717.039	17.6	10.4	4.325	41.352	7.590	0.215	1.380475	2.050432	0.027679
597	1	1	0	5	4	45.651	67020.500	17.2	12.8	3.927	41.534	7.624	0.215	1.386754	2.041147	0.027634
598	1	3	1	4	8	45.961	67488.312	189.1	198.4	10.174	41.815	7.678	0.215	1.396434	2.026999	0.027567
599	1	5	1	1	8	46.182	67823.141	29.3	27.9	2.171	42.016	7.716	0.215	1.403362	2.016992	0.027520
600	1	1	4	2	8	46.276	67965.383	169.6	225.6	72.993	42.101	7.732	0.215	1.406305	2.012770	0.027500

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
601	1	4	1	3	8	46.446	68223.047	79.9	102.7	28.579	42.255	7.761	0.215	1.411636	2.005169	0.027465	
602	1	2	4	1	8	46.487	68284.055	77.5	109.7	44.588	42.292	7.768	0.215	1.412899	2.003377	0.027457	
603	1	2	2	4	8	46.680	68577.414	6.2	6.8	2.261	42.468	7.801	0.215	1.418969	1.994807	0.027418	
604	1	3	0	4	4	47.109	69226.711	73.1	113.2	60.636	42.856	7.875	0.216	1.432404	1.976097	0.027336	
605	1	0	4	2	4	47.120	69243.266	193.9	294.9	150.170	42.866	7.877	0.216	1.432746	1.975625	0.027334	
606	1	2	3	3	8	47.297	69511.859	14.4	12.3	2.176	43.027	7.908	0.216	1.438304	1.967991	0.027300	
607	1	5	0	1	4	47.347	69588.219	27.2	32.3	6.256	43.073	7.916	0.216	1.439884	1.965832	0.027291	
608	1	2	4	0	4	47.417	69693.789	0.1	0.2	0.126	43.136	7.928	0.216	1.442068	1.962854	0.027278	
609	1	4	2	2	8	47.563	69915.844	3.9	6.2	3.881	43.268	7.954	0.216	1.446663	1.956620	0.027252	
610	1	4	0	3	4	47.632	70020.375	25.4	22.8	2.580	43.331	7.966	0.216	1.448826	1.953699	0.027239	
611	1	3	3	2	8	47.674	70083.039	127.1	136.6	10.302	43.368	7.973	0.216	1.450122	1.951952	0.027232	
612	1	3	2	3	8	49.034	72150.062	161.7	178.2	18.144	44.601	8.208	0.216	1.492892	1.896031	0.027007	
613	1	1	4	1	8	49.205	72411.008	83.7	120.0	50.941	44.757	8.238	0.216	1.498291	1.889198	0.026980	
614	1	1	2	4	8	49.435	72761.125	99.2	169.1	116.433	44.965	8.277	0.216	1.505536	1.880107	0.026946	
615	1	1	3	3	8	50.169	73880.125	204.0	214.8	11.915	45.630	8.405	0.216	1.528690	1.851631	0.026841	
616	1	0	2	4	4	50.467	74335.578	35.5	39.8	5.220	45.901	8.457	0.216	1.538114	1.840286	0.026801	
617	1	2	1	4	8	50.602	74541.469	237.5	220.2	15.976	46.023	8.480	0.216	1.542374	1.835203	0.026783	
618	1	4	2	1	8	50.761	74783.719	10.1	8.4	1.838	46.167	8.508	0.216	1.547386	1.829258	0.026762	
619	1	3	3	1	8	50.895	74988.430	576.1	692.9	137.315	46.288	8.531	0.216	1.551622	1.824264	0.026745	
620	1	0	3	3	4	51.249	75530.016	942.4	1082.7	157.505	46.609	8.592	0.216	1.562828	1.811184	0.026701	
621	1	0	4	0	2	51.402	75763.562	739.6	872.4	153.139	46.747	8.619	0.216	1.567661	1.805600	0.026682	
622	1	4	1	2	8	51.732	76269.602	5.7	5.3	1.952	47.047	8.677	0.216	1.578131	1.793621	0.026642	
623	1	4	2	0	4	51.979	76647.141	133.6	169.3	44.410	47.270	8.720	0.216	1.585943	1.784786	0.026614	
624	1	2	0	4	4	52.146	76904.109	0.4	2.1	7.793	47.422	8.749	0.216	1.591260	1.778822	0.026595	
625	1	2	3	2	8	52.915	78083.258	24.9	47.0	41.203	48.118	8.883	0.216	1.615659	1.751960	0.026511	
626	1	4	0	2	4	53.385	78806.117	1801.1	1722.4	73.744	48.544	8.965	0.216	1.630616	1.735890	0.026463	
627	1	3	1	3	8	53.640	79196.930	248.6	283.1	38.522	48.774	9.010	0.217	1.638702	1.727324	0.026438	
628	1	1	1	4	8	54.166	80007.227	4.8	17.1	42.395	49.250	9.102	0.217	1.655468	1.709830	0.026387	
629	1	2	2	3	8	54.793	80973.227	781.7	816.5	35.995	49.818	9.212	0.217	1.675457	1.689431	0.026331	
630	1	3	2	2	8	55.380	81880.094	185.8	236.5	63.154	50.349	9.315	0.217	1.694221	1.670720	0.026280	
631	1	3	0	3	4	55.489	82048.133	52.4	65.7	16.586	50.448	9.334	0.217	1.697698	1.667298	0.026271	
632	1	4	1	1	8	55.923	82720.164	9.5	25.2	40.707	50.841	9.410	0.217	1.711603	1.653753	0.026236	
633	1	1	0	4	4	56.072	82950.141	7.3	17.9	25.403	50.975	9.437	0.217	1.716362	1.649168	0.026225	
634	1	1	3	2	8	57.030	84435.445	648.3	851.7	260.760	51.842	9.606	0.217	1.747095	1.620158	0.026153	
635	1	2	3	1	8	57.425	85048.789	5.7	6.0	1.312	52.199	9.675	0.217	1.759786	1.608474	0.026125	
636	1	4	1	0	4	57.563	85263.492	1.7	2.3	0.792	52.324	9.700	0.217	1.764228	1.604423	0.026116	
637	1	0	0	4	2	57.591	85306.078	778.5	739.6	36.460	52.349	9.705	0.217	1.765110	1.603622	0.026114	
638	1	4	0	1	4	58.027	85985.297	18.6	11.5	5.760	52.744	9.782	0.217	1.779164	1.590955	0.026084	
639	1	2	3	0	4	59.205	87820.391	352.9	491.4	188.204	53.808	9.991	0.217	1.817134	1.557710	0.026011	
640	1	1	2	3	8	59.400	88124.805	430.6	447.0	17.203	53.985	10.025	0.217	1.823433	1.552329	0.026000	
641	1	4	0	0	2	59.865	88852.602	656.8	643.5	13.963	54.405	10.108	0.218	1.838492	1.539614	0.025973	
642	1	3	2	1	8	60.613	90023.898	883.1	1037.3	176.857	55.081	10.241	0.218	1.862728	1.519582	0.025932	
643	1	2	1	3	8	61.454	91343.523	4.4	31.2	188.539	55.841	10.391	0.218	1.890033	1.497629	0.025890	
644	1	3	1	2	8	62.285	92651.367	239.3	310.0	89.452	56.591	10.540	0.218	1.917095	1.476489	0.025850	
645	1	1	3	1	8	62.794	93453.992	254.1	428.5	286.926	57.051	10.631	0.218	1.933702	1.463808	0.025828	
646	1	2	2	2	8	64.107	95531.508	0.0	0.0	0.013	58.236	10.868	0.218	1.976689	1.431975	0.025773	
647	1	2	0	3	4	64.276	95798.680	1032.7	999.5	32.015	58.388	10.898	0.218	1.982217	1.427981	0.025766	
648	1	0	3	1	4	64.946	96862.539	1440.6	1872.2	546.875	58.993	11.019	0.219	2.004230	1.412297	0.025741	
649	1	3	0	2	4	65.228	97310.617	71.2	134.8	117.391	59.247	11.070	0.219	2.013501	1.405794	0.025731	
650	1	1	1	3	8	68.166	102007.961	1189.0	1108.2	73.859	61.896	11.605	0.219	2.110696	1.341059	0.025636	
651	1	3	1	1	8	70.014	104986.430	2422.9	2464.6	42.249	63.560	11.943	0.220	2.172325	1.303013	0.025586	
652	1	0	1	3	4	70.940	106488.312	14.2	66.1	235.309	64.395	12.114	0.220	2.203402	1.284636	0.025563	
653	1	1	2	2	8	71.835	107943.312	1235.3	1426.7	216.054	65.200	12.280	0.220	2.233508	1.267320	0.025543	
654	1	1	0	3	4	72.072	108329.188	935.0	868.4	60.776	65.413	12.324	0.220	2.241492	1.262806	0.025538	
655	1	2	2	1	8	72.626	109233.766	4551.1	5227.0	756.328	65.911	12.427	0.220	2.260209	1.252348	0.025526	
656	1	3	0	1	4	74.262	111916.688	1196.9	1344.6	161.757	67.382	12.732	0.221	2.315723	1.222326	0.025494	
657	1	0	2	2	4	75.099	113295.031	4996.1	5275.3	287.385	68.134	12.889	0.221	2.344243	1.207456	0.025479	
658	1	2	1	2	8	75.542	114028.000	6455.2	6528.0	72.976	68.532	12.972	0.221	2.359409	1.199694	0.025471	

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 BRAGG R-Factors and weight fractions for Pattern #  1
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=> Phase:  1     VOSO4 Nuclear
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=> Bragg R-factor:   11.4       Vol:  325.587( 2.991)  Fract(%):  100.00( 1.65)
=> Rf-factor=  10.5             ATZ:         651.994   Brindley:  1.0000

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Pattern#  2 Phase No:   1 Phase name: VOSO4 Nuclear
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No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
1	1	1	6	5	8	123.103	29078.863	0.0	0.0	0.000	120.385	5.072	0.055	0.835386	3.388336	0.043828	
2	1	4	5	5	8	123.214	29103.881	0.0	0.0	0.000	120.494	5.076	0.055	0.836105	3.385423	0.043764	
3	1	7	1	5	8	123.229	29107.342	0.0	0.0	0.000	120.509	5.077	0.055	0.836204	3.385020	0.043755	
4	1	3	7	1	8	123.232	29108.051	0.0	0.0	0.000	120.512	5.077	0.055	0.836225	3.384938	0.043753	
5	1	8	3	1	8	123.258	29113.818	0.0	0.0	0.000	120.537	5.078	0.055	0.836390	3.384267	0.043739	
6	1	2	5	6	8	123.268	29116.035	0.0	0.0	0.000	120.547	5.078	0.055	0.836454	3.384010	0.043733	
7	1	0	7	3	4	123.499	29168.291	0.0	0.0	0.000	120.773	5.087	0.055	0.837955	3.377947	0.043600	
8	1	4	4	6	8	123.587	29188.084	0.0	0.0	0.000	120.859	5.091	0.055	0.838524	3.375657	0.043550	
9	1	5	5	4	8	123.855	29248.600	0.0	0.0	0.000	121.121	5.101	0.055	0.840263	3.368672	0.043399	
10	1	5	3	6	8	124.119	29308.184	0.0	0.0	0.000	121.380	5.112	0.055	0.841974	3.361824	0.043251	
11	1	6	1	6	8	124.124	29309.361	0.0	0.0	0.000	121.385	5.112	0.055	0.842008	3.361688	0.043248	
12	1	8	3	0	4	124.171	29319.875	0.0	0.0	0.000	121.431	5.114	0.055	0.842310	3.360483	0.043222	
13	1	1	4	7	8	124.344	29358.979	0.0	0.0	0.000	121.600	5.120	0.055	0.843433	3.356007	0.043126	
14	1	7	0	5	4	124.389	29369.182	0.0	0.0	0.000	121.645	5.122	0.055	0.843727	3.354841	0.043101	
15	1	1	2	8	8	124.544	29404.139	0.1	0.1	0.001	121.796	5.128	0.055	0.844731	3.350853	0.043016	
16	1	3	6	4	8	124.593	29415.119	0.7	0.6	0.005	121.844	5.130	0.055	0.845046	3.349602	0.042990	
17	1	2	7	2	8	124.710	29441.383	0.9	0.7	0.015	121.958	5.135	0.055	0.845801	3.346614	0.042926	
18	1	5	6	1	8	124.831	29468.641	1.1	0.8	0.035	122.076	5.140	0.055	0.846584	3.343518	0.042861	
19	1	6	3	5	8	124.921	29489.141	0.5	0.4	0.027	122.165	5.143	0.055	0.847173	3.341194	0.042812	
20	1	6	4	4	8	125.038	29515.512	1.4	1.0	0.116	122.280	5.148	0.055	0.847930	3.338209	0.042749	
21	1	7	4	2	8	125.056	29519.492	11.6	8.7	1.051	122.297	5.148	0.055	0.848045	3.337759	0.042739	
22	1	4	6	3	8	125.108	29531.154	1.9	1.4	0.208	122.348	5.151	0.055	0.848380	3.336441	0.042711	
23	1	8	1	3	8	125.240	29560.984	4.7	3.4	0.684	122.478	5.156	0.055	0.849237	3.333074	0.042641	
24	1	6	0	6	4	125.310	29576.742	0.4	0.3	0.061	122.546	5.158	0.055	0.849689	3.331298	0.042604	
25	1	0	2	8	4	125.412	29599.660	0.2	0.1	0.026	122.646	5.162	0.055	0.850348	3.328719	0.042550	
26	1	2	1	8	8	125.524	29624.832	0.0	0.0	0.000	122.755	5.167	0.055	0.851071	3.325891	0.042491	
27	1	6	5	2	8	125.597	29641.309	3.0	2.4	0.447	122.827	5.170	0.055	0.851544	3.324042	0.042452	
28	1	4	2	7	8	125.654	29654.195	0.4	0.3	0.049	122.883	5.172	0.055	0.851915	3.322597	0.042422	
29	1	3	3	7	8	125.761	29678.283	50.3	47.0	3.136	122.987	5.176	0.055	0.852607	3.319901	0.042366	
30	1	1	5	6	8	125.843	29696.826	0.1	0.2	0.003	123.068	5.179	0.055	0.853139	3.317827	0.042323	
31	1	5	4	5	8	126.125	29760.287	0.1	0.2	0.037	123.344	5.190	0.055	0.854962	3.310753	0.042178	
32	1	8	2	2	8	126.389	29819.627	0.0	0.0	0.006	123.602	5.201	0.055	0.856667	3.304164	0.042043	
33	1	8	0	3	4	126.459	29835.377	3.1	4.0	1.281	123.670	5.204	0.055	0.857120	3.302420	0.042007	
34	1	2	0	8	4	126.750	29901.021	0.2	0.4	0.220	123.956	5.215	0.055	0.859006	3.295170	0.041860	
35	1	1	7	2	8	127.378	30042.268	28.1	36.1	10.056	124.571	5.240	0.055	0.863063	3.279677	0.041548	
36	1	2	7	1	8	127.613	30095.074	0.0	0.0	0.006	124.801	5.249	0.055	0.864580	3.273923	0.041434	
37	1	7	4	1	8	127.984	30178.514	5.1	4.8	0.331	125.164	5.263	0.055	0.866977	3.264871	0.041255	
38	1	7	2	4	8	128.203	30227.568	3.6	3.0	0.467	125.378	5.272	0.055	0.868387	3.259572	0.041151	
39	1	1	1	8	8	128.246	30237.258	42.5	35.3	5.900	125.420	5.274	0.055	0.868665	3.258528	0.041130	
40	1	6	5	1	8	128.564	30308.709	3.0	2.2	0.537	125.731	5.286	0.055	0.870718	3.250846	0.040980	
41	1	2	7	0	4	128.627	30322.838	0.3	0.3	0.063	125.793	5.289	0.055	0.871124	3.249331	0.040951	
42	1	7	3	3	8	128.879	30379.363	22.6	16.6	4.341	126.040	5.298	0.055	0.872747	3.243286	0.040834	
43	1	2	6	4	8	129.126	30434.826	0.0	0.0	0.001	126.281	5.308	0.055	0.874341	3.237375	0.040720	
44	1	8	2	1	8	129.414	30499.422	1.9	1.6	0.257	126.563	5.319	0.055	0.876197	3.230519	0.040589	
45	1	4	1	7	8	129.458	30509.375	140.8	119.1	18.009	126.607	5.321	0.055	0.876482	3.229465	0.040569	
46	1	3	5	5	8	129.479	30514.178	109.2	92.9	13.576	126.628	5.322	0.055	0.876620	3.228956	0.040559	
47	1	1	0	8	4	129.555	30531.104	21.6	18.8	2.427	126.701	5.325	0.055	0.877107	3.227166	0.040525	
48	1	6	5	0	4	129.601	30541.400	281.0	246.6	29.579	126.746	5.327	0.055	0.877402	3.226078	0.040504	
49	1	3	4	6	8	129.912	30611.266	26.1	24.3	1.612	127.051	5.339	0.055	0.879410	3.218715	0.040365	
50	1	4	6	2	8	130.113	30656.250	175.6	167.0	8.091	127.248	5.347	0.055	0.880702	3.213992	0.040276	
51	1	8	1	2	8	130.262	30689.621	2.5	2.4	0.133	127.394	5.353	0.055	0.881661	3.210497	0.040210	
52	1	5	2	6	8	130.411	30723.098	4.0	3.7	0.299	127.540	5.358	0.055	0.882622	3.206999	0.040145	
53	1	2	3	7	8	130.427	30726.592	3.1	2.8	0.242	127.555	5.359	0.055	0.882723	3.206634	0.040138	
54	1	8	2	0	4	130.471	30736.568	4.8	4.3	0.418	127.599	5.361	0.055	0.883009	3.205594	0.040119	
55	1	1	7	1	8	130.476	30737.770	8.3	7.4	0.728	127.604	5.361	0.055	0.883044	3.205468	0.040116	
56	1	0	0	8	2	130.532	30750.148	46.5	41.1	4.658	127.658	5.363	0.055	0.883399	3.204178	0.040092	
57	1	4	0	7	4	130.805	30811.307	4.0	3.2	0.627	127.925	5.374	0.055	0.885156	3.197818	0.039974	
58	1	5	5	3	8	130.811	30812.834	25.3	20.3	3.958	127.932	5.374	0.055	0.885200	3.197659	0.039971	
59	1	6	2	5	8	131.342	30931.740	0.1	0.1	0.021	128.451	5.395	0.055	0.888616	3.185367	0.039745	
60	1	0	7	1	4	131.474	30961.324	11.3	8.5	2.069	128.581	5.400	0.055	0.889466	3.182323	0.039689	

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
61	1	8	0	2	4	131.634	30996.990	115.3	85.9	21.488	128.737	5.406	0.055	0.890491	3.178662	0.039623	
62	1	3	6	3	8	131.682	31007.705	8.0	5.9	1.507	128.784	5.408	0.055	0.890799	3.177563	0.039603	
63	1	1	6	4	8	132.094	31100.018	1.8	1.2	0.386	129.188	5.424	0.055	0.893451	3.168131	0.039432	
64	1	6	4	3	8	132.207	31125.369	21.3	13.7	4.778	129.298	5.429	0.055	0.894179	3.165551	0.039386	
65	1	4	5	4	8	132.231	31130.629	0.9	0.6	0.197	129.322	5.429	0.055	0.894330	3.165016	0.039376	
66	1	7	1	4	8	132.250	31134.867	5.4	3.4	1.215	129.340	5.430	0.055	0.894452	3.164585	0.039369	
67	1	3	2	7	8	132.319	31150.236	34.2	21.6	7.804	129.407	5.433	0.055	0.894893	3.163024	0.039341	
68	1	4	3	6	8	132.552	31202.500	2.7	1.7	0.630	129.636	5.442	0.055	0.896395	3.157726	0.039246	
69	1	0	6	4	4	133.130	31331.633	54.9	39.7	10.822	130.202	5.465	0.055	0.900105	3.144711	0.039015	
70	1	4	6	1	8	133.419	31396.336	1.0	0.7	0.227	130.485	5.476	0.055	0.901963	3.138231	0.038902	
71	1	1	3	7	8	133.487	31411.539	0.7	0.5	0.170	130.552	5.478	0.055	0.902400	3.136712	0.038875	

72	1	8	1	1	8	133.580	31432.188	0.2	0.1	0.038	130.642	5.482	0.055	0.902993	3.134651	0.038839
73	1	7	0	4	4	133.686	31455.951	0.4	0.2	0.086	130.746	5.486	0.055	0.903676	3.132283	0.038798
74	1	6	3	4	8	134.347	31603.473	18.3	16.1	1.909	131.393	5.512	0.055	0.907914	3.117662	0.038546
75	1	7	3	2	8	134.369	31608.357	29.8	26.3	2.986	131.415	5.513	0.055	0.908054	3.117180	0.038537
76	1	0	3	7	4	134.556	31650.238	33.8	30.4	3.010	131.598	5.520	0.055	0.909258	3.113055	0.038467
77	1	4	6	0	4	134.579	31655.203	37.3	33.5	3.399	131.620	5.521	0.055	0.909400	3.112567	0.038458
78	1	2	5	5	8	134.587	31657.084	1.9	1.7	0.175	131.628	5.521	0.055	0.909454	3.112382	0.038455
79	1	5	1	6	8	134.677	31677.188	0.9	0.8	0.101	131.717	5.525	0.055	0.910032	3.110407	0.038422
80	1	8	1	0	4	134.743	31691.951	0.1	0.1	0.013	131.781	5.527	0.055	0.910456	3.108958	0.038397
81	1	4	4	5	8	135.002	31749.754	1.1	0.8	0.229	132.035	5.537	0.055	0.912116	3.103298	0.038301
82	1	8	0	1	4	135.060	31762.656	5.7	3.8	1.247	132.092	5.540	0.055	0.912487	3.102037	0.038280
83	1	2	4	6	8	135.073	31765.535	1.5	1.0	0.324	132.104	5.540	0.055	0.912570	3.101756	0.038275
84	1	5	3	5	8	135.696	31904.508	0.0	0.0	0.000	132.715	5.564	0.055	0.916562	3.088245	0.038048
85	1	6	1	5	8	135.703	31906.025	1.4	0.8	0.339	132.721	5.565	0.055	0.916606	3.088098	0.038046
86	1	5	4	4	8	135.846	31937.912	1.9	1.2	0.421	132.861	5.570	0.055	0.917522	3.085015	0.037994
87	1	7	2	3	8	135.963	31963.838	23.9	16.9	4.848	132.975	5.575	0.055	0.918267	3.082513	0.037953
88	1	5	0	6	4	136.195	32015.527	0.3	0.2	0.046	133.203	5.584	0.055	0.919752	3.077536	0.037870
89	1	8	0	0	2	136.263	32030.771	40.9	32.6	6.551	133.270	5.586	0.055	0.920190	3.076072	0.037846
90	1	5	5	2	8	136.563	32097.467	17.8	14.8	2.450	133.563	5.598	0.055	0.922106	3.069680	0.037741
91	1	3	1	7	8	136.780	32145.982	22.5	18.8	2.998	133.776	5.607	0.055	0.923499	3.065047	0.037666
92	1	2	6	3	8	137.064	32209.199	38.2	31.8	5.247	134.054	5.618	0.055	0.925315	3.059031	0.037568
93	1	6	0	5	4	137.256	32251.834	136.4	111.5	19.979	134.242	5.625	0.055	0.926540	3.054987	0.037503
94	1	3	6	2	8	137.553	32317.922	6.6	5.1	1.117	134.533	5.637	0.055	0.928439	3.048740	0.037402
95	1	2	2	7	8	137.783	32369.033	6.8	5.0	1.313	134.758	5.645	0.055	0.929907	3.043926	0.037325
96	1	1	5	5	8	137.957	32407.715	1.7	1.2	0.366	134.928	5.652	0.055	0.931019	3.040293	0.037267
97	1	7	3	1	8	138.018	32421.438	21.0	14.0	4.564	134.988	5.655	0.055	0.931413	3.039006	0.037247
98	1	6	4	2	8	138.152	32451.205	2.1	1.3	0.469	135.120	5.660	0.055	0.932268	3.036218	0.037202
99	1	3	0	7	4	138.371	32499.740	3.2	1.9	0.740	135.333	5.668	0.055	0.933662	3.031684	0.037131
100	1	1	4	6	8	138.480	32524.092	0.1	0.1	0.034	135.441	5.673	0.055	0.934362	3.029414	0.037095
101	1	0	5	5	4	139.137	32670.045	142.2	113.6	22.459	136.084	5.698	0.055	0.938555	3.015880	0.036884
102	1	0	4	6	4	139.674	32789.281	96.6	84.2	10.624	136.610	5.719	0.055	0.941980	3.004913	0.036714
103	1	3	5	4	8	140.061	32875.152	24.4	21.4	2.547	136.989	5.734	0.055	0.944447	2.997065	0.036594
104	1	4	2	6	8	140.294	32926.840	61.7	53.9	6.715	137.217	5.743	0.055	0.945932	2.992360	0.036523
105	1	5	5	1	8	140.398	32949.914	4.2	3.7	0.466	137.319	5.747	0.055	0.946595	2.990264	0.036491
106	1	3	3	6	8	140.443	32959.824	10.9	9.5	1.210	137.363	5.749	0.055	0.946880	2.989365	0.036477
107	1	1	6	3	8	140.628	33000.793	46.3	40.3	5.108	137.544	5.756	0.055	0.948057	2.985654	0.036421
108	1	4	5	3	8	140.793	33037.371	85.1	74.7	8.980	137.705	5.762	0.055	0.949108	2.982348	0.036372
109	1	7	1	3	8	140.816	33042.434	55.7	49.0	5.820	137.728	5.763	0.055	0.949253	2.981891	0.036365
110	1	1	2	7	8	141.404	33172.766	0.0	0.0	0.001	138.304	5.786	0.055	0.952997	2.970176	0.036190
111	1	3	6	1	8	141.475	33188.535	57.8	54.7	2.989	138.373	5.788	0.055	0.953450	2.968765	0.036169
112	1	6	4	1	8	142.127	33332.930	3.1	2.9	0.187	139.012	5.814	0.055	0.957598	2.955904	0.035980
113	1	6	2	4	8	142.426	33399.066	0.3	0.3	0.026	139.305	5.825	0.055	0.959498	2.950051	0.035894
114	1	7	2	2	8	142.452	33404.836	47.7	42.6	4.542	139.330	5.826	0.055	0.959664	2.949542	0.035887
115	1	7	0	3	4	142.552	33426.980	22.9	20.1	2.437	139.428	5.830	0.055	0.960300	2.947587	0.035859
116	1	2	1	7	8	142.840	33490.633	1.2	1.0	0.179	139.710	5.841	0.055	0.962129	2.941985	0.035778
117	1	6	3	3	8	143.353	33604.168	8.8	6.3	1.757	140.213	5.861	0.055	0.965391	2.932045	0.035635
118	1	3	4	5	8	143.365	33606.828	95.1	68.2	18.948	140.225	5.861	0.055	0.965467	2.931813	0.035632
119	1	6	4	0	4	143.530	33643.207	1.9	1.4	0.388	140.386	5.868	0.055	0.966512	2.928643	0.035587
120	1	2	6	2	8	143.720	33685.195	1.2	0.9	0.246	140.572	5.875	0.055	0.967718	2.924992	0.035535

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
121	1	5	2	5	8	144.036	33754.980	4.5	3.4	0.854	140.881	5.887	0.055	0.969723	2.918945	0.035450	
122	1	2	0	7	4	144.653	33891.230	210.1	149.7	42.197	141.486	5.911	0.055	0.973637	2.907211	0.035285	
123	1	5	4	3	8	145.178	34007.066	42.0	28.7	8.932	142.000	5.931	0.055	0.976965	2.897308	0.035148	
124	1	4	1	6	8	145.643	34109.590	0.0	0.0	0.002	142.455	5.949	0.055	0.979910	2.888600	0.035029	
125	1	2	5	4	8	146.587	34317.605	0.1	0.1	0.003	143.379	5.985	0.055	0.985886	2.871090	0.034792	
126	1	7	2	1	8	146.820	34368.965	9.9	9.4	0.394	143.608	5.994	0.055	0.987362	2.866800	0.034735	
127	1	1	1	7	8	146.885	34383.207	21.3	20.3	0.993	143.671	5.997	0.055	0.987771	2.865613	0.034719	
128	1	4	3	5	8	146.933	34393.891	100.4	94.9	5.133	143.719	5.999	0.055	0.988078	2.864722	0.034707	
129	1	2	3	6	8	147.024	34413.949	123.1	115.3	7.163	143.808	6.002	0.055	0.988654	2.863052	0.034685	
130	1	4	4	4	8	147.123	34435.746	122.4	113.9	7.771	143.905	6.006	0.055	0.989280	2.861240	0.034661	
131	1	4	0	6	4	147.566	34533.102	48.5	44.0	4.044	144.338	6.023	0.055	0.992077	2.853174	0.034555	
132	1	1	6	2	8	147.842	34593.840	28.0	24.5	2.991	144.609	6.033	0.055	0.993822	2.848164	0.034489	
133	1	5	3	4	8	148.022	34633.449	19.0	16.3	2.269	144.785	6.040	0.055	0.994960	2.844907	0.034446	
134	1	6	1	4	8	148.031	34635.387	85.9	73.7	10.316	144.794	6.041	0.055	0.995016	2.844748	0.034444	
135	1	4	5	2	8	148.033	34635.988	3.2	2.7	0.382	144.796	6.041	0.055	0.995033	2.844699	0.034444	
136	1	7	1	2	8	148.060	34641.820	33.3	28.4	4.053	144.822	6.042	0.055	0.995201	2.844219	0.034437	
137	1	2	6	1	8	148.209	34674.535	17.4	14.7	2.231	144.968	6.048	0.055	0.996140	2.841536	0.034403	
138	1	0	1	7	4	148.311	34696.973	9.2	7.8	1.225	145.068	6.051	0.055	0.996785	2.839699	0.034379	
139	1	1	0	7	4	148.857	34817.117	14.3	11.0	2.576	145.603	6.072	0.055	1.000237	2.829900	0.034252	
140	1	0	6	2	4	149.296	34913.465	0.1	0.1	0.024	146.033	6.089	0.055	1.003004	2.822090	0.034153	
141	1	3	2	6	8	149.746	35012.309	21.8	17.0	3.702	146.474	6.106	0.055	1.005844	2.814123	0.034052	
142	1	2	6	0	4	149.800	35024.207	0.1	0.1	0.012	146.527	6.109	0.055	1.006186	2.813167	0.034040	
143	1	5	1	5	8	149.840	35032.789	4.8	3.8	0.748	146.565	6.110	0.055	1.006432	2.812478	0.034031	
144	1	6	0	4	4	150.050	35079.043	12.4	10.7	1.478	146.772	6.118	0.055	1.007761	2.808769	0.033984	
145	1	7	0	2	4	150.081	35085.723	16.8	14.6	1.909	146.802	6.119	0.055	1.007953	2.808235	0.033978	
146	1	3	5	3	8	150.352	35145.297	21.6	19.9	1.525	147.068	6.130	0.055	1.009665	2.803475	0.033918	
147	1	2	4	5	8	150.385	35152.402	0.1	0.1	0.010	147.099	6.131	0.055	1.009869	2.802908	0.033911	
148	1	1	5	4	8	150.966	35279.879	0.1	0.0	0.006	147.669	6.153	0.055	1.013531	2.792780	0.033786	
149	1	6	3	2	8	151.016	35290.785	362.5	310.6	43.592	147.718	6.155	0.055	1.013844	2.791917	0.033775	
150	1	1	3	6	8	151.444	35384.594	19.8	16.8	2.504	148.137	6.171	0.055	1.016539	2.784515	0.033684	
151	1	5	0	5	4	151.935	35492.094	2.1	2.0	0.130	148.618	6.190	0.055	1.019627	2.776082	0.033582	

152	1	1	6	1	8	152.739	35668.039	12.5	12.8	0.361	149.405	6.221	0.055	1.024682	2.762388	0.033417
153	1	4	5	1	8	152.950	35714.238	57.7	54.8	2.714	149.612	6.229	0.055	1.026009	2.758814	0.033374
154	1	7	1	1	8	152.979	35720.633	23.4	22.0	1.301	149.641	6.230	0.055	1.026193	2.758320	0.033369
155	1	5	4	2	8	153.152	35758.316	50.2	44.7	4.771	149.810	6.237	0.055	1.027276	2.755414	0.033334
156	1	6	2	3	8	153.286	35787.621	211.4	182.9	24.205	149.941	6.242	0.055	1.028118	2.753157	0.033307
157	1	4	5	0	4	154.701	36096.668	0.1	0.0	0.024	151.327	6.296	0.055	1.036996	2.729586	0.033033
158	1	1	4	5	8	155.123	36188.797	0.4	0.2	0.098	151.741	6.312	0.055	1.039643	2.722637	0.032953
159	1	7	0	1	4	155.210	36207.910	4.3	3.4	0.873	151.827	6.315	0.055	1.040192	2.721200	0.032936
160	1	0	6	0	2	156.142	36411.078	238.6	245.6	7.284	152.739	6.350	0.055	1.046028	2.706016	0.032765
161	1	6	3	1	8	156.245	36433.410	7.5	7.6	0.114	152.840	6.354	0.055	1.046670	2.704357	0.032746
162	1	3	1	6	8	156.296	36444.551	52.1	52.7	0.644	152.890	6.356	0.055	1.046990	2.703531	0.032737
163	1	4	2	5	8	157.681	36746.070	7.5	7.2	0.275	154.247	6.409	0.055	1.055652	2.681346	0.032492
164	1	2	2	6	8	157.794	36770.547	0.9	0.9	0.054	154.357	6.413	0.055	1.056355	2.679562	0.032472
165	1	3	3	5	8	157.892	36791.934	107.2	98.8	7.693	154.454	6.417	0.055	1.056970	2.678004	0.032455
166	1	6	3	0	4	158.112	36839.676	59.2	53.9	4.793	154.669	6.425	0.055	1.058341	2.674533	0.032418
167	1	3	4	4	8	158.128	36843.188	64.8	58.9	5.232	154.685	6.426	0.055	1.058442	2.674279	0.032415
168	1	2	5	3	8	158.503	36924.676	0.0	0.0	0.000	155.052	6.440	0.055	1.060783	2.668377	0.032351
169	1	5	4	1	8	158.613	36948.512	17.4	16.4	0.972	155.159	6.444	0.055	1.061468	2.666655	0.032333
170	1	3	0	6	4	158.677	36962.488	55.9	52.8	2.866	155.222	6.447	0.055	1.061869	2.665647	0.032322
171	1	5	2	4	8	159.028	37038.652	8.6	8.5	0.212	155.566	6.460	0.055	1.064057	2.660166	0.032263
172	1	4	4	3	8	159.181	37071.965	2.4	2.4	0.060	155.716	6.466	0.055	1.065014	2.657775	0.032238
173	1	3	5	2	8	159.258	37088.742	15.3	15.4	0.478	155.792	6.469	0.055	1.065496	2.656573	0.032225
174	1	5	3	3	8	160.319	37318.969	27.1	17.4	6.297	156.831	6.509	0.055	1.072111	2.640184	0.032053
175	1	6	1	3	8	160.330	37321.402	0.0	0.0	0.007	156.842	6.509	0.055	1.072180	2.640012	0.032051
176	1	6	2	2	8	162.753	37846.000	16.8	7.3	4.120	159.216	6.601	0.055	1.087251	2.603418	0.031678
177	1	6	0	3	4	162.902	37878.215	20.9	11.5	5.095	159.362	6.606	0.055	1.088177	2.601203	0.031656
178	1	4	3	4	8	162.946	37887.699	5.4	3.1	1.297	159.405	6.608	0.055	1.088449	2.600553	0.031649
179	1	1	2	6	8	163.289	37961.762	2.3	1.9	0.366	159.741	6.621	0.055	1.090577	2.595479	0.031599
180	1	1	5	3	8	164.074	38131.434	87.4	90.7	3.579	160.511	6.650	0.055	1.095451	2.583930	0.031485

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
181	1	0	2	6	4	165.251	38385.324	409.3	392.9	15.509	161.664	6.695	0.055	1.102745	2.566839	0.031320	
182	1	4	1	5	8	165.376	38412.309	27.5	26.4	1.024	161.786	6.699	0.055	1.103520	2.565036	0.031303	
183	1	3	5	1	8	165.421	38421.895	144.9	139.9	4.721	161.830	6.701	0.055	1.103796	2.564396	0.031297	
184	1	2	1	6	8	165.506	38440.266	14.5	14.3	0.254	161.913	6.704	0.055	1.104324	2.563170	0.031285	
185	1	0	5	3	4	166.065	38560.766	20.7	25.1	5.188	162.461	6.725	0.055	1.107785	2.555161	0.031209	
186	1	5	1	4	8	166.930	38746.895	5.0	5.5	0.818	163.309	6.758	0.055	1.113132	2.542886	0.031094	
187	1	2	3	5	8	167.403	38848.566	0.0	0.0	0.007	163.772	6.776	0.055	1.116053	2.536231	0.031032	
188	1	2	4	4	8	167.683	38908.914	0.4	0.6	0.377	164.047	6.786	0.055	1.117787	2.532298	0.030996	
189	1	4	0	5	4	168.201	39020.199	0.1	0.2	0.194	164.554	6.805	0.054	1.120984	2.525075	0.030930	
190	1	2	0	6	4	168.338	39049.508	4.1	7.1	5.227	164.688	6.811	0.054	1.121826	2.523180	0.030913	
191	1	2	5	2	8	169.031	39198.469	621.0	704.8	93.186	165.368	6.837	0.054	1.126105	2.513592	0.030826	
192	1	6	2	1	8	169.345	39265.688	161.3	174.0	13.493	165.675	6.848	0.054	1.128036	2.509289	0.030788	
193	1	5	0	4	4	169.836	39371.070	0.1	0.1	0.009	166.156	6.867	0.054	1.131064	2.502572	0.030728	
194	1	4	4	2	8	169.853	39374.801	132.4	150.2	19.725	166.173	6.867	0.054	1.131171	2.502335	0.030726	
195	1	5	3	2	8	171.237	39671.141	77.8	72.7	4.649	167.529	6.919	0.054	1.139684	2.483643	0.030562	
196	1	6	1	2	8	171.250	39674.062	23.5	21.9	1.480	167.542	6.920	0.054	1.139768	2.483460	0.030560	
197	1	3	2	5	8	171.444	39715.570	140.9	127.6	11.852	167.732	6.927	0.054	1.140961	2.480864	0.030538	
198	1	6	2	0	4	171.725	39775.645	0.1	0.1	0.002	168.007	6.937	0.054	1.142687	2.477118	0.030505	
199	1	1	1	6	8	171.874	39807.484	1.3	1.4	0.059	168.153	6.943	0.054	1.143601	2.475136	0.030488	
200	1	3	4	3	8	173.373	40127.949	33.3	37.4	4.688	169.623	6.999	0.054	1.152808	2.455369	0.030321	
201	1	1	3	5	8	173.999	40261.438	9.0	10.0	1.145	170.236	7.022	0.054	1.156643	2.447229	0.030253	
202	1	1	4	4	8	174.314	40328.629	14.2	15.0	0.869	170.545	7.034	0.054	1.158573	2.443151	0.030219	
203	1	6	0	2	4	174.390	40344.914	0.8	0.8	0.037	170.619	7.037	0.054	1.159041	2.442165	0.030211	
204	1	5	2	3	8	174.559	40380.871	59.2	61.2	2.253	170.785	7.043	0.054	1.160074	2.439991	0.030193	
205	1	1	0	6	4	175.048	40485.242	7.5	8.3	0.949	171.265	7.061	0.054	1.163072	2.433700	0.030142	
206	1	1	5	2	8	175.828	40651.312	65.7	74.8	10.193	172.029	7.090	0.054	1.167843	2.423758	0.030061	
207	1	0	3	5	4	176.375	40767.797	2.8	3.6	0.951	172.565	7.110	0.054	1.171189	2.416833	0.030005	
208	1	2	5	1	8	176.444	40782.426	1.5	2.0	0.580	172.633	7.113	0.054	1.171610	2.415966	0.029999	
209	1	0	4	4	4	176.703	40837.555	22.6	31.8	12.622	172.887	7.122	0.054	1.173193	2.412704	0.029973	
210	1	4	4	1	8	177.379	40981.133	0.0	0.0	0.001	173.549	7.147	0.054	1.177318	2.404252	0.029906	
211	1	0	0	6	2	177.469	41000.199	10.0	12.0	2.414	173.637	7.151	0.054	1.177866	2.403133	0.029897	
212	1	4	2	4	8	177.958	41104.227	722.5	718.8	4.197	174.117	7.169	0.054	1.180855	2.397052	0.029849	
213	1	3	3	4	8	178.261	41168.445	134.3	138.4	4.162	174.413	7.180	0.054	1.182699	2.393312	0.029820	
214	1	5	3	1	8	178.954	41315.551	16.8	19.9	3.494	175.093	7.206	0.054	1.186926	2.384791	0.029755	
215	1	6	1	1	8	178.970	41318.852	1.5	1.7	0.305	175.108	7.206	0.054	1.187020	2.384600	0.029753	
216	1	2	5	0	4	179.139	41354.668	199.5	231.7	36.702	175.274	7.213	0.054	1.188049	2.382535	0.029737	
217	1	4	3	3	8	179.770	41488.367	236.6	260.0	25.258	175.892	7.236	0.054	1.191890	2.374857	0.029679	
218	1	4	4	0	4	180.117	41561.902	5.4	6.6	1.318	176.232	7.249	0.054	1.194003	2.370656	0.029647	
219	1	3	1	5	8	181.450	41844.023	315.2	305.1	9.685	177.539	7.298	0.054	1.202108	2.354672	0.029528	
220	1	6	1	0	4	181.782	41914.305	631.6	581.6	45.156	177.865	7.310	0.054	1.204127	2.350724	0.029499	
221	1	6	0	1	4	182.559	42078.289	94.4	107.9	15.152	178.626	7.339	0.054	1.208838	2.341563	0.029432	
222	1	2	2	5	8	183.797	42339.570	152.6	174.4	24.473	179.840	7.384	0.054	1.216344	2.327112	0.029328	
223	1	1	5	1	8	184.208	42426.242	21.7	24.9	3.679	180.243	7.400	0.054	1.218834	2.322358	0.029294	
224	1	5	1	3	8	185.149	42624.297	76.8	75.4	1.476	181.165	7.434	0.054	1.224524	2.311568	0.029218	
225	1	3	0	5	4	185.192	42633.355	169.7	167.0	2.867	181.207	7.436	0.054	1.224784	2.311077	0.029214	
226	1	6	0	0	2	185.545	42707.691	12.3	14.0	1.871	181.553	7.449	0.054	1.226919	2.307054	0.029186	
227	1	2	4	3	8	186.175	42840.277	1.7	3.0	2.088	182.171	7.472	0.054	1.230728	2.299914	0.029137	
228	1	0	5	1	4	187.031	43019.992	99.9	151.1	75.789	183.010	7.503	0.054	1.235891	2.290306	0.029071	
229	1	3	4	2	8	187.398	43097.094	31.0	46.8	23.466	183.370	7.517	0.054	1.238106	2.286209	0.029043	
230	1	5	2	2	8	188.894	43410.871	124.2	125.5	1.799	184.837	7.571	0.054	1.247120	2.269684	0.028933	
231	1	5	0	3	4	189.127	43459.504	82.6	83.0	1.051	185.065	7.580	0.054	1.248518	2.267144	0.028916	

232	1	4	1	4	8	189.213	43477.672	0.1	0.2	0.006	185.150	7.583	0.054	1.249040	2.266196	0.028910
233	1	2	3	4	8	192.254	44113.328	1099.5	1140.0	41.221	188.131	7.694	0.054	1.267301	2.233541	0.028699
234	1	1	2	5	8	192.611	44187.773	2.6	2.9	0.348	188.481	7.707	0.054	1.269440	2.229778	0.028676
235	1	4	0	4	4	193.462	44365.113	0.0	0.0	0.001	189.315	7.738	0.054	1.274534	2.220865	0.028620
236	1	1	4	3	8	195.349	44757.859	119.2	125.8	7.040	191.166	7.806	0.054	1.285817	2.201378	0.028501
237	1	4	3	2	8	195.532	44795.805	5.2	5.5	0.342	191.345	7.813	0.054	1.286907	2.199513	0.028490
238	1	2	1	5	8	196.263	44947.562	4.0	6.4	3.717	192.062	7.839	0.054	1.291267	2.192086	0.028445
239	1	3	4	1	8	197.623	45229.633	184.8	212.3	30.911	193.395	7.888	0.054	1.299370	2.178416	0.028364
240	1	3	2	4	8	198.422	45395.277	207.7	215.0	7.556	194.179	7.917	0.054	1.304129	2.170467	0.028318

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
241	1	5	2	1	8	199.377	45592.730	48.0	63.4	20.010	195.115	7.952	0.054	1.309802	2.161067	0.028264	
242	1	4	2	3	8	200.502	45825.285	0.1	0.1	0.013	196.219	7.992	0.054	1.316483	2.150100	0.028202	
243	1	3	3	3	8	200.933	45914.328	153.8	158.0	4.390	196.642	8.008	0.054	1.319041	2.145930	0.028179	
244	1	2	0	5	4	201.010	45930.180	176.6	180.4	4.008	196.717	8.011	0.054	1.319496	2.145190	0.028174	
245	1	1	3	4	8	202.395	46215.637	28.1	33.6	6.489	198.075	8.060	0.054	1.327697	2.131939	0.028101	
246	1	5	1	2	8	202.491	46235.539	93.0	112.9	23.691	198.170	8.064	0.054	1.328268	2.131022	0.028096	
247	1	2	4	2	8	203.832	46511.562	1.0	5.2	20.134	199.485	8.112	0.054	1.336198	2.118375	0.028027	
248	1	1	1	5	8	207.078	47177.605	0.6	0.6	0.083	202.669	8.228	0.054	1.355332	2.088469	0.027870	
249	1	4	3	1	8	207.213	47205.203	663.7	718.2	57.737	202.801	8.233	0.054	1.356125	2.087248	0.027864	
250	1	5	0	2	4	207.711	47307.121	61.2	71.0	11.058	203.289	8.251	0.054	1.359053	2.082751	0.027840	
251	1	0	1	5	4	211.095	47998.105	301.4	274.4	24.210	206.609	8.371	0.053	1.378904	2.052767	0.027690	
252	1	4	3	0	4	211.590	48099.055	14.1	13.9	0.308	207.095	8.389	0.053	1.381804	2.048459	0.027669	
253	1	1	0	5	4	212.665	48317.676	13.7	19.0	7.205	208.149	8.427	0.053	1.388085	2.039191	0.027625	
254	1	3	1	4	8	214.329	48655.727	151.5	163.9	13.240	209.781	8.486	0.053	1.397796	2.025023	0.027557	
255	1	5	1	1	8	215.529	48899.094	23.5	28.8	6.444	210.959	8.528	0.053	1.404788	2.014944	0.027510	
256	1	1	4	2	8	216.007	48995.898	135.9	161.0	29.114	211.428	8.545	0.053	1.407569	2.010963	0.027492	
257	1	4	1	3	8	216.948	49186.328	64.1	78.4	17.244	212.351	8.579	0.053	1.413040	2.003178	0.027456	
258	1	2	4	1	8	217.144	49225.965	62.1	78.2	19.922	212.543	8.585	0.053	1.414178	2.001565	0.027449	
259	1	2	2	4	8	218.203	49439.738	5.0	10.0	9.987	213.581	8.623	0.053	1.420320	1.992910	0.027410	
260	1	3	0	4	4	220.531	49909.266	58.6	72.7	17.098	215.866	8.705	0.053	1.433808	1.974161	0.027327	
261	1	0	4	2	4	220.569	49916.871	155.4	190.7	42.519	215.904	8.706	0.053	1.434027	1.973861	0.027326	
262	1	2	3	3	8	221.541	50112.402	11.5	15.6	5.352	216.857	8.740	0.053	1.439644	1.966159	0.027293	
263	1	5	0	1	4	221.838	50172.031	21.8	31.1	13.039	217.148	8.750	0.053	1.441357	1.963822	0.027282	
264	1	2	4	0	4	222.187	50242.133	0.1	0.2	0.079	217.491	8.763	0.053	1.443371	1.961082	0.027271	
265	1	4	2	2	8	223.004	50406.254	3.1	3.9	1.018	218.293	8.791	0.053	1.448086	1.954697	0.027244	
266	1	4	0	3	4	223.384	50482.434	20.4	23.0	2.906	218.665	8.805	0.053	1.450274	1.951747	0.027231	
267	1	3	3	2	8	223.595	50524.828	101.9	114.6	14.127	218.873	8.812	0.053	1.451492	1.950109	0.027224	
268	1	3	2	3	8	231.068	52016.078	129.6	159.2	35.730	226.206	9.072	0.053	1.494334	1.894202	0.027000	
269	1	1	4	1	8	231.996	52200.309	67.1	85.8	23.493	227.117	9.104	0.053	1.499626	1.887517	0.026974	
270	1	1	2	4	8	233.283	52455.422	79.5	114.7	49.602	228.380	9.149	0.053	1.506955	1.878337	0.026939	
271	1	1	3	3	8	237.361	53260.918	163.6	182.8	21.222	232.383	9.289	0.053	1.530096	1.849930	0.026835	
272	1	0	2	4	4	239.035	53590.289	28.5	34.0	6.508	234.026	9.347	0.053	1.539558	1.838560	0.026795	
273	1	2	1	4	8	239.798	53740.105	190.3	203.1	13.452	234.774	9.373	0.053	1.543862	1.833434	0.026777	
274	1	4	2	1	8	240.694	53915.980	8.1	9.3	1.360	235.654	9.403	0.053	1.548914	1.827453	0.026756	
275	1	3	3	1	8	241.434	54061.168	461.4	526.1	72.123	236.381	9.429	0.053	1.553085	1.822546	0.026739	
276	1	0	3	3	4	243.421	54450.074	755.1	854.7	110.277	238.332	9.497	0.053	1.564258	1.809528	0.026695	
277	1	0	4	0	2	244.274	54616.613	592.9	696.9	119.610	239.169	9.526	0.053	1.569042	1.804010	0.026677	
278	1	4	1	2	8	246.179	54988.098	4.5	9.0	8.668	241.039	9.590	0.052	1.579715	1.791823	0.026637	
279	1	4	2	0	4	247.573	55259.520	107.0	139.1	40.972	242.408	9.638	0.052	1.587512	1.783022	0.026608	
280	1	2	0	4	4	248.522	55443.730	0.4	1.3	3.432	243.339	9.670	0.052	1.592804	1.777098	0.026589	
281	1	2	3	2	8	252.899	56291.312	19.9	42.2	46.323	247.637	9.818	0.052	1.617154	1.750340	0.026506	
282	1	4	0	2	4	255.628	56817.324	1443.7	1436.5	8.049	250.317	9.909	0.052	1.632265	1.734136	0.026458	
283	1	3	1	3	8	257.085	57097.461	199.1	264.3	84.505	251.748	9.958	0.052	1.640313	1.725627	0.026433	
284	1	1	1	4	8	260.125	57680.059	3.9	18.2	65.920	254.733	10.060	0.052	1.657050	1.708198	0.026383	
285	1	2	2	3	8	263.773	58376.168	626.3	661.4	36.474	258.316	10.181	0.052	1.677048	1.687828	0.026326	
286	1	3	2	2	8	267.220	59031.023	148.9	171.1	25.057	261.702	10.296	0.052	1.695861	1.669104	0.026276	
287	1	3	0	3	4	267.866	59153.484	42.0	53.5	14.343	262.337	10.317	0.052	1.699379	1.665649	0.026267	
288	1	4	1	1	8	270.435	59639.254	7.6	20.0	31.902	264.861	10.402	0.052	1.713334	1.652082	0.026232	
289	1	1	0	4	4	271.298	59802.043	5.9	17.5	34.237	265.708	10.430	0.052	1.718011	1.647585	0.026221	
290	1	1	3	2	8	276.981	60869.652	519.9	640.6	145.358	271.291	10.616	0.052	1.748682	1.618688	0.026149	
291	1	2	3	1	8	279.351	61312.500	4.6	6.2	2.134	273.620	10.693	0.052	1.761404	1.606996	0.026122	
292	1	4	1	0	4	280.212	61473.137	1.4	1.4	0.014	274.466	10.721	0.052	1.766019	1.602797	0.026112	
293	1	0	0	4	2	280.358	61500.297	623.4	612.7	10.888	274.609	10.726	0.052	1.766799	1.602089	0.026110	
294	1	4	0	1	4	283.011	61993.980	14.9	26.5	20.369	277.216	10.812	0.051	1.780982	1.589331	0.026081	
295	1	2	3	0	4	290.132	63310.406	283.0	354.6	87.673	284.214	11.042	0.051	1.818800	1.556284	0.026008	
296	1	1	2	3	8	291.332	63531.070	345.2	381.9	39.777	285.393	11.080	0.051	1.825140	1.550878	0.025997	
297	1	4	0	0	2	294.224	64061.543	526.8	553.3	27.406	288.235	11.173	0.051	1.840379	1.538036	0.025970	
298	1	3	2	1	8	298.830	64902.410	708.0	836.5	148.275	292.763	11.320	0.051	1.864536	1.518109	0.025930	
299	1	2	1	3	8	304.074	65853.680	3.5	27.5	184.997	297.918	11.486	0.051	1.891864	1.496180	0.025887	
300	1	3	1	2	8	309.315	66798.133	191.8	261.4	92.597	303.071	11.650	0.051	1.918997	1.475026	0.025848	

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
301	1	1	3	1	8	312.508	67370.391	203.6	299.9	138.387	306.210	11.750	0.051	1.935437	1.462496	0.025825	
302	1	2	2	2	8	320.944	68871.492	0.0	0.0	0.019	314.506	12.012	0.050	1.978561	1.430620	0.025771	
303	1	2	0	3	4	322.045	69066.203	828.6	898.9	74.561	315.588	12.046	0.050	1.984154	1.426587	0.025764	
304	1	0	3	1	4	326.360	69826.930	1155.7	1518.5	465.066	319.833	12.178	0.050	2.006009	1.411045	0.025739	
305	1	3	0	2	4	328.246	70158.086	57.1	128.7	157.732	321.688	12.236	0.050	2.015522	1.404385	0.025728	
306	1	1	1	3	8	347.769	73541.094	952.9	1081.5	142.370	340.894	12.826	0.050	2.112710	1.339781	0.025634	
307	1	3	1	1	8	360.429	75692.000	1942.7	2207.8	293.675	353.353	13.201	0.049	2.174502	1.301709	0.025584	
308	1	0	1	3	4	366.852	76770.648	11.4	22.7	22.156	359.674	13.390	0.049	2.205490	1.283419	0.025562	

309	1	1	2	2	8	373.135	77817.828	988.6	1097.6	117.925	365.859	13.572	0.049	2.235574	1.266149	0.025542
310	1	1	0	3	4	374.830	78099.016	747.9	830.0	88.767	367.528	13.621	0.049	2.243652	1.261590	0.025536
311	1	2	2	1	8	378.765	78749.602	3650.4	4222.6	644.607	371.403	13.735	0.049	2.262342	1.251167	0.025525
312	1	3	0	1	4	390.611	80689.828	960.3	1158.3	232.523	383.067	14.073	0.049	2.318082	1.221083	0.025493
313	1	0	2	2	4	396.689	81675.109	4005.9	4465.8	499.008	389.053	14.245	0.048	2.346387	1.206352	0.025478
314	1	2	1	2	8	399.998	82208.453	5158.2	5631.5	502.714	392.312	14.338	0.048	2.361709	1.198526	0.025470
315	1	2	2	0	4	405.706	83123.805	10.7	56.5	234.117	397.934	14.498	0.048	2.388005	1.185328	0.025457
316	1	2	0	2	4	441.495	88730.227	39.8	92.9	120.433	433.198	15.475	0.047	2.549068	1.110433	0.025393
317	1	1	2	1	8	469.884	93023.125	736.3	940.4	252.998	461.186	16.224	0.047	2.672396	1.059188	0.025356
318	1	1	1	2	8	510.032	98879.477	2411.7	2673.8	281.850	500.786	17.246	0.046	2.840639	0.996455	0.025317
319	1	2	1	1	8	523.651	100812.508	11.4	121.4	1132.962	514.224	17.583	0.045	2.896172	0.977348	0.025307
320	1	0	2	0	2	585.155	109233.227	2920.3	3918.5	1295.927	574.940	19.051	0.044	3.138085	0.902005	0.025272
321	1	2	1	0	4	594.863	110519.039	2741.2	3220.5	544.633	584.527	19.276	0.044	3.175024	0.891511	0.025267
322	1	1	0	2	4	597.661	110887.461	1171.8	1385.6	244.508	587.290	19.340	0.044	3.185608	0.888549	0.025266
323	1	2	0	1	4	618.741	113634.648	2868.3	3271.4	444.402	608.113	19.819	0.043	3.264530	0.867068	0.025258
324	1	0	0	2	2	693.578	123000.594	287.5	568.9	537.394	682.073	21.452	0.042	3.533598	0.801044	0.025236
325	1	2	0	0	2	736.486	128123.086	15.7	257.0	3818.320	724.502	22.346	0.041	3.680758	0.769018	0.025227

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 BRAGG R-Factors and weight fractions for Pattern #  2
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=> Phase:  1     VOSO4 Nuclear
=> Bragg R-factor:   14.0       Vol:  326.520( 0.000)  Fract(%):  100.00( 0.00)
=> Rf-factor=  8.28             ATZ:         651.994   Brindley:  1.0000
```

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-------------------------------------------------------------------------------------------------------------
Pattern#  3 Phase No:   1 Phase name: VOSO4 Nuclear
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No.	Code	H	K	L	Mult	Hw	ETA/M	2theta/TOF	Icalc	Iobs	Sigma	StrFactor^2	d-hkl	CORR
1	1	1	0	1	4	0.134834	0.000000	17.419	613.5	762.4	185.293	1708.4188	5.098137	1.000000
2	1	0	1	1	4	0.130248	0.000000	18.937	439.0	862.0	830.413	1450.8103	4.692774	1.000000
3	1	1	1	1	8	0.119794	0.000000	22.500	408.9	485.6	91.510	965.0206	3.957122	1.000000
4	1	2	0	0	2	0.114953	0.000000	24.214	107.4	355.8	822.104	1181.8676	3.680758	1.000000
5	1	0	0	2	2	0.112129	0.000000	25.238	689.5	706.1	18.770	8270.8066	3.533598	1.000000
6	1	2	0	1	4	0.106483	0.000000	27.357	2320.4	2159.3	150.090	16491.5312	3.264530	1.000000
7	1	1	0	2	4	0.104704	0.000000	28.049	475.4	359.0	87.905	3561.0671	3.185608	1.000000
8	1	2	1	0	4	0.104462	0.000000	28.144	8.0	4.2	2.004	60.3759	3.175024	1.000000
9	1	0	2	0	2	0.103606	0.000000	28.482	1746.5	1696.9	48.595	27025.6875	3.138085	1.000000
10	1	2	1	1	8	0.097721	0.000000	30.919	277.6	248.2	26.796	1279.0918	2.896172	1.000000
11	1	1	1	2	8	0.096308	0.000000	31.539	449.7	468.6	20.447	2161.4563	2.840639	1.000000
12	1	1	2	1	8	0.091939	0.000000	33.581	243.0	444.8	369.195	1336.5267	2.672396	1.000000
13	1	2	0	2	4	0.088724	0.000000	35.258	59.3	207.3	517.171	725.0848	2.549068	1.000000
14	1	2	2	0	4	0.084719	0.000000	37.722	89.9	295.8	677.329	1272.9370	2.388005	1.000000
15	1	2	1	2	8	0.084111	0.000000	38.158	17.8	64.7	170.884	128.9409	2.361709	1.000000
16	1	0	2	2	4	0.083765	0.000000	38.417	5.7	41.5	262.317	83.3219	2.346387	1.000000
17	1	3	0	1	4	0.083145	0.000000	38.905	5.6	11.3	12.010	85.1833	2.318082	1.000000
18	1	2	2	1	8	0.082012	0.000000	39.904	189.1	317.5	215.563	1514.4487	2.262342	1.000000
19	1	1	0	3	4	0.081663	0.000000	40.251	1.2	2.7	3.042	20.2191	2.243652	1.000000
20	1	1	2	2	8	0.081517	0.000000	40.402	379.0	507.6	172.318	3118.6741	2.235574	1.000000
21	1	0	1	3	4	0.081007	0.000000	40.978	488.4	622.2	170.525	8292.5078	2.205490	1.000000
22	1	3	1	1	8	0.080539	0.000000	41.589	38.9	68.0	50.850	341.4664	2.174503	1.000000
23	1	1	1	3	8	0.079817	0.000000	42.864	48.0	84.8	65.092	450.3593	2.112710	1.000000
24	1	3	0	2	4	0.079420	0.000000	45.042	47.3	99.2	108.947	990.3688	2.015522	1.000000
25	1	0	3	1	4	0.079442	0.000000	45.267	315.6	512.6	320.064	6679.8301	2.006009	1.000000
26	1	2	0	3	4	0.079539	0.000000	45.794	209.9	198.7	10.928	4561.2671	1.984154	1.000000
27	1	2	2	2	8	0.079575	0.000000	45.931	78.5	65.9	10.903	858.7982	1.978561	1.000000
28	1	1	3	1	8	0.080018	0.000000	47.015	49.6	42.1	7.215	571.0631	1.935437	1.000000
29	1	3	1	2	8	0.080270	0.000000	47.442	52.6	43.7	7.954	618.1785	1.918997	1.000000
30	1	2	1	3	8	0.080796	0.000000	48.165	58.5	59.3	3.774	710.7715	1.891864	1.000000
31	1	3	2	1	8	0.081475	0.000000	48.917	1.7	13.2	91.966	20.7892	1.864536	1.000000
32	1	4	0	0	2	0.082211	0.000000	49.602	222.2	288.1	85.387	11542.8174	1.840379	1.000000
33	1	1	2	3	8	0.082746	0.000000	50.045	2.2	5.0	6.124	29.5690	1.825140	1.000000
34	1	2	3	0	4	0.082985	0.000000	50.231	78.2	216.8	384.115	2088.1670	1.818800	1.000000
35	1	4	0	1	4	0.084626	0.000000	51.375	70.8	71.7	3.429	1989.1326	1.780982	1.000000
36	1	0	0	4	2	0.085342	0.000000	51.818	98.6	119.5	25.263	5649.1660	1.766799	1.000000
37	1	4	1	0	4	0.085383	0.000000	51.842	76.8	88.0	12.903	2201.8342	1.766019	1.000000
38	1	2	3	1	8	0.085629	0.000000	51.988	44.7	68.4	36.413	644.2196	1.761404	1.000000
39	1	1	3	2	8	0.086341	0.000000	52.395	101.3	118.8	20.781	1486.7444	1.748681	1.000000
40	1	1	0	4	4	0.088261	0.000000	53.404	12.3	35.9	68.676	378.0764	1.718011	1.000000
41	1	4	1	1	8	0.088580	0.000000	53.561	5.8	2.9	2.103	89.4394	1.713334	1.000000
42	1	3	0	3	4	0.089577	0.000000	54.037	46.1	71.0	38.347	1450.5143	1.699379	1.000000
43	1	3	2	2	8	0.089838	0.000000	54.158	70.3	65.4	5.136	1110.2814	1.695861	1.000000
44	1	2	2	3	8	0.091311	0.000000	54.816	2.6	3.0	2.593	41.4319	1.677048	1.000000
45	1	1	1	4	8	0.093018	0.000000	55.534	2.7	27.0	243.627	44.8639	1.657050	1.000000
46	1	3	1	3	8	0.094564	0.000000	56.151	47.6	87.9	74.617	814.6120	1.640313	1.000000
47	1	4	0	2	4	0.095347	0.000000	56.452	225.7	260.0	39.530	7823.8931	1.632265	1.000000
48	1	2	3	2	8	0.096887	0.000000	57.028	163.5	326.7	325.912	2897.8904	1.617154	1.000000
49	1	2	0	4	4	0.099574	0.000000	57.982	15.2	47.9	102.869	559.6502	1.592804	1.000000
50	1	4	2	0	4	0.100192	0.000000	58.194	53.7	55.9	2.950	1989.9320	1.587512	1.000000
51	1	4	1	2	8	0.101127	0.000000	58.509	121.8	250.5	264.644	2284.0901	1.579715	1.000000

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    52   1      0   4   0     2  0.102451  0.000000      58.946      246.7      205.7     34.236      18806.0879  1.569043      1.000000
    53   1      0   3   3     4  0.103062  0.000000      59.144      351.2      546.7    304.279      13488.0898  1.564258      1.000000
    54   1      3   3   1     8  0.104532  0.000000      59.612        5.2        7.2      2.794        101.7405  1.553085      1.000000
    55   1      4   2   1     8  0.105097  0.000000      59.789      121.5      130.1      9.279       2397.0217  1.548915      1.000000
    56   1      2   1   4     8  0.105792  0.000000      60.005      384.5      612.3    341.873       8080.6782  1.543862      1.000000

    ------------------------------------------------------
    BRAGG R-Factors and weight fractions for Pattern #  3
    ------------------------------------------------------

=> Phase:  1     VOSO4 Nuclear
=> Bragg R-factor:   25.4       Vol:  326.520( 0.000)  Fract(%):  100.00( 0.00)
=> Rf-factor=  17.7             ATZ:         651.994   Brindley:  1.0000

    ---------------------------------------------------------------------
     SYMBOLIC NAMES AND FINAL VALUES AND SIGMA OF REFINED PARAMETERS:
    ---------------------------------------------------------------------

     ->  Parameter number    1 :      Cell_A_ph1_pat1     7.3539782    ( +/-    0.39001860E-01 )
     ->  Parameter number    2 :             X_V1_ph1    0.16364004    ( +/-    0.12658078E-02 )
     ->  Parameter number    3 :           Zero_pat1    -1.9953272    ( +/-     2.1815798     )
     ->  Parameter number    4 :             Z_V1_ph1    0.23747978    ( +/-    0.14008972E-02 )
     ->  Parameter number    5 :             X_S1_ph1    0.87405801    ( +/-    0.12579196E-02 )
     ->  Parameter number    6 :           Dtt1_pat1     48329.039    ( +/-     256.27936     )
     ->  Parameter number    7 :             Z_S1_ph1    0.87407881    ( +/-    0.92349324E-03 )
     ->  Parameter number    8 :             X_O1_ph1    0.71441048    ( +/-    0.52903622E-03 )
     ->  Parameter number    9 :           Dtt2_pat1    -3.2745945    ( +/-     1.0731602     )
     ->  Parameter number   10 :             Z_O1_ph1    0.98820972    ( +/-    0.69793494E-03 )
     ->  Parameter number   11 :             X_O2_ph1    0.44627253E-01( +/-    0.54321694E-03 )
     ->  Parameter number   12 :           Zero_pat2    -5.3567719    ( +/-     8.9365711     )
     ->  Parameter number   13 :             Z_O2_ph1    0.97938156    ( +/-    0.67112118E-03 )
     ->  Parameter number   14 :             X_O3_ph1    0.37422553    ( +/-    0.78570709E-03 )
     ->  Parameter number   15 :           Dtt1_pat2     34808.738    ( +/-     10.998049     )
     ->  Parameter number   16 :             Z_O3_ph1    0.16945940    ( +/-    0.48556097E-03 )
     ->  Parameter number   17 :             X_O4_ph1    0.11908086    ( +/-    0.86413400E-03 )
     ->  Parameter number   18 :             Y_O4_ph1    0.56241012    ( +/-    0.36183369E-03 )
     ->  Parameter number   19 :             Z_O4_ph1    0.25823894    ( +/-    0.39830123E-03 )
     ->  Parameter number   20 :           Dtt2_pat2    -3.1474333    ( +/-     3.0181901     )
     ->  Parameter number   21 :       Scale_ph1_pat1     1.1250159    ( +/-    0.80381203E-02 )
     ->  Parameter number   22 :      Cell_B_ph1_pat1     6.2706499    ( +/-    0.33256516E-01 )
     ->  Parameter number   23 :      Cell_C_ph1_pat1     7.0604458    ( +/-    0.37445270E-01 )

---------------------------------------------------------------------
=> Number of bytes for floating point variables: 4
=> Dimensions of dynamic allocated arrays in this run of FullProf:
---------------------------------------------------------------------

=> Total approximate array memory (dynamic + static): 121369011 bytes

   MaxPOINT=    70000 Max.num. of points(+int. Inten.)/diffraction pattern
   MaxREFLT=    20000 Max.num. of reflections/diffraction pattern
   MaxPARAM=      500 Max.num. of refinable parameters
   MaxOVERL=     2024 Max.num. of overlapping reflections

-----------------------------------------------------------
=> Number of bytes for floating point arrays: 4
=> Dimensions of fixed arrays in this release of FullProf:
-----------------------------------------------------------

   NPATT   =       80 Max.num. of powder diffraction patterns
   NATS    =      830 Max.num. of atoms (all kind) in asymmetric unit
   MPAR    =     1800 Max.num. of non atomic parameters/phase
   IEXCL   =       30 Max.num. of excluded regions
   IBACP   =      277 Max.num. of background points for interpolation
   NPHT    =       16 Max.num. of phases
   NMAGM   =        8 Max.num. of rotation-matrices sets for magnetic structure
   NBASIS  =       12 Max.num. of basis functions associated to a single atom
   NIREPS  =        9 Max.num. of irreducible representations to be combined
   N_EQ    =      384 Max.num. of user-supplied symmetry operators/propagation vectors
   NGL     =      300 Max.num. of global parameters/diffraction pattern
   N_LINC  =       30 Max.num. of global linear restraints
   NAT_P   =       64 Max.num. of atomic parameters per atom
   NCONST  =      500 Max.num. of slack constraints per phase
   N_SPE   =       30 Max.num. of different chemical species
   N_FORM  =       60 Max.num. of scattering factor values in a table
   NPR     =      150 Max.num. of points defining a numerical profile
   INPR    =       25 Max.num. of different numerical peak shapes
   NPRC    =      150 Max.num. of terms in the table for correcting intensities
   NSOL    =       10 Max.num. of solutions to be stored in Montecarlo searchs


              CPU Time:    25.656 seconds
                            0.428 minutes
```

```
=> Run finished at:     Date: 10/06/2021  Time: 17:15:45.419
```

pcrfile.pdf

end of pcrfile.pdf

Appendix:B Pcr-out-file

appendix B

Pcrout

```
       ***********************************************************
       ** PROGRAM FullProf.2k (Version 6.00 - Mar2017-ILL JRC) **
       ***********************************************************
                     M U L T I -- P A T T E R N
           Rietveld, Profile Matching & Integrated Intensity
                Refinement of X-ray and/or Neutron Data


   Date: 10/06/2021  Time: 17:15:19.747

=> PCR file code: VOSO4_test-working_beforerefinement (1) (1)
=> DAT file code: hrp77265_abscor_b1_T -> Relative contribution: 0.3333
=> DAT file code: hrp77265_abscor_b2_T -> Relative contribution: 0.3333
=> DAT file code: PK752.dat            -> Relative contribution: 0.3333

==> CONDITIONS OF THIS RUN FOR PATTERN No.:  1

=> Global Refinement of neutron powder data
=> Neutron Time-Of-Flight data
=> Abcisa variable is T.O.F. in microsecs
=> Title:Multi-pattern b-VOSO4 hrpd

=> Number of phases:    1
=> Number of excluded regions:    2
=> Number of scattering factors supplied:    0
=> Maximum Likelihood weighting scheme ( w=1/(calculated variance) )
=> Asymmetry correction as in J.Appl.Cryst. 26,128(1993)
=> Background linearly interpolated between the   60 points given
=> The    9th default profile function was selected
=> T.O.F Profile Function #1
   Decay double Exponential convoluted with pseudo-Voigt:
   Omega(DT) = (1-eta)N {Exp(u).Erfc(y)+ Exp(v).Erfc(z)} +
               2N eta/pi{-Im[Exp(p)E1(p)]-Im[Exp(q)E1(q)]}

==> CONDITIONS OF THIS RUN FOR PATTERN No.:  2

=> Global Refinement of neutron powder data
=> Neutron Time-Of-Flight data
=> Abcisa variable is T.O.F. in microsecs
=> Title:Multi-pattern b-VOSO4 hrpd

=> Number of phases:    1
=> Number of excluded regions:    2
=> Number of scattering factors supplied:    0
=> Maximum Likelihood weighting scheme ( w=1/(calculated variance) )
=> Asymmetry correction as in J.Appl.Cryst. 26,128(1993)
=> Background linearly interpolated between the   20 points given
=> The    9th default profile function was selected
=> T.O.F Profile Function #1
   Decay double Exponential convoluted with pseudo-Voigt:
   Omega(DT) = (1-eta)N {Exp(u).Erfc(y)+ Exp(v).Erfc(z)} +
               2N eta/pi{-Im[Exp(p)E1(p)]-Im[Exp(q)E1(q)]}

==> CONDITIONS OF THIS RUN FOR PATTERN No.:  3

=> Global Refinement of X-ray powder diffraction data
=> Global Refinement of X-ray powder diffraction data
   Bragg-Brentano(X-rays) or Debye-Scherrer geometry(Neutrons)
=> Title:Multi-pattern b-VOSO4 hrpd
```

```
=> Number of phases:    1
=> Number of excluded regions:    2
=> Number of scattering factors supplied:    0
=> Conventional weights: w=1.0/Variance(yobs)
=> Asymmetry correction as in J.Appl.Cryst. 26,128(1993)
=> Background linearly interpolated between the   76 points given
=> The    7th default profile function was selected
=> T-C-H Pseudo-Voigt function
   This function is convoluted with asymmetry due to axial
   divergence as formulated by:
   van Laar and Yelon, J. Appl. Cryst. 17, 47(1984).
   and using the method of:
   Finger, Cox and Jephcoat, J. Appl. Cryst. 27, 892 (1994).
   Fortran 90 module adapted from function PROFVAL (in F77) :
   L.W. Finger, J. Appl. Cryst. 31, 111 (1998).


==> INPUT/OUTPUT OPTIONS:

=> Generate bacground file *.bac
=> Generate file *.PRF for plot
=> Output Integrated Intensities
=> Generate bacground file *.bac
=> Generate file *.PRF for plot
=> Output Integrated Intensities
=> Generate file *.PRF for plot
=> Output Integrated Intensities
=> Generate new input file *.PCR

=> X-Y type of data: 2theta/TOF/E(Kev) Intens sigma for pattern:  1
=> Plot pattern at each cycle
=> Absorption correction type: 2
=> Base of peaks: 2.0*HW*    6.00

=> X-Y type of data: 2theta/TOF/E(Kev) Intens sigma for pattern:  2
=> Plot pattern at each cycle
=> Absorption correction type: 2
=> Base of peaks: 2.0*HW*    2.00

=> X-Y type of data: 2theta/TOF/E(Kev) Intens sigma for pattern:  3
=> Wavelengths:  1.54397 0.00000
=> Alpha2/Alpha1 ratio:   0.0000
=> Cos(Monochromator angle)=   0.9100
=> Asymmetry correction for angles lower than    0.000 degrees
=> Absorption correction (AC), muR-eff =   0.0000  0.0000
=> Base of peaks: 2.0*HW*    8.00

=> Number of cycles:   40
=> Relaxation factors ==>    for coordinates:  0.20
=> for anisotropic temperature factors:  0.20
=> for halfwidth/strain/size parameters:  0.20
=> for lattice constants and propagation vectors:  0.20
=> EPS-value for convergence:    0.1
=> Background ==>
   Position   Intensity
   31417.23        1.56        0.00
   33050.90        1.51        0.00
   35443.45        1.64        0.00
   35710.23        1.62        0.00
   37522.09        1.77        0.00
   39461.37        1.77        0.00
   39782.26        1.80        0.00
   41563.17        1.82        0.00
   42905.91        1.91        0.00
   44212.39        1.91        0.00
   46553.28        2.05        0.00
   47398.70        2.00        0.00
   48506.18        2.04        0.00
   49938.23        2.08        0.00
   52079.98        2.12        0.00
   52393.35        2.12        0.00
   55532.64        2.21        0.00
   57896.95        2.31        0.00
   58630.96        2.33        0.00
   60597.76        2.35        0.00

   60725.13        2.36        0.00
   62442.95        2.38        0.00
   64673.28        2.42        0.00
   66184.39        2.42        0.00
   66363.30        2.46        0.00
   70276.38        2.56        0.00
   70784.12        2.50        0.00
```

```
   71918.41        2.60        0.00
   73620.88        2.60        0.00
   77101.43        2.69        0.00
   77495.59        2.71        0.00
   80215.43        2.74        0.00
   80311.73        2.71        0.00
   83430.16        2.83        0.00
   85841.77        2.89        0.00
   86384.20        2.85        0.00
   87479.36        2.95        0.00
   89121.45        3.01        0.00
   91258.53        3.04        0.00
   91807.65        3.05        0.00

   94830.47        3.06        0.00
   96148.00        3.17        0.00
   97806.02        3.28        0.00
  100241.52        3.23        0.00
  101725.73        3.37        0.00
  104040.15        3.30        0.00
  104352.69        3.26        0.00
  107369.06        3.33        0.00
  108828.16        3.51        0.00
  110937.52        3.42        0.00
  111170.70        3.42        0.00
  112816.73        3.53        0.00
  115037.91        3.40        0.00
  116008.16        3.37        0.00
  117373.22        3.37        0.00
  119254.08        3.34        0.00
  120259.88        3.37        0.00
  121930.72        3.24        0.00
  123254.51        3.21        0.00
  124704.84        3.28        0.00


=> Excluded regions for Pattern#  1
   From     to
   100.0000  31360.0000
115000.0000 300000.0000

=> Background ==>
   Position   Intensity
   29924.81        1.10        0.00
   32293.23        1.20        0.00
   39060.15        1.41        0.00
   46729.32        1.50        0.00
   56090.23        1.61        0.00
   63195.49        1.71        0.00
   72443.61        1.80        0.00
   79436.09        1.89        0.00
   83834.59        1.90        0.00
   87105.26        1.90        0.00
   91954.89        2.00        0.00
   95225.57        2.00        0.00
  100187.98        2.00        0.00
  105263.16        2.10        0.00
  112030.08        2.10        0.00
  116541.36        2.10        0.00
  120601.51        2.09        0.00
  127142.86        2.00        0.00
  133909.78        1.90        0.00
  135150.38        1.90        0.00


=> Excluded regions for Pattern#  2
   From     to
   100.0000  29000.0000
135000.0000 300000.0000

=> Background ==>
   Position   Intensity
      13.66    12101.32        0.00
      14.24    12213.08        0.00
      14.82    12101.32        0.00
      15.31    12078.97        0.00
      15.98    12324.83        0.00
      16.70    12324.83        0.00
      17.54    11944.87        0.00
      18.17    11654.31        0.00
      19.06    11028.50        0.00
```

```
     19.51    10782.64        0.00
     20.13    10670.89        0.00
     20.62    10916.75        0.00
     21.70    11028.50        0.00
     22.05    10872.04        0.00
     22.72    10804.99        0.00
     23.39    10804.99        0.00
     23.88    10492.08        0.00
     24.06    10156.83        0.00
     24.38     9754.52        0.00
     24.60     9285.16        0.00

     24.73     9151.05        0.00
     25.13     8435.84        0.00
     25.54     8055.88        0.00
     25.76     7698.27        0.00
     25.98     7385.36        0.00
     26.07     7072.45        0.00
     26.34     6692.49        0.00
     26.61     6468.99        0.00
     26.74     6089.03        0.00
     27.59     5843.17        0.00
     28.08     5910.23        0.00
     28.62     5284.41        0.00
     29.15     4993.85        0.00
     29.78     4882.10        0.00
     30.40     4815.05        0.00
     31.07     4680.95        0.00
     31.79     4591.54        0.00
     32.37     4412.74        0.00
     33.08     4435.09        0.00
     33.79     4211.58        0.00

     34.33     4211.58        0.00
     35.09     4211.58        0.00
     35.98     4122.18        0.00
     36.43     4278.64        0.00
     36.70     4569.19        0.00
     37.01     4815.05        0.00
     38.04     4904.45        0.00
     38.21     4658.60        0.00
     38.39     4435.09        0.00
     39.02     4390.39        0.00
     40.00     4300.99        0.00
     40.49     4368.04        0.00
     41.16     4233.94        0.00
     42.01     4166.88        0.00
     43.08     4166.88        0.00
     43.75     4055.13        0.00
     44.38     3853.98        0.00
     45.36     3563.42        0.00
     46.12     3496.37        0.00
     46.74     3451.67        0.00

     47.59     3272.86        0.00
     48.35     3272.86        0.00
     49.02     3138.76        0.00
     49.82     3138.76        0.00
     50.58     3004.66        0.00
     51.03     3049.36        0.00
     52.14     2892.90        0.00
     52.86     2870.55        0.00
     53.57     2803.50        0.00
     54.38     2781.15        0.00
     54.96     2758.80        0.00
     55.58     2647.05        0.00
     56.52     2736.45        0.00
     57.37     2669.40        0.00
     58.44     2624.70        0.00
     59.20     2647.05        0.00


=> Excluded regions for Pattern#  3
   From     to
     0.0000     13.6500
    60.0000    120.0000

=> Number of Least-Squares parameters varied:    23

=>--------------------------->
=>------->  PATTERN number:  1
=>--------------------------->
```

```
=> Global parameters and codes ==>
=> Zero-point:    -1.9860   31.0000
=> D-spacing to T.O.F. coefficient dtt1 and code:  48329.055    61.000
=> D-spacing to T.O.F. coefficient dtt2 and code:     -3.264    91.000
=> T.O.F. 2theta average detector angle      :    168.330

=> Reading Intensity data  =>>

-> No recognizable heading in input data file X,Y,sigma
   First 6 lines are considered as COMMENTS (except for TSAMP keyword)
-> COMMENT:     31370.14550        1.78958093        0.07817861
-> COMMENT:     31379.55654        1.70332124        0.07721400
-> COMMENT:     31388.97041        1.52623027        0.07186282
-> COMMENT:     31398.38710        1.66464591        0.07488378
-> COMMENT:     31407.80662        1.64923724        0.07479645
-> COMMENT:     31417.22896        1.51009650        0.07020225
==> T.O.F. range, and number of points:
   TOFmin:   31426.654297  TOFmax:  125005.390625
   No. of points:   4604

=>--------------------------->
=>------->  PATTERN number:  2
=>--------------------------->
=> Global parameters and codes ==>
=> Zero-point:    -5.4160  121.0000
=> D-spacing to T.O.F. coefficient dtt1 and code:  34808.883   151.000
=> D-spacing to T.O.F. coefficient dtt2 and code:     -3.173   201.000
=> T.O.F. 2theta average detector angle      :     89.580

=> Reading Intensity data  =>>

-> No recognizable heading in input data file X,Y,sigma
   First 6 lines are considered as COMMENTS (except for TSAMP keyword)
-> COMMENT:     29421.77496        1.50198738        0.09937595
-> COMMENT:     29442.37020        1.61397357        0.09610834
-> COMMENT:     29462.97986        1.40734600        0.08841921
-> COMMENT:     29483.60395        1.48815299        0.09451091
-> COMMENT:     29504.24247        1.35736807        0.08246329
-> COMMENT:     29524.89544        1.44424067        0.08349656
==> T.O.F. range, and number of points:
   TOFmin:   29545.562500  TOFmax:  135554.000000
   No. of points:   2178

=>--------------------------->
=>------->  PATTERN number:  3
=>--------------------------->
=> Global parameters and codes ==>
=> Zero-point:    -0.1171    0.0000
=> Displacement peak-shift parameter and code:     0.00    0.00
=> Transparency peak-shift parameter and code:     0.00    0.00

=> Reading Intensity data  =>>

-> No recognizable heading in input data file X,Y,sigma
   First 6 lines are considered as COMMENTS (except for TSAMP keyword)
-> COMMENT: 4.000 1790
-> COMMENT: 4.005 1766
-> COMMENT: 4.010 1802
-> COMMENT: 4.015 1842
-> COMMENT: 4.020 1853
-> COMMENT: 4.025 1878
==> Angular range, step and number of points:
    2Thmin:       4.030000  2Thmax:     100.000000  Step:       0.005000  No. of points:  19195
------------------------------------------------------------------------------
=> Phase  No. 1
     VOSO4 Nuclear
------------------------------------------------------------------------------
=>-------> Pattern#  1
=> Crystal Structure Refinement
=> Preferred orientation vector:   1.0000  0.0000  0.0000
=>-------> Pattern#  2
=> Crystal Structure Refinement
=> Preferred orientation vector:   1.0000  0.0000  0.0000
=>-------> Pattern#  3
=> Crystal Structure Refinement
=> The    2th profile function was selected for phase no.  1
=> Preferred orientation vector:   0.0000  0.0000  1.0000

=>-------> Data for PHASE: 1
=> Number of atoms:    6
=> Number of distance  constraints:    0
=> Number of angle     constraints:    0
```

```
=> Symmetry information on space group: P n m a
-> The multiplicity of the general position is:   8
-> The space group is Centric (-1 at origin)
-> Lattice type  P: { 000 }
-> Reduced set of symmetry operators:

 No.  IT   Symmetry symbol    Rotation part     Associated Translation
  1: ( 1)   1            -->     ( x, y, z) + {  0.0000  0.0000  0.0000}
  2: ( 4)   2 ( x, 0, 0) -->     ( x,-y,-z) + {  0.5000  0.5000  0.5000}
  3: ( 3)   2 ( 0, y, 0) -->     (-x, y,-z) + {  0.0000  0.5000  0.0000}
  4: ( 2)   2 ( 0, 0, z) -->     (-x,-y, z) + {  0.5000  0.0000  0.5000}


       Information on Space Group:
       ---------------------------

=>   Number of Space group:  62
=>  Hermann-Mauguin Symbol: P n m a
=>             Hall Symbol: -P 2ac 2n
=>            Setting Type: IT (Generated from Hermann-Mauguin symbol)
=>          Crystal System: Orthorhombic
=>              Laue Class: mmm
=>             Point Group: mmm
=>         Bravais Lattice: P
=>          Lattice Symbol: oP
=>  Reduced Number of S.O.:   4
=>    General multiplicity:   8
=>          Centrosymmetry: Centric (-1 at origin)
=>  Generators (exc. -1&L):   2
=>         Asymmetric unit:  0.000 <= x <=  0.500
                             0.000 <= y <=  0.250
                             0.000 <= z <=  1.000

=> List of S.O. without inversion and lattice centring translations
=> SYMM(  1): x,y,z                              => SYMM(  2): x+1/2,-y+1/2,-z+1/2
=> SYMM(  3): -x,y+1/2,-z                        => SYMM(  4): -x+1/2,-y,z+1/2


=> Initial parameters ==>
Atom    Ntyp                 X         Y         Z         B         occ.         in  fin  Spc  Mult
                           B11       B22       B33       B12       B13       B23
V1     V                 0.16364   0.25000   0.23748   0.05000   0.50000           0    0    0    4
                Codes:   21.00000   0.00000  41.00000   0.00000   0.00000
S1     S                 0.87406   0.25000   0.87408   0.05000   0.50000           0    0    0    4
                Codes:   51.00000   0.00000  71.00000   0.00000   0.00000
O1     O                 0.71441   0.25000   0.98821   0.05000   0.50000           0    0    0    4
                Codes:   81.00000   0.00000 101.00000   0.00000   0.00000
O2     O                 0.04463   0.25000   0.97938   0.05000   0.50000           0    0    0    4
                Codes:  111.00000   0.00000 131.00000   0.00000   0.00000
O3     O                 0.37423   0.25000   0.16946   0.05000   0.50000           0    0    0    4
                Codes:  141.00000   0.00000 161.00000   0.00000   0.00000
O4     O                 0.11908   0.56241   0.25824   0.05000   1.00000           0    0    0    8
                Codes:  171.00000 181.00000 191.00000   0.00000   0.00000

=> IT IS ASSUMED THAT THE FIRST GIVEN SITE IS FULLY OCCUPIED
   OR THE FIRST AND SECOND ATOMS ARE IN THE SAME SITE WITH TOTAL FULL OCCUPATION
 (If this is not the case, change the order of atoms to obtain correct values for the content of the unit cell)
   The given occupation factors have been obtained mutiplying m/M by   1.0000
     -> Atom: V    ,  Chemical element: V   Atomic Mass:    50.9414
     -> Atom: S    ,  Chemical element: S   Atomic Mass:    32.0600
     -> Atom: O    ,  Chemical element: O   Atomic Mass:    15.9994
     -> Atom: O    ,  Chemical element: O   Atomic Mass:    15.9994
     -> Atom: O    ,  Chemical element: O   Atomic Mass:    15.9994
     -> Atom: O    ,  Chemical element: O   Atomic Mass:    15.9994
=> The given value of ATZ is        651.99 the program has calculated:         651.99
   The value of ATZ given in the input PCR file will be used for quantitative analysis
=> The chemical content of the unit cell is:
      4.0000 V    +   4.0000 S    +   4.0000 O    +   4.0000 O    +   4.0000 O    +   8.0000 O
=> The normalized site occupation numbers in % are:
    100.0000 V1     :      100.0000 S1     :      100.0000 O1     :      100.0000 O2     :      100.0000 O3     :      100.0000 O4
=> The density (volumic mass) of the compound is:    3.325 g/cm3

=>-------> PROFILE PARAMETERS FOR PATTERN:  1

=> Overall scale factor:    1.12500
=> T.O.F. Extinction parameter:   0.0000
=> Overall temperature factor:      0.00000
=> T.O.F. Gaussian variances Sig-2, Sig-1, Sig-0:     -2.64100   166.84900     0.00000
=> T.O.F. <Unused> Xt,Yt parameters:       0.0000      0.0000
=> T.O.F. Gaussian and <unused> Size parameters Z1,Z0  :      0.00000     0.00000
=> T.O.F. Lorentzian FWHM Gam-2, Gam-1, Gam-0:      0.00000     5.49800     0.00000
=> T.O.F. Lorentzian strain and size parameters (LStr,LSiz):      0.00000     0.00000
=> Direct cell parameters:    7.3540   6.2706   7.0604  90.0000  90.0000  90.0000
```

```
=> Preferred orientation parameters:   0.0000  0.0000
=> T.O.F. Peak shape parameter alpha0,beta0,alpha1,beta1/kappa:      0.00000     0.02518     2.83057     0.00908
=> Strain parameters s2,s1,s0:      0.00000     0.00000     0.00000


==> CODEWORDS FOR PROFILE PARAMETERS of PATTERN#  1

=> Codeword - Overall scale factor:   211.000
=> Codeword  - T.O.F. Extinction parameter:   0.0000
=> Codeword  - Overall temperature factor:      0.00000
=> Codewords - T.O.F. Gaussian variances Sig-2, Sig-1, Sig-0:      0.00000     0.00000     0.00000
=> Codewords - T.O.F. <Unused> Xt,Yt parameters:       0.0000      0.0000
=> Codewords - T.O.F. Gaussian and <unused> Size parameters Z1,Z0  :      0.00000     0.00000
=> Codewords - T.O.F. Lorentzian FWHM Gam-2, Gam-1, Gam-0:      0.00000     0.00000     0.00000
=> Codewords - T.O.F. Lorentzian strain and size parameters (LStr,LSiz):      0.00000     0.00000
=> Codewords - Direct cell parameters:   11.0000 221.0000 231.0000   0.0000   0.0000   0.0000
=> Codewords - Preferred orientation parameters:   0.0000  0.0000
=> Codewords - T.O.F. Peak shape parameter alpha0,beta0,alpha1,beta1/kappa:      0.00000     0.00000     0.00000     0.00000
=> Codewords - Strain parameters s2,s1,s0:      0.00000     0.00000     0.00000


=> Cell constraints according to Laue symmetry: mmm

       Metric information:
       -------------------

=> Direct cell parameters:

        a =       7.3540      b =       6.2706      c =       7.0604
    alpha =       90.000   beta =       90.000  gamma =       90.000
                     Direct Cell Volume =     325.5859

=> Reciprocal cell parameters:

        a*=     0.135981      b*=     0.159473      c*=     0.141634
    alpha*=       90.000   beta*=       90.000  gamma*=       90.000
                   Reciprocal Cell Volume =   0.00307139

=> Direct and Reciprocal Metric Tensors:

                  GD                                        GR
    54.0809      0.0000      0.0000          0.018491    0.000000    0.000000
     0.0000     39.3210      0.0000          0.000000    0.025432    0.000000
     0.0000      0.0000     49.8498          0.000000    0.000000    0.020060

=>  Cartesian frame: x // a; y is in the ab-plane; z is x ^ y

    Crystal_to_Orthonormal_Matrix              Orthonormal_to_Crystal Matrix
            Cr_Orth_cel                                Orth_Cr_cel
     7.3540      0.0000      0.0000          0.135981   -0.000000   -0.000000
     0.0000      6.2706      0.0000          0.000000    0.159473   -0.000000
     0.0000      0.0000      7.0604          0.000000    0.000000    0.141634

    Busing-Levy B-matrix: Hc=B.H            Inverse of the Busing-Levy B-matrix
              BL_M                                       BL_Minv
   0.135981    0.000000    0.000000            7.3540     -0.0000     -0.0000
   0.000000    0.159473   -0.000000            0.0000      6.2706      0.0000
   0.000000    0.000000    0.141634            0.0000      0.0000      7.0604

=>-------> PROFILE PARAMETERS FOR PATTERN:  2

=> Overall scale factor:    1.26420
=> T.O.F. Extinction parameter:   0.0000
=> Overall temperature factor:      0.00000
=> T.O.F. Gaussian variances Sig-2, Sig-1, Sig-0:    252.28700  3568.98804     0.00000
=> T.O.F. <Unused> Xt,Yt parameters:       0.0000      0.0000
=> T.O.F. Gaussian and <unused> Size parameters Z1,Z0  :      0.00000     0.00000
=> T.O.F. Lorentzian FWHM Gam-2, Gam-1, Gam-0:      0.00000     6.07100     0.00000
=> T.O.F. Lorentzian strain and size parameters (LStr,LSiz):      0.00000     0.00000
=> Direct cell parameters:    7.3615   6.2762   7.0672  90.0000  90.0000  90.0000
=> Preferred orientation parameters:   0.0000  0.0000
=> T.O.F. Peak shape parameter alpha0,beta0,alpha1,beta1/kappa:      0.00000     0.02518     2.83057     0.00908
=> Strain parameters s2,s1,s0:      0.00000     0.00000     0.00000


==> CODEWORDS FOR PROFILE PARAMETERS of PATTERN#  2

=> Codeword - Overall scale factor:   0.00000
=> Codeword  - T.O.F. Extinction parameter:   0.0000
=> Codeword  - Overall temperature factor:      0.00000
=> Codewords - T.O.F. Gaussian variances Sig-2, Sig-1, Sig-0:      0.00000     0.00000     0.00000
=> Codewords - T.O.F. <Unused> Xt,Yt parameters:       0.0000      0.0000
=> Codewords - T.O.F. Gaussian and <unused> Size parameters Z1,Z0  :      0.00000     0.00000
```

```
=> Codewords - T.O.F. Lorentzian FWHM Gam-2, Gam-1, Gam-0:      0.00000     0.00000     0.00000
=> Codewords - T.O.F. Lorentzian strain and size parameters (LStr,LSiz):      0.00000     0.00000
=> Codewords - Direct cell parameters:    0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
=> Codewords - Preferred orientation parameters:   0.0000  0.0000
=> Codewords - T.O.F. Peak shape parameter alpha0,beta0,alpha1,beta1/kappa:      0.00000     0.00000     0.00000     0.00000
=> Codewords - Strain parameters s2,s1,s0:      0.00000     0.00000     0.00000


=> Cell constraints according to Laue symmetry: mmm

=>-------> PROFILE PARAMETERS FOR PATTERN:  3

=> Overall scale factor:   0.223100E-02
=> ETA (p-Voigt) OR M (Pearson VII):   0.0000
=> Overall temperature factor:      0.00000
=> Halfwidth U,V,W:      0.37277    -0.14637     0.23141
=> X and Y parameters:       0.0000      0.0000
=> Direct cell parameters:    7.3615   6.2762   7.0672  90.0000  90.0000  90.0000
=> Preferred orientation parameters:   0.0000  0.0000
=> Asymmetry parameters     :      0.00000     0.00000     0.00000     0.00000
=> Strain parameters        :      0.00000     0.00000     0.00000
=> Size   parameters        :     -0.19498     0.00000

==> CODEWORDS FOR PROFILE PARAMETERS of PATTERN#  3

=> Overall scale factor:    0.000
=> ETA (p-Voigt) OR M (Pearson VII):    0.000
=> Overall temperature factor:    0.000
=> Halfwidth U,V,W:    0.000   0.000   0.000
=> X and Y parameters:    0.000   0.000
=> Direct cell parameters:    0.000   0.000   0.000   0.000   0.000   0.000
=> Preferred orientation parameters:    0.000   0.000
=> Asymmetry parameters     :    0.000   0.000   0.000   0.000
=> Strain parameters        :    0.000   0.000   0.000
=> Size   parameters        :    0.000   0.000

=> Cell constraints according to Laue symmetry: mmm

=> Laue symmetry mmm   will be used to generate HKL for pattern#   1
=> Reflections generated between S(1/d)min:  0.3866 A-1 and S(1/d)max:  1.8173 A-1
=>                                  dmax:  2.5865 A   and      dmin:  0.5503 A
=> The number of reflections generated is:   1090
=> The max. scatt. variable (gen.ref.) is:    125005.3906
=> Scattering coefficients from internal table

=> Scattering lengths:

V     -0.0382
S      0.2847
O      0.5803

=> Laue symmetry mmm   will be used to generate HKL for pattern#   2
=> Reflections generated between S(1/d)min:  0.2568 A-1 and S(1/d)max:  1.4310 A-1
=>                                  dmax:  3.8942 A   and      dmin:  0.6988 A
=> The number of reflections generated is:    541
=> The max. scatt. variable (gen.ref.) is:    135554.0000
=> Scattering coefficients from internal table

=> Scattering lengths:

V     -0.0382
S      0.2847
O      0.5803

=> Laue symmetry mmm   will be used to generate HKL for pattern#   3
=> Reflections generated between S(1/d)min:  0.0455 A-1 and S(1/d)max:  1.0019 A-1
=>                                  dmax: 21.9556 A   and      dmin:  0.9982 A
=> The number of reflections generated is:    190
=> The max. scatt. variable (gen.ref.) is:       101.3230
=> Scattering coefficients from internal table


=> X-ray scattering coeff. (A1, B1, A2,...C, f(0), Z, Dfp,Dfpp)

V      10.2971   6.8657   7.3511   0.4385   2.0703  26.8938   2.0571 102.4780   1.2199  22.9955  23.0000   0.0350   2.1100
S       6.9053   1.4679   5.2034  22.2151   1.4379   0.2536   1.5863  56.1720   0.8669  15.9998  16.0000   0.3190   0.5570
O       3.0485  13.2771   2.2868   5.7011   1.5463   0.3239   0.8670  32.9089   0.2508   7.9994   8.0000   0.0470   0.0320

    ---------------------------------------------------------------
     SYMBOLIC NAMES AND INITIAL VALUES OF PARAMETERS TO BE VARIED:
    ---------------------------------------------------------------

     ->  Parameter number    1   -> Symbolic Name:      Cell_A_ph1_pat1     7.3539691
```

```
     ->  Parameter number    2   -> Symbolic Name:             X_V1_ph1    0.16364001
     ->  Parameter number    3   -> Symbolic Name:            Zero_pat1    -1.9859999
     ->  Parameter number    4   -> Symbolic Name:             Z_V1_ph1    0.23748000
     ->  Parameter number    5   -> Symbolic Name:             X_S1_ph1    0.87405998
     ->  Parameter number    6   -> Symbolic Name:            Dtt1_pat1     48329.055
     ->  Parameter number    7   -> Symbolic Name:             Z_S1_ph1    0.87408000
     ->  Parameter number    8   -> Symbolic Name:             X_O1_ph1    0.71441001
     ->  Parameter number    9   -> Symbolic Name:            Dtt2_pat1    -3.2639999
     ->  Parameter number   10   -> Symbolic Name:             Z_O1_ph1    0.98821002
     ->  Parameter number   11   -> Symbolic Name:             X_O2_ph1    0.44629999E-01
     ->  Parameter number   12   -> Symbolic Name:            Zero_pat2    -5.4159999
     ->  Parameter number   13   -> Symbolic Name:             Z_O2_ph1    0.97938001
     ->  Parameter number   14   -> Symbolic Name:             X_O3_ph1    0.37423000
     ->  Parameter number   15   -> Symbolic Name:            Dtt1_pat2     34808.883
     ->  Parameter number   16   -> Symbolic Name:             Z_O3_ph1    0.16946000
     ->  Parameter number   17   -> Symbolic Name:             X_O4_ph1    0.11908000
     ->  Parameter number   18   -> Symbolic Name:             Y_O4_ph1    0.56241000
     ->  Parameter number   19   -> Symbolic Name:             Z_O4_ph1    0.25824001
     ->  Parameter number   20   -> Symbolic Name:            Dtt2_pat2    -3.1730001
     ->  Parameter number   21   -> Symbolic Name:       Scale_ph1_pat1     1.1250000
     ->  Parameter number   22   -> Symbolic Name:      Cell_B_ph1_pat1     6.2706432
     ->  Parameter number   23   -> Symbolic Name:      Cell_C_ph1_pat1     7.0604382


=> No optimization for routine tasks
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

=> CYCLE No.:    1
------------------------------------------------------------------------------
=> Phase  1 Name: VOSO4 Nuclear
------------------------------------------------------------------------------
=> New parameters, shifts, and standard deviations

Atom        x       dx      sx       y       dy      sy       z       dz      sz       B       dB      sB      occ.    docc.   socc.

V1       0.16364 0.00000 0.00127  0.25000 0.00000 0.00000  0.23748-0.00000 0.00140  0.05000 0.00000 0.00000  0.50000 0.00000 0.00000
S1       0.87406-0.00000 0.00126  0.25000 0.00000 0.00000  0.87408-0.00000 0.00092  0.05000 0.00000 0.00000  0.50000 0.00000 0.00000
O1       0.71441 0.00000 0.00053  0.25000 0.00000 0.00000  0.98821-0.00000 0.00070  0.05000 0.00000 0.00000  0.50000 0.00000 0.00000
O2       0.04463-0.00000 0.00054  0.25000 0.00000 0.00000  0.97938 0.00000 0.00067  0.05000 0.00000 0.00000  0.50000 0.00000 0.00000
O3       0.37423-0.00000 0.00079  0.25000 0.00000 0.00000  0.16946-0.00000 0.00049  0.05000 0.00000 0.00000  0.50000 0.00000 0.00000
O4       0.11908 0.00000 0.00086  0.56241 0.00000 0.00036  0.25824-0.00000 0.00040  0.05000 0.00000 0.00000  1.00000 0.00000 0.00000

==> PROFILE PARAMETERS FOR PATTERN#  1

=> Overall scale factor:      1.125015855     0.000015825     0.008038120
=> T.O.F. extinct. parameter :     0.000000    0.000000    0.000000
=> Overall tem. factor:     0.000000    0.000000    0.000000
=> T.O.F. FWHM: sig2,sig1,sig0:
       -2.641000    0.000000    0.000000
      166.848999    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Cell parameters:
        7.353978    0.000009    0.039002
        6.270650    0.000007    0.033257
        7.060446    0.000008    0.037445
       90.000000    0.000000    0.000000
       90.000000    0.000000    0.000000
       90.000000    0.000000    0.000000
=> Preferred orientation:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> T.O.F. shape a0,b0,a1,b1/kappa:
        0.000000    0.000000    0.000000
        0.025178    0.000000    0.000000
        2.830569    0.000000    0.000000
        0.009083    0.000000    0.000000
=> Xtof and Ytof parameters:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Strain parameters s2,s1,s0:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Size   parameters z1,z0:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000

=> T.O.F. FWHM: GAM2,GAM1,GAM0:
        0.000000    0.000000    0.000000
        5.498000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> STRAIN PARAMETER  LSTR :
        0.000000    0.000000    0.000000
```

```
=> Absorption parameters:
      0.021680  0.000000  0.000000
      0.000000  0.000000  0.000000

==> PROFILE PARAMETERS FOR PATTERN#  2

=> Overall scale factor:      1.264199972     0.000000000     0.000000000
=> T.O.F. extinct. parameter :     0.000000    0.000000    0.000000
=> Overall tem. factor:     0.000000    0.000000    0.000000
=> T.O.F. FWHM: sig2,sig1,sig0:
      252.287003    0.000000    0.000000
     3568.988037    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Cell parameters:
       7.361516    0.000000    0.000000
       6.276170    0.000000    0.000000
       7.067196    0.000000    0.000000
      90.000000    0.000000    0.000000
      90.000000    0.000000    0.000000
      90.000000    0.000000    0.000000
=> Preferred orientation:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> T.O.F. shape a0,b0,a1,b1/kappa:
        0.000000    0.000000    0.000000
        0.025178    0.000000    0.000000
        2.830569    0.000000    0.000000
        0.009083    0.000000    0.000000
=> Xtof and Ytof parameters:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Strain parameters s2,s1,s0:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Size   parameters z1,z0:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000

=> T.O.F. FWHM: GAM2,GAM1,GAM0:
        0.000000    0.000000    0.000000
        6.071000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> STRAIN PARAMETER  LSTR :
        0.000000    0.000000    0.000000

=> Absorption parameters:
      0.029020  0.000000  0.000000
      0.000000  0.000000  0.000000

==> PROFILE PARAMETERS FOR PATTERN#  3

=> Overall scale factor:      0.002231000     0.000000000     0.000000000
=> Eta(p-Voigt) or m(Pearson VII):   0.000000  0.000000  0.000000
=> Overall tem. factor:     0.000000    0.000000    0.000000
=> Halfwidth parameters:
        0.372771    0.000000    0.000000
       -0.146366    0.000000    0.000000
        0.231411    0.000000    0.000000
=> Cell parameters:
       7.361516    0.000000    0.000000
       6.276170    0.000000    0.000000
       7.067196    0.000000    0.000000
      90.000000    0.000000    0.000000
      90.000000    0.000000    0.000000
      90.000000    0.000000    0.000000
=> Preferred orientation:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Asymmetry parameters:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> X and Y parameters:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Strain parameters:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Size   parameters (G,L):
```

```
       -0.194981    0.000000    0.000000
        0.000000    0.000000    0.000000

==> GLOBAL PARAMETERS FOR PATTERN#  1


=> Zero-point:    -1.9953   -0.0093    2.1816

=> T.O.F.- dtt1 (    TOFo=dtt1*dsp    ):  48329.04     -0.01    256.28
=> T.O.F.- dtt2 (TOF=TOFo+dtt2*dsp*dsp):     -3.27     -0.01      1.07

==> RELIABILITY FACTORS WITH ALL NON-EXCLUDED POINTS FOR PATTERN:  1

=> R-Factors:   5.04      8.25     Chi2:  41.1     DW-Stat.:  0.5884   Patt#:  1
=> Expected :            1.29                                1.9088
=> Deviance :  89.1         Dev*:  0.1941E-01
=> GoF-index:  6.4         Sqrt(Residual/N)
=> N-P+C:  4317

=>    SumYdif       SumYobs      SumYcal      SumwYobsSQ     Residual    Condition
     673.2        0.1336E+05    0.1317E+05    0.2611E+08    0.1776E+06    0.9488E+18


=> Conventional Rietveld Rp,Rwp,Re and Chi2:   22.2      23.2      3.61      41.15
=> (Values obtained using Ynet, but true sigma(y))
=>  SumYnet, Sum(w Ynet**2):      3031.        0.3309E+07


==> RELIABILITY FACTORS FOR POINTS WITH BRAGG CONTRIBUTIONS FOR PATTERN:  1

=> R-Factors:   5.33      8.57     Chi2:  45.0     DW-Stat.:  0.5968   Patt#:
=> Expected :            1.28                                1.9041
=> Deviance :  86.2         Dev*:  0.2082E-01
=> GoF-index:  6.7         Sqrt(Residual/N)
=> N-P+C:  3890

=>    SumYdif       SumYobs      SumYcal      SumwYobsSQ     Residual    Condition
     640.8        0.1202E+05    0.1186E+05    0.2386E+08    0.1751E+06    0.9488E+18


=> Conventional Rietveld Rp,Rwp,Re and Chi2:   21.3      23.0      3.43      45.01
=> (Values obtained using Ynet, but true sigma(y))
=>  SumYnet, Sum(w Ynet**2):      3004.        0.3306E+07


==> GLOBAL PARAMETERS FOR PATTERN#  2


=> Zero-point:    -5.3568    0.0592    8.9366

=> T.O.F.- dtt1 (    TOFo=dtt1*dsp    ):  34808.74     -0.14     11.00
=> T.O.F.- dtt2 (TOF=TOFo+dtt2*dsp*dsp):     -3.15      0.03      3.02

==> RELIABILITY FACTORS WITH ALL NON-EXCLUDED POINTS FOR PATTERN:  2

=> R-Factors:   5.33      6.97     Chi2:  73.0     DW-Stat.:  0.1314   Patt#:  2
=> Expected :           0.816                                1.8730
=> Deviance :  26.9         Dev*:  0.1149E-01
=> GoF-index:  8.5         Sqrt(Residual/N)
=> N-P+C:  2164

=>    SumYdif       SumYobs      SumYcal      SumwYobsSQ     Residual    Condition
     270.6         5073.         4936.        0.3248E+08    0.1579E+06    0.9488E+18


=> Conventional Rietveld Rp,Rwp,Re and Chi2:   19.2      19.3      2.25      72.99
=> (Values obtained using Ynet, but true sigma(y))
=>  SumYnet, Sum(w Ynet**2):      1411.        0.4260E+07


==> RELIABILITY FACTORS FOR POINTS WITH BRAGG CONTRIBUTIONS FOR PATTERN:  2

=> R-Factors:   5.99      7.93     Chi2:  88.9     DW-Stat.:  0.1375   Patt#:
=> Expected :           0.841                                1.8575
=> Deviance :  25.9         Dev*:  0.1410E-01
=> GoF-index:  9.4         Sqrt(Residual/N)
=> N-P+C:  1699

=>    SumYdif       SumYobs      SumYcal      SumwYobsSQ     Residual    Condition
     247.6         4133.         4018.        0.2400E+08    0.1510E+06    0.9488E+18


=> Conventional Rietveld Rp,Rwp,Re and Chi2:   17.8      18.8      2.00      88.85
```

```
=> (Values obtained using Ynet, but true sigma(y))
=>  SumYnet, Sum(w Ynet**2):      1389.        0.4253E+07


==> GLOBAL PARAMETERS FOR PATTERN#  3


=> Zero-point:    -0.1171    0.0000    0.0000

=> Cos( theta)-shift parameter :   0.0000  0.0000  0.0000
=> Sin(2theta)-shift parameter :   0.0000  0.0000  0.0000

==> RELIABILITY FACTORS WITH ALL NON-EXCLUDED POINTS FOR PATTERN:  3

=> R-Factors:   2.46      4.50     Chi2:  12.4     DW-Stat.:  0.0358   Patt#:  3
=> Expected :            1.28                                1.9371
=> Deviance : 0.126E+06     Dev*:   13.59
=> GoF-index:  3.5         Sqrt(Residual/N)
=> N-P+C:  9262

=>    SumYdif       SumYobs      SumYcal      SumwYobsSQ     Residual    Condition
    0.1398E+07    0.5689E+08    0.5622E+08    0.5689E+08    0.1150E+06    0.9488E+18


=> Conventional Rietveld Rp,Rwp,Re and Chi2:   44.1      33.7      9.56      12.41
=> (Values obtained using Ynet, but true sigma(y))
=>  SumYnet, Sum(w Ynet**2):     0.3169E+07    0.1013E+07


==> RELIABILITY FACTORS FOR POINTS WITH BRAGG CONTRIBUTIONS FOR PATTERN:  3

=> R-Factors:   2.90      5.08     Chi2:  14.7     DW-Stat.:  0.0367   Patt#:
=> Expected :            1.33                                1.9309
=> Deviance : 0.123E+06     Dev*:   16.10
=> GoF-index:  3.8         Sqrt(Residual/N)
=> N-P+C:  7643

=>    SumYdif       SumYobs      SumYcal      SumwYobsSQ     Residual    Condition
    0.1261E+07    0.4347E+08    0.4287E+08    0.4347E+08    0.1122E+06    0.9488E+18


=> Conventional Rietveld Rp,Rwp,Re and Chi2:   40.6      33.3      8.70      14.68
=> (Values obtained using Ynet, but true sigma(y))
=>  SumYnet, Sum(w Ynet**2):     0.3103E+07    0.1010E+07


=> Global user-weigthed Chi2 (Bragg contrib.):   51.2

=> ---------> Pattern#  1
=> Phase:  1
=>    Bragg R-factor:  11.4
=>    RF-factor     :  10.5

=> ---------> Pattern#  2
=> Phase:  1
=>    Bragg R-factor:  14.0
=>    RF-factor     :  8.28

=> ---------> Pattern#  3
=> Phase:  1
=>    Bragg R-factor:  25.4
=>    RF-factor     :  17.7


  Standard deviations have to be multiplied by: 2.5620
  (correlated residuals) See references:
 -J.F.Berar & P.Lelann, J. Appl. Cryst. 24, 1-5 (1991)
 -J.F.Berar, Acc. in Pow. Diff. II,NIST Sp.Pub. 846, 63(1992)



  Standard deviations have to be multiplied by: 5.0247
  (correlated residuals) See references:
 -J.F.Berar & P.Lelann, J. Appl. Cryst. 24, 1-5 (1991)
 -J.F.Berar, Acc. in Pow. Diff. II,NIST Sp.Pub. 846, 63(1992)



  Standard deviations have to be multiplied by: 5.8240
  (correlated residuals) See references:
 -J.F.Berar & P.Lelann, J. Appl. Cryst. 24, 1-5 (1991)
 -J.F.Berar, Acc. in Pow. Diff. II,NIST Sp.Pub. 846, 63(1992)
```

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

=> CYCLE No.:    1
=>  Convergence reached at this CYCLE !!!!
=>  Parameter shifts set to zero
------------------------------------------------------------------------------
=> Phase  1 Name: VOSO4 Nuclear
------------------------------------------------------------------------------
=> New parameters, shifts, and standard deviations

Atom        x       dx      sx       y       dy      sy       z       dz      sz       B       dB      sB      occ.    docc.   socc.

V1       0.16364 0.00000 0.00127  0.25000 0.00000 0.00000  0.23748 0.00000 0.00140  0.05000 0.00000 0.00000  0.50000 0.00000 0.00000
S1       0.87406 0.00000 0.00126  0.25000 0.00000 0.00000  0.87408 0.00000 0.00092  0.05000 0.00000 0.00000  0.50000 0.00000 0.00000
O1       0.71441 0.00000 0.00053  0.25000 0.00000 0.00000  0.98821 0.00000 0.00070  0.05000 0.00000 0.00000  0.50000 0.00000 0.00000
O2       0.04463 0.00000 0.00054  0.25000 0.00000 0.00000  0.97938 0.00000 0.00067  0.05000 0.00000 0.00000  0.50000 0.00000 0.00000
O3       0.37423 0.00000 0.00079  0.25000 0.00000 0.00000  0.16946 0.00000 0.00049  0.05000 0.00000 0.00000  0.50000 0.00000 0.00000
O4       0.11908 0.00000 0.00086  0.56241 0.00000 0.00036  0.25824 0.00000 0.00040  0.05000 0.00000 0.00000  1.00000 0.00000 0.00000

==> PROFILE PARAMETERS FOR PATTERN#  1

=> Overall scale factor:      1.125015855     0.000000000     0.008038120
=> T.O.F. extinct. parameter :     0.000000    0.000000    0.000000
=> Overall tem. factor:     0.000000    0.000000    0.000000
=> T.O.F. FWHM: sig2,sig1,sig0:
       -2.641000    0.000000    0.000000
      166.848999    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Cell parameters:
        7.353978    0.000000    0.039002
        6.270650    0.000000    0.033257
        7.060446    0.000000    0.037445
       90.000000    0.000000    0.000000
       90.000000    0.000000    0.000000
       90.000000    0.000000    0.000000
=> Preferred orientation:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> T.O.F. shape a0,b0,a1,b1/kappa:
        0.000000    0.000000    0.000000
        0.025178    0.000000    0.000000
        2.830569    0.000000    0.000000
        0.009083    0.000000    0.000000
=> Xtof and Ytof parameters:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Strain parameters s2,s1,s0:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Size   parameters z1,z0:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000

=> T.O.F. FWHM: GAM2,GAM1,GAM0:
        0.000000    0.000000    0.000000
        5.498000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> STRAIN PARAMETER  LSTR :
        0.000000    0.000000    0.000000

=> Absorption parameters:
       0.021680  0.000000  0.000000
       0.000000  0.000000  0.000000

==> PROFILE PARAMETERS FOR PATTERN#  2

=> Overall scale factor:      1.264199972     0.000000000     0.000000000
=> T.O.F. extinct. parameter :     0.000000    0.000000    0.000000
=> Overall tem. factor:     0.000000    0.000000    0.000000
=> T.O.F. FWHM: sig2,sig1,sig0:
      252.287003    0.000000    0.000000
     3568.988037    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Cell parameters:
        7.361516    0.000000    0.000000
        6.276170    0.000000    0.000000
        7.067196    0.000000    0.000000
       90.000000    0.000000    0.000000
       90.000000    0.000000    0.000000
       90.000000    0.000000    0.000000
=> Preferred orientation:
        0.000000    0.000000    0.000000
```

```
        0.000000    0.000000    0.000000
=> T.O.F. shape a0,b0,a1,b1/kappa:
        0.000000    0.000000    0.000000
        0.025178    0.000000    0.000000
        2.830569    0.000000    0.000000
        0.009083    0.000000    0.000000
=> Xtof and Ytof parameters:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Strain parameters s2,s1,s0:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Size   parameters z1,z0:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000

=> T.O.F. FWHM: GAM2,GAM1,GAM0:
        0.000000    0.000000    0.000000
        6.071000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> STRAIN PARAMETER  LSTR :
        0.000000    0.000000    0.000000

=> Absorption parameters:
      0.029020  0.000000  0.000000
      0.000000  0.000000  0.000000

==> PROFILE PARAMETERS FOR PATTERN#  3

=> Overall scale factor:      0.002231000     0.000000000     0.000000000
=> Eta(p-Voigt) or m(Pearson VII):   0.000000  0.000000  0.000000
=> Overall tem. factor:     0.000000    0.000000    0.000000
=> Halfwidth parameters:
        0.372771    0.000000    0.000000
       -0.146366    0.000000    0.000000
        0.231411    0.000000    0.000000
=> Cell parameters:
       7.361516    0.000000    0.000000
       6.276170    0.000000    0.000000
       7.067196    0.000000    0.000000
      90.000000    0.000000    0.000000
      90.000000    0.000000    0.000000
      90.000000    0.000000    0.000000
=> Preferred orientation:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Asymmetry parameters:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> X and Y parameters:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Strain parameters:
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
=> Size   parameters (G,L):
       -0.194981    0.000000    0.000000
        0.000000    0.000000    0.000000

==> GLOBAL PARAMETERS FOR PATTERN#  1


=> Zero-point:    -1.9953    0.0000    2.1816

=> T.O.F.- dtt1 (    TOFo=dtt1*dsp    ):  48329.04      0.00    256.28
=> T.O.F.- dtt2 (TOF=TOFo+dtt2*dsp*dsp):     -3.27      0.00      1.07

==> RELIABILITY FACTORS WITH ALL NON-EXCLUDED POINTS FOR PATTERN:  1

=> R-Factors:   5.04      8.25     Chi2:  41.1     DW-Stat.:  0.5884   Patt#:  1
=> Expected :            1.29                                1.9088
=> Deviance :  89.1         Dev*:  0.1941E-01
=> GoF-index:  6.4          Sqrt(Residual/N)
=> N-P+C:  4317

=>    SumYdif       SumYobs      SumYcal      SumwYobsSQ     Residual    Condition
     673.2        0.1336E+05    0.1317E+05    0.2611E+08    0.1776E+06    0.9488E+18
```

```
=> Conventional Rietveld Rp,Rwp,Re and Chi2:   22.2      23.2      3.61      41.15
=> (Values obtained using Ynet, but true sigma(y))
=>  SumYnet, Sum(w Ynet**2):      3031.        0.3309E+07

=> N-sigma of the GoF: 1865.181

==> RELIABILITY FACTORS FOR POINTS WITH BRAGG CONTRIBUTIONS FOR PATTERN:  1

=> R-Factors:   5.33      8.57     Chi2:  45.0     DW-Stat.:  0.5968   Patt#:
=> Expected :             1.28                                1.9041
=> Deviance :  86.2         Dev*:  0.2082E-01
=> GoF-index:  6.7         Sqrt(Residual/N)
=> N-P+C:  3890

=>    SumYdif       SumYobs      SumYcal      SumwYobsSQ     Residual    Condition
     640.8        0.1202E+05    0.1186E+05    0.2386E+08    0.1751E+06    0.9488E+18


=> Conventional Rietveld Rp,Rwp,Re and Chi2:   21.3      23.0      3.43      45.01
=> (Values obtained using Ynet, but true sigma(y))
=>  SumYnet, Sum(w Ynet**2):      3004.        0.3306E+07

=> N-sigma of the GoF:     1941.074

==> GLOBAL PARAMETERS FOR PATTERN#  2


=> Zero-point:    -5.3568    0.0000    8.9366

=> T.O.F.- dtt1 (    TOFo=dtt1*dsp    ):  34808.74      0.00     11.00
=> T.O.F.- dtt2 (TOF=TOFo+dtt2*dsp*dsp):     -3.15      0.00      3.02

==> RELIABILITY FACTORS WITH ALL NON-EXCLUDED POINTS FOR PATTERN:  2

=> R-Factors:   5.33      6.97     Chi2:  73.0     DW-Stat.:  0.1314   Patt#:  2
=> Expected :           0.816                                1.8730
=> Deviance :  26.9         Dev*:  0.1149E-01
=> GoF-index:  8.5         Sqrt(Residual/N)
=> N-P+C:  2164

=>    SumYdif       SumYobs      SumYcal      SumwYobsSQ     Residual    Condition
     270.6         5073.         4936.        0.3248E+08    0.1579E+06    0.9488E+18


=> Conventional Rietveld Rp,Rwp,Re and Chi2:   19.2      19.3      2.25      72.99
=> (Values obtained using Ynet, but true sigma(y))
=>  SumYnet, Sum(w Ynet**2):      1411.        0.4260E+07

=> N-sigma of the GoF: 2367.961

==> RELIABILITY FACTORS FOR POINTS WITH BRAGG CONTRIBUTIONS FOR PATTERN:  2

=> R-Factors:   5.99      7.93     Chi2:  88.9     DW-Stat.:  0.1375   Patt#:
=> Expected :           0.841                                1.8575
=> Deviance :  25.9         Dev*:  0.1410E-01
=> GoF-index:  9.4         Sqrt(Residual/N)
=> N-P+C:  1699

=>    SumYdif       SumYobs      SumYcal      SumwYobsSQ     Residual    Condition
     247.6         4133.         4018.        0.2400E+08    0.1510E+06    0.9488E+18


=> Conventional Rietveld Rp,Rwp,Re and Chi2:   17.8      18.8      2.00      88.85
=> (Values obtained using Ynet, but true sigma(y))
=>  SumYnet, Sum(w Ynet**2):      1389.        0.4253E+07

=> N-sigma of the GoF:     2560.634

==> GLOBAL PARAMETERS FOR PATTERN#  3


=> Zero-point:    -0.1171    0.0000    0.0000

=> Cos( theta)-shift parameter :   0.0000  0.0000  0.0000
=> Sin(2theta)-shift parameter :   0.0000  0.0000  0.0000

==> RELIABILITY FACTORS WITH ALL NON-EXCLUDED POINTS FOR PATTERN:  3

=> R-Factors:   2.46      4.50     Chi2:  12.4     DW-Stat.:  0.0358   Patt#:  3
=> Expected :           1.28                                1.9371
=> Deviance : 0.126E+06     Dev*:   13.59
=> GoF-index:  3.5         Sqrt(Residual/N)
=> N-P+C:  9262
```

```
=>    SumYdif       SumYobs      SumYcal      SumwYobsSQ     Residual    Condition
    0.1398E+07    0.5689E+08    0.5622E+08    0.5689E+08    0.1150E+06    0.9488E+18


=> Conventional Rietveld Rp,Rwp,Re and Chi2:   44.1      33.7      9.56      12.41
=> (Values obtained using Ynet, but true sigma(y))
=>  SumYnet, Sum(w Ynet**2):     0.3169E+07    0.1013E+07

=> N-sigma of the GoF:  776.663

==> RELIABILITY FACTORS FOR POINTS WITH BRAGG CONTRIBUTIONS FOR PATTERN:  3

=> R-Factors:   2.90      5.08     Chi2:  14.7     DW-Stat.:  0.0367   Patt#:
=> Expected :            1.33                                1.9309
=> Deviance : 0.123E+06     Dev*:   16.10
=> GoF-index:  3.8         Sqrt(Residual/N)
=> N-P+C:  7643

=>    SumYdif       SumYobs      SumYcal      SumwYobsSQ     Residual    Condition
    0.1261E+07    0.4347E+08    0.4287E+08    0.4347E+08    0.1122E+06    0.9488E+18


=> Conventional Rietveld Rp,Rwp,Re and Chi2:   40.6      33.3      8.70      14.68
=> (Values obtained using Ynet, but true sigma(y))
=>  SumYnet, Sum(w Ynet**2):     0.3103E+07    0.1010E+07

=> N-sigma of the GoF:      845.557

=> Global user-weigthed Chi2 (Bragg contrib.):   51.2

=> ---------> Pattern#  1
=> Phase:  1
=>    Bragg R-factor:  11.4
=>    RF-factor     :  10.5

=> ---------> Pattern#  2
=> Phase:  1
=>    Bragg R-factor:  14.0
=>    RF-factor     :  8.28

=> ---------> Pattern#  3
=> Phase:  1
=>    Bragg R-factor:  25.4
=>    RF-factor     :  17.7

-------------------------------------------------------------------------------------------------------------
Pattern#  1 Phase No:   1 Phase name: VOSO4 Nuclear
-------------------------------------------------------------------------------------------------------------

  No.  Code     H   K   L  Mult     Hw     2theta/TOF      Icalc       Iobs      Sigma    HwG    HwL     ETA     d-hkl  TOF_alpha  TOF_beta     CORR

    1   1      6   8   2     8    21.604   31369.666        0.1        0.0      0.001  19.677  3.569  0.213  0.649085  4.360860  0.076349
    2   1      1   8   6     8    21.628   31404.418        0.2        0.0      0.021  19.699  3.573  0.213  0.649804  4.356034  0.076123
    3   1      3   6   8     8    21.639   31420.838        0.0        0.0      0.005  19.709  3.574  0.213  0.650144  4.353758  0.076016
    4   1      5   6   7     8    21.662   31454.432        8.3        2.9      1.896  19.730  3.578  0.213  0.650839  4.349108  0.075800
    5   1     11   2   1     8    21.669   31465.020        0.6        0.3      0.157  19.737  3.580  0.213  0.651058  4.347645  0.075731
    6   1      6   4   8     8    21.682   31483.328        0.7        0.4      0.171  19.748  3.582  0.213  0.651437  4.345116  0.075614
    7   1      4   9   0     4    21.684   31487.416        0.4        0.2      0.092  19.751  3.582  0.213  0.651521  4.344553  0.075588
    8   1     10   0   5     4    21.708   31522.447       12.7       10.1      2.038  19.773  3.586  0.213  0.652246  4.339724  0.075364
    9   1      0   8   6     4    21.712   31527.738       80.6       63.6     13.106  19.776  3.587  0.213  0.652356  4.338996  0.075330
   10   1     11   1   2     8    21.743   31573.037        9.8       12.0      2.561  19.804  3.592  0.213  0.653293  4.332770  0.075043
   11   1     10   4   2     8    21.775   31619.164        0.8        0.5      0.187  19.833  3.597  0.213  0.654248  4.326450  0.074753
   12   1      2   5   9     8    21.782   31629.949        0.8        0.4      0.192  19.840  3.598  0.213  0.654471  4.324975  0.074685
   13   1      7   7   3     8    21.791   31642.766       11.4        5.6      2.838  19.848  3.600  0.213  0.654736  4.323223  0.074605
   14   1      4   4   9     8    21.814   31677.445        0.8        0.1      0.146  19.869  3.604  0.213  0.655453  4.318490  0.074389
   15   1      4   1  10     8    21.816   31679.695        0.6        0.1      0.117  19.871  3.604  0.213  0.655500  4.318183  0.074375
   16   1      7   6   5     8    21.836   31708.406        0.4        0.2      0.105  19.888  3.607  0.213  0.656094  4.314273  0.074197
   17   1      9   2   6     8    21.842   31718.279        3.8        2.0      0.928  19.895  3.608  0.213  0.656298  4.312930  0.074136
   18   1      8   5   5     8    21.847   31724.707       22.6       13.3      5.346  19.899  3.609  0.213  0.656431  4.312057  0.074096
   19   1     11   0   2     4    21.861   31745.791        2.6        1.8      0.510  19.912  3.611  0.213  0.656868  4.309193  0.073967
   20   1      5   3   9     8    21.869   31756.705       17.9       13.2      3.370  19.919  3.613  0.213  0.657093  4.307711  0.073900
   21   1      6   1   9     8    21.869   31757.084        0.8        0.6      0.158  19.919  3.613  0.213  0.657101  4.307660  0.073897
   22   1      2   9   3     8    21.876   31767.426        0.3        0.3      0.054  19.925  3.614  0.213  0.657315  4.306258  0.073834
   23   1      9   5   3     8    21.878   31770.053        1.0        0.8      0.158  19.927  3.614  0.213  0.657370  4.305902  0.073818
   24   1      6   8   1     8    21.881   31775.078       41.1       34.3      5.616  19.930  3.615  0.213  0.657474  4.305221  0.073787
   25   1      8   4   6     8    21.885   31781.059        0.9        0.8      0.101  19.934  3.615  0.213  0.657597  4.304410  0.073750
   26   1      2   3  10     8    21.902   31805.924        4.2        4.4      0.227  19.949  3.618  0.213  0.658112  4.301045  0.073599
   27   1      3   9   2     8    21.913   31821.420        4.6        4.9      0.364  19.959  3.620  0.213  0.658432  4.298951  0.073504
   28   1      6   6   6     8    21.928   31843.836        0.1        0.1      0.010  19.973  3.623  0.213  0.658896  4.295925  0.073368
   29   1      2   7   7     8    21.930   31845.982        0.8        0.6      0.112  19.974  3.623  0.213  0.658941  4.295635  0.073355
   30   1      4   0  10     4    21.935   31854.219       27.9       21.6      4.808  19.979  3.624  0.213  0.659111  4.294525  0.073306
   31   1      7   4   7     8    21.964   31895.600        3.2        2.4      0.617  20.005  3.629  0.213  0.659967  4.288953  0.073056
```

32	1	3	8	5	8	21.965	31898.076	17.4	12.8	3.327	20.007	3.629	0.213	0.660019	4.288620	0.073042
33	1	6	8	0	4	21.976	31913.750	0.0	0.0	0.006	20.016	3.631	0.213	0.660343	4.286513	0.072948
34	1	7	2	8	8	21.984	31925.348	5.5	3.9	1.112	20.024	3.632	0.213	0.660583	4.284956	0.072878
35	1	6	0	9	4	21.989	31932.895	57.5	40.6	11.635	20.028	3.633	0.213	0.660739	4.283944	0.072833
36	1	6	5	7	8	22.019	31975.746	0.1	0.1	0.006	20.055	3.638	0.213	0.661626	4.278203	0.072578
37	1	11	1	1	8	22.026	31986.488	2.7	2.4	0.329	20.062	3.639	0.213	0.661848	4.276766	0.072515
38	1	8	6	3	8	22.042	32010.225	1.3	0.7	0.328	20.076	3.642	0.213	0.662339	4.273595	0.072374
39	1	1	5	9	8	22.044	32012.555	9.2	4.8	2.275	20.078	3.642	0.213	0.662387	4.273283	0.072361
40	1	10	4	1	8	22.059	32034.457	2.7	1.2	0.649	20.092	3.644	0.213	0.662841	4.270362	0.072232
41	1	3	2	10	8	22.068	32047.691	8.5	3.2	1.952	20.100	3.646	0.213	0.663114	4.268599	0.072154
42	1	2	6	8	8	22.072	32053.389	0.3	0.1	0.071	20.103	3.646	0.213	0.663232	4.267840	0.072121
43	1	10	2	4	8	22.079	32064.598	3.4	1.2	0.763	20.110	3.648	0.213	0.663464	4.266348	0.072055
44	1	5	8	3	8	22.086	32073.988	6.8	2.6	1.578	20.116	3.649	0.213	0.663658	4.265099	0.072000
45	1	8	2	7	8	22.097	32090.604	2.2	1.0	0.554	20.127	3.651	0.213	0.664002	4.262890	0.071903
46	1	4	7	6	8	22.116	32118.342	0.3	0.2	0.063	20.144	3.654	0.213	0.664576	4.259209	0.071742
47	1	7	5	6	8	22.117	32119.502	1.2	0.9	0.236	20.145	3.654	0.213	0.664600	4.259055	0.071735
48	1	0	5	9	4	22.133	32143.209	58.7	38.4	12.969	20.159	3.657	0.213	0.665091	4.255914	0.071598
49	1	1	9	3	8	22.141	32155.104	9.3	6.3	2.017	20.167	3.658	0.213	0.665337	4.254340	0.071529
50	1	10	3	3	8	22.144	32158.607	1.8	1.2	0.375	20.169	3.658	0.213	0.665409	4.253876	0.071509
51	1	11	0	1	4	22.149	32166.160	0.2	0.1	0.043	20.174	3.659	0.213	0.665566	4.252877	0.071466
52	1	10	4	0	4	22.156	32176.564	0.5	0.4	0.106	20.180	3.660	0.213	0.665781	4.251502	0.071406
53	1	1	3	10	8	22.169	32195.033	11.1	9.1	1.619	20.192	3.663	0.213	0.666163	4.249063	0.071300
54	1	1	7	7	8	22.197	32236.580	1.6	1.7	0.110	20.217	3.667	0.213	0.667023	4.243587	0.071063
55	1	3	9	1	8	22.203	32244.836	21.2	20.6	0.608	20.223	3.668	0.213	0.667194	4.242500	0.071016
56	1	9	1	6	8	22.208	32252.654	17.8	16.4	1.318	20.227	3.669	0.213	0.667355	4.241472	0.070971
57	1	4	8	4	8	22.212	32259.195	126.3	115.2	9.945	20.231	3.670	0.213	0.667491	4.240612	0.070934
58	1	0	9	3	4	22.232	32287.518	11.9	13.4	1.762	20.249	3.673	0.213	0.668077	4.236892	0.070774
59	1	6	7	4	8	22.270	32343.312	0.2	0.2	0.006	20.284	3.679	0.213	0.669231	4.229583	0.070460
60	1	7	7	2	8	22.272	32345.797	9.9	9.6	0.461	20.285	3.680	0.213	0.669283	4.229259	0.070446

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
61	1	0	7	7	4	22.288	32370.008	2.1	1.5	0.415	20.300	3.682	0.213	0.669784	4.226095	0.070311	
62	1	9	3	5	8	22.293	32376.967	15.0	10.0	3.262	20.305	3.683	0.213	0.669928	4.225187	0.070272	
63	1	9	4	4	8	22.306	32395.295	10.0	6.3	2.275	20.316	3.685	0.213	0.670307	4.222796	0.070170	
64	1	9	0	6	4	22.334	32436.873	5.7	4.0	1.181	20.342	3.690	0.213	0.671167	4.217383	0.069940	
65	1	1	6	8	8	22.344	32451.764	14.6	10.4	2.962	20.351	3.692	0.213	0.671475	4.215448	0.069858	
66	1	4	5	8	8	22.356	32469.236	1.4	0.9	0.288	20.362	3.694	0.213	0.671837	4.213180	0.069761	
67	1	7	1	8	8	22.357	32470.438	7.8	5.3	1.680	20.363	3.694	0.213	0.671862	4.213024	0.069755	
68	1	2	9	2	8	22.363	32478.984	5.3	3.4	1.208	20.368	3.695	0.213	0.672038	4.211915	0.069708	
69	1	9	5	2	8	22.365	32481.791	1.2	0.8	0.282	20.370	3.695	0.213	0.672097	4.211551	0.069693	
70	1	5	7	5	8	22.384	32510.143	0.2	0.1	0.045	20.388	3.698	0.213	0.672683	4.207879	0.069538	
71	1	2	8	5	8	22.419	32560.508	34.9	33.1	1.776	20.419	3.704	0.213	0.673725	4.201369	0.069264	
72	1	0	6	8	4	22.437	32587.893	26.3	20.3	4.543	20.436	3.707	0.213	0.674292	4.197839	0.069116	
73	1	3	4	9	8	22.443	32596.729	0.2	0.1	0.037	20.442	3.708	0.213	0.674475	4.196701	0.069068	
74	1	3	1	10	8	22.445	32599.184	21.7	15.9	4.173	20.443	3.709	0.213	0.674526	4.196385	0.069055	
75	1	10	1	4	8	22.457	32616.977	15.3	11.1	2.955	20.454	3.711	0.213	0.674894	4.194096	0.068959	
76	1	4	6	7	8	22.463	32625.377	2.6	1.8	0.512	20.459	3.712	0.213	0.675068	4.193016	0.068914	
77	1	8	1	7	8	22.476	32644.354	55.8	36.0	12.486	20.471	3.714	0.213	0.675460	4.190578	0.068813	
78	1	7	0	8	4	22.486	32658.438	18.0	11.1	4.146	20.480	3.715	0.213	0.675752	4.188771	0.068737	
79	1	5	2	9	8	22.491	32666.109	38.7	24.6	8.771	20.485	3.716	0.213	0.675910	4.187788	0.068696	
80	1	2	2	10	8	22.527	32719.682	1.2	1.1	0.034	20.518	3.722	0.213	0.677019	4.180931	0.068412	
81	1	8	6	2	8	22.540	32738.605	65.9	52.6	10.364	20.530	3.724	0.213	0.677410	4.178514	0.068312	
82	1	6	3	8	8	22.544	32744.490	1.8	1.5	0.302	20.534	3.725	0.213	0.677532	4.177763	0.068281	
83	1	3	0	10	4	22.575	32789.441	24.5	17.9	4.752	20.562	3.730	0.213	0.678462	4.172036	0.068045	
84	1	7	7	1	8	22.576	32790.793	6.6	4.7	1.298	20.562	3.730	0.213	0.678490	4.171864	0.068038	
85	1	5	8	2	8	22.587	32806.828	14.4	9.9	3.069	20.572	3.732	0.213	0.678822	4.169825	0.067955	
86	1	10	0	4	4	22.588	32807.543	1.5	1.0	0.314	20.573	3.732	0.213	0.678837	4.169734	0.067951	
87	1	8	0	7	4	22.607	32835.406	0.8	0.6	0.166	20.590	3.735	0.213	0.679413	4.166196	0.067806	
88	1	1	9	2	8	22.646	32893.648	13.5	10.4	2.417	20.626	3.742	0.213	0.680618	4.158819	0.067505	
89	1	10	3	2	8	22.649	32897.398	0.1	0.1	0.026	20.629	3.742	0.213	0.680696	4.158345	0.067485	
90	1	2	9	1	8	22.671	32929.574	0.0	0.0	0.003	20.649	3.746	0.213	0.681362	4.154282	0.067320	
91	1	9	5	1	8	22.673	32932.500	12.0	8.0	2.590	20.651	3.746	0.213	0.681422	4.153912	0.067305	
92	1	5	4	8	8	22.676	32936.898	13.8	8.9	3.090	20.653	3.747	0.213	0.681513	4.153358	0.067283	
93	1	4	3	9	8	22.694	32963.051	32.1	16.4	7.850	20.670	3.750	0.213	0.682055	4.150063	0.067149	
94	1	1	8	5	8	22.704	32978.340	0.7	0.3	0.179	20.679	3.752	0.213	0.682371	4.148139	0.067072	
95	1	7	6	4	8	22.731	33017.344	0.0	0.0	0.012	20.703	3.756	0.213	0.683178	4.143239	0.066874	
96	1	8	5	4	8	22.744	33035.746	0.6	0.0	0.155	20.715	3.758	0.213	0.683559	4.140930	0.066781	
97	1	3	7	6	8	22.772	33077.727	6.5	3.0	1.627	20.741	3.763	0.213	0.684427	4.135675	0.066570	
98	1	8	3	6	8	22.774	33079.844	0.4	0.2	0.100	20.742	3.763	0.213	0.684471	4.135410	0.066560	
99	1	2	9	0	4	22.777	33083.992	0.1	0.1	0.033	20.745	3.764	0.213	0.684557	4.134892	0.066539	
100	1	10	2	3	8	22.790	33104.020	17.0	7.6	4.147	20.757	3.766	0.213	0.684971	4.132390	0.066439	
101	1	1	2	10	8	22.817	33143.754	2.4	0.7	0.565	20.782	3.770	0.213	0.685794	4.127436	0.066241	
102	1	8	6	1	8	22.856	33200.242	2.6	0.6	0.517	20.817	3.777	0.213	0.686962	4.120414	0.065963	
103	1	7	3	7	8	22.862	33209.066	0.0	0.0	0.000	20.823	3.778	0.213	0.687145	4.119318	0.065919	
104	1	3	8	4	8	22.878	33231.645	22.9	13.9	5.366	20.837	3.780	0.213	0.687612	4.116519	0.065809	
105	1	5	1	9	8	22.891	33250.738	6.8	4.5	1.498	20.849	3.783	0.213	0.688007	4.114156	0.065716	
106	1	5	8	1	8	22.905	33271.398	4.9	3.4	1.057	20.862	3.785	0.213	0.688435	4.111601	0.065615	
107	1	0	2	10	4	22.917	33288.820	17.6	12.1	3.689	20.872	3.787	0.213	0.688795	4.109450	0.065530	
108	1	2	4	9	8	22.927	33304.629	0.7	0.5	0.140	20.882	3.789	0.213	0.689122	4.107499	0.065454	
109	1	2	1	10	8	22.929	33307.250	22.6	16.7	4.285	20.884	3.789	0.213	0.689176	4.107176	0.065441	
110	1	4	8	3	8	22.937	33318.293	0.0	0.0	0.006	20.891	3.790	0.213	0.689405	4.105814	0.065388	
111	1	9	2	5	8	22.953	33342.355	29.6	23.5	4.762	20.906	3.793	0.213	0.689903	4.102851	0.065272	

112	1	5	6	6	8	22.959	33350.355	0.0	0.0	0.004	20.911	3.794	0.213	0.690068	4.101867	0.065233
113	1	8	6	0	4	22.964	33358.520	19.7	15.7	3.161	20.916	3.795	0.213	0.690237	4.100863	0.065194
114	1	1	9	1	8	22.967	33361.965	3.8	3.0	0.611	20.918	3.795	0.213	0.690309	4.100440	0.065178
115	1	10	3	1	8	22.969	33365.883	5.7	4.6	0.899	20.920	3.796	0.213	0.690390	4.099958	0.065159
116	1	6	7	3	8	23.000	33410.996	0.9	0.8	0.156	20.948	3.801	0.213	0.691323	4.094422	0.064943
117	1	8	4	5	8	23.003	33415.301	0.3	0.2	0.043	20.951	3.801	0.213	0.691412	4.093894	0.064923
118	1	5	0	9	4	23.029	33452.699	3.3	2.9	0.367	20.974	3.806	0.213	0.692186	4.089318	0.064745
119	1	3	5	8	8	23.035	33461.398	0.1	0.1	0.008	20.980	3.807	0.213	0.692366	4.088255	0.064704
120	1	9	4	3	8	23.039	33468.305	14.4	12.1	1.873	20.984	3.807	0.213	0.692509	4.087411	0.064672

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
121	1	6	6	5	8	23.053	33488.293	73.4	56.4	12.772	20.997	3.810	0.213	0.692923	4.084971	0.064577	
122	1	5	5	7	8	23.062	33501.980	2.9	2.3	0.458	21.005	3.811	0.213	0.693206	4.083302	0.064513	
123	1	0	9	1	4	23.068	33509.926	5.0	4.2	0.681	21.010	3.812	0.213	0.693370	4.082334	0.064476	
124	1	2	0	10	4	23.068	33510.250	1.7	1.4	0.224	21.010	3.812	0.213	0.693377	4.082295	0.064474	
125	1	10	3	0	4	23.079	33526.547	9.6	8.8	0.793	21.020	3.814	0.213	0.693714	4.080310	0.064398	
126	1	3	6	7	8	23.151	33632.367	3.9	0.0	0.628	21.086	3.826	0.213	0.695904	4.067472	0.063907	
127	1	6	4	7	8	23.204	33709.035	0.0	0.0	0.000	21.134	3.835	0.213	0.697490	4.058221	0.063556	
128	1	10	1	3	8	23.207	33712.922	2.3	0.0	0.389	21.136	3.835	0.213	0.697571	4.057754	0.063538	
129	1	6	2	8	8	23.228	33744.156	0.0	0.0	0.000	21.156	3.839	0.213	0.698217	4.053997	0.063396	
130	1	1	4	9	8	23.233	33752.172	12.4	7.0	2.996	21.161	3.840	0.213	0.698383	4.053035	0.063360	
131	1	1	1	10	8	23.235	33754.891	0.4	0.2	0.102	21.162	3.840	0.213	0.698439	4.052708	0.063347	
132	1	9	3	4	8	23.248	33774.195	26.1	17.3	5.736	21.174	3.842	0.213	0.698838	4.050392	0.063260	
133	1	4	7	5	8	23.272	33807.996	5.4	4.5	0.786	21.195	3.846	0.213	0.699538	4.046342	0.063108	
134	1	7	5	5	8	23.272	33809.355	1.0	0.8	0.137	21.196	3.846	0.213	0.699566	4.046180	0.063102	
135	1	2	7	6	8	23.278	33818.152	8.7	7.5	1.097	21.202	3.847	0.213	0.699748	4.045127	0.063063	
136	1	7	4	6	8	23.319	33877.590	1.7	0.9	0.501	21.239	3.854	0.213	0.700978	4.038030	0.062797	
137	1	10	2	2	8	23.342	33911.570	0.4	0.2	0.091	21.260	3.858	0.213	0.701681	4.033984	0.062647	
138	1	10	0	3	4	23.350	33923.480	16.6	11.6	3.464	21.267	3.859	0.213	0.701927	4.032568	0.062594	
139	1	5	7	4	8	23.352	33925.449	3.4	2.4	0.694	21.268	3.859	0.213	0.701968	4.032334	0.062586	
140	1	9	1	5	8	23.379	33964.750	27.1	18.4	5.770	21.293	3.864	0.213	0.702781	4.027668	0.062413	
141	1	1	0	10	4	23.380	33966.246	2.1	1.4	0.458	21.294	3.864	0.213	0.702812	4.027490	0.062406	
142	1	6	5	6	8	23.385	33973.672	7.9	5.3	1.731	21.298	3.865	0.213	0.702966	4.026610	0.062374	
143	1	2	8	4	8	23.391	33982.691	0.6	0.4	0.121	21.304	3.866	0.213	0.703152	4.025541	0.062334	
144	1	4	2	9	8	23.391	33983.500	2.6	1.8	0.564	21.305	3.866	0.213	0.703169	4.025445	0.062331	
145	1	3	3	9	8	23.405	34002.648	4.5	3.4	0.867	21.316	3.868	0.213	0.703565	4.023179	0.062247	
146	1	8	2	6	8	23.479	34111.523	28.4	25.4	2.666	21.384	3.881	0.213	0.705818	4.010337	0.061776	
147	1	0	0	10	2	23.486	34122.430	2.9	2.7	0.217	21.391	3.882	0.213	0.706044	4.009056	0.061729	
148	1	4	8	2	8	23.500	34142.027	2.0	1.9	0.049	21.403	3.884	0.213	0.706449	4.006754	0.061645	
149	1	7	6	3	8	23.509	34155.574	15.5	14.3	1.166	21.412	3.886	0.213	0.706730	4.005165	0.061588	
150	1	8	5	3	8	23.523	34175.949	27.7	22.9	3.926	21.424	3.888	0.213	0.707151	4.002777	0.061501	
151	1	9	0	5	4	23.526	34180.098	34.4	28.4	4.850	21.427	3.888	0.213	0.707237	4.002292	0.061483	
152	1	2	5	8	8	23.559	34228.496	10.3	9.4	0.787	21.457	3.894	0.213	0.708238	3.996633	0.061278	
153	1	6	7	2	8	23.568	34241.793	48.7	42.8	5.095	21.465	3.895	0.213	0.708514	3.995080	0.061222	
154	1	7	2	7	8	23.576	34253.270	1.6	1.4	0.133	21.472	3.897	0.213	0.708751	3.993742	0.061174	
155	1	1	7	6	8	23.599	34287.008	2.7	2.6	0.100	21.493	3.901	0.213	0.709449	3.989812	0.061033	
156	1	4	4	8	8	23.600	34288.707	8.6	8.4	0.333	21.494	3.901	0.213	0.709484	3.989614	0.061025	
157	1	9	4	2	8	23.610	34303.496	6.5	6.5	0.272	21.504	3.902	0.213	0.709790	3.987895	0.060964	
158	1	5	3	8	8	23.669	34389.297	1.1	1.0	0.071	21.557	3.912	0.213	0.711566	3.977945	0.060608	
159	1	6	1	8	8	23.669	34389.773	38.4	35.6	2.611	21.557	3.912	0.213	0.711576	3.977890	0.060606	
160	1	3	8	3	8	23.671	34392.977	9.6	8.7	0.856	21.559	3.913	0.213	0.711642	3.977519	0.060593	
161	1	2	6	7	8	23.684	34411.562	108.6	92.2	13.665	21.571	3.915	0.213	0.712026	3.975371	0.060516	
162	1	10	2	1	8	23.693	34425.426	39.3	35.8	3.147	21.579	3.916	0.213	0.712313	3.973770	0.060459	
163	1	1	8	4	8	23.716	34458.527	6.4	8.5	2.690	21.600	3.920	0.213	0.712998	3.969953	0.060324	
164	1	10	1	2	8	23.790	34567.027	58.5	49.3	7.680	21.667	3.932	0.213	0.715243	3.957491	0.059885	
165	1	10	2	0	4	23.814	34601.973	4.3	4.1	0.196	21.689	3.936	0.213	0.715966	3.953495	0.059745	
166	1	6	0	8	4	23.822	34613.355	2.8	2.8	0.113	21.696	3.938	0.213	0.716202	3.952195	0.059699	
167	1	0	8	4	4	23.827	34621.633	7.1	7.5	0.515	21.701	3.939	0.213	0.716373	3.951250	0.059666	
168	1	4	1	9	8	23.842	34643.223	2.2	2.5	0.436	21.715	3.941	0.213	0.716820	3.948787	0.059580	
169	1	4	8	1	8	23.858	34666.590	1.0	1.1	0.228	21.729	3.944	0.213	0.717303	3.946126	0.059488	
170	1	1	5	8	8	23.891	34714.875	36.7	28.7	6.176	21.759	3.949	0.213	0.718302	3.940637	0.059297	
171	1	4	6	6	8	23.919	34755.930	15.3	10.7	3.146	21.785	3.954	0.213	0.719152	3.935982	0.059136	
172	1	6	7	1	8	23.930	34771.043	0.4	0.3	0.094	21.794	3.956	0.213	0.719465	3.934272	0.059077	
173	1	8	1	6	8	23.935	34778.875	3.1	2.0	0.709	21.799	3.957	0.213	0.719627	3.933385	0.059047	
174	1	10	0	2	4	23.945	34794.109	6.2	4.2	1.335	21.809	3.958	0.213	0.719942	3.931663	0.058988	
175	1	2	3	9	8	23.955	34808.488	0.1	0.0	0.010	21.818	3.960	0.213	0.720239	3.930040	0.058932	
176	1	9	4	1	8	23.974	34835.656	37.3	31.5	4.852	21.834	3.963	0.213	0.720802	3.926974	0.058827	
177	1	4	8	0	4	23.981	34846.895	14.5	13.1	1.215	21.841	3.964	0.213	0.721034	3.925708	0.058783	
178	1	4	0	9	4	23.998	34871.816	0.0	0.0	0.001	21.857	3.967	0.213	0.721550	3.922902	0.058687	
179	1	9	2	4	8	24.000	34874.426	16.8	18.1	1.367	21.859	3.967	0.213	0.721604	3.922609	0.058677	
180	1	1	6	7	8	24.022	34905.902	6.7	7.3	0.540	21.878	3.971	0.213	0.722255	3.919072	0.058557	

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
181	1	4	5	7	8	24.037	34927.648	154.7	131.7	19.167	21.892	3.973	0.213	0.722705	3.916631	0.058473	
182	1	7	1	7	8	24.038	34929.145	7.7	6.5	0.976	21.893	3.974	0.213	0.722736	3.916464	0.058468	
183	1	3	7	5	8	24.040	34932.398	37.8	31.8	4.884	21.895	3.974	0.213	0.722803	3.916099	0.058455	
184	1	8	3	5	8	24.041	34934.898	34.5	29.1	4.421	21.896	3.974	0.213	0.722855	3.915819	0.058446	
185	1	6	7	0	4	24.054	34952.988	42.8	39.7	2.849	21.907	3.976	0.213	0.723229	3.913792	0.058377	
186	1	8	4	4	8	24.057	34957.922	31.7	30.4	1.241	21.910	3.977	0.213	0.723331	3.913239	0.058358	
187	1	9	3	3	8	24.083	34995.477	4.3	4.8	0.486	21.934	3.981	0.213	0.724108	3.909040	0.058216	
188	1	8	0	6	4	24.093	35010.188	12.7	13.2	0.600	21.943	3.983	0.213	0.724413	3.907398	0.058161	

189	1	6	6	4	8	24.114	35041.520	6.0	5.0	0.814	21.962	3.986	0.213	0.725061	3.903904	0.058043
190	1	7	6	2	8	24.116	35044.672	12.5	10.2	1.880	21.964	3.987	0.213	0.725126	3.903553	0.058031
191	1	8	5	2	8	24.131	35066.684	5.3	3.7	1.110	21.978	3.989	0.213	0.725582	3.901103	0.057949
192	1	10	1	1	8	24.162	35111.746	0.4	0.2	0.100	22.006	3.994	0.213	0.726514	3.896096	0.057781
193	1	3	2	9	8	24.172	35126.105	3.6	1.5	0.912	22.015	3.996	0.213	0.726811	3.894503	0.057727
194	1	7	0	7	4	24.198	35163.484	5.9	4.1	1.213	22.038	4.000	0.213	0.727585	3.890363	0.057589
195	1	5	7	3	8	24.198	35163.816	9.0	6.4	1.868	22.038	4.000	0.213	0.727592	3.890326	0.057588
196	1	2	8	3	8	24.241	35227.578	54.3	55.9	1.799	22.078	4.008	0.213	0.728911	3.883285	0.057354
197	1	5	6	5	8	24.259	35253.965	0.5	0.5	0.014	22.094	4.011	0.213	0.729457	3.880378	0.057258
198	1	6	3	7	8	24.271	35270.969	5.5	5.3	0.307	22.105	4.012	0.213	0.729809	3.878508	0.057196
199	1	10	1	0	4	24.290	35299.121	6.5	5.4	0.869	22.122	4.016	0.213	0.730391	3.875414	0.057094
200	1	3	8	2	8	24.292	35301.246	7.5	6.1	1.084	22.124	4.016	0.213	0.730435	3.875181	0.057086
201	1	1	3	9	8	24.305	35320.383	58.5	41.0	12.010	22.136	4.018	0.213	0.730831	3.873081	0.057017
202	1	10	0	1	4	24.325	35349.809	10.1	7.4	1.948	22.154	4.021	0.213	0.731440	3.869858	0.056911
203	1	4	7	4	8	24.365	35408.305	0.4	0.2	0.109	22.190	4.028	0.213	0.732650	3.863465	0.056702
204	1	7	5	4	8	24.366	35409.867	1.8	0.6	0.489	22.191	4.028	0.213	0.732683	3.863294	0.056696
205	1	3	4	8	8	24.402	35463.453	3.2	0.8	0.726	22.225	4.034	0.213	0.733792	3.857456	0.056506
206	1	7	3	6	8	24.403	35464.188	0.4	0.1	0.090	22.225	4.034	0.213	0.733807	3.857377	0.056504
207	1	0	3	9	4	24.425	35496.102	1.3	0.5	0.335	22.245	4.038	0.213	0.734467	3.853908	0.056391
208	1	5	4	7	8	24.435	35511.777	5.1	2.5	1.318	22.255	4.040	0.213	0.734791	3.852207	0.056336
209	1	10	0	0	2	24.455	35541.039	0.4	0.3	0.093	22.273	4.043	0.213	0.735397	3.849035	0.056234
210	1	5	2	8	8	24.463	35552.848	10.2	7.4	2.062	22.280	4.045	0.213	0.735641	3.847757	0.056193
211	1	9	1	4	8	24.488	35588.516	15.8	12.2	2.737	22.302	4.049	0.213	0.736379	3.843901	0.056068
212	1	7	6	1	8	24.504	35612.656	2.9	2.4	0.413	22.317	4.051	0.213	0.736879	3.841295	0.055985
213	1	8	5	1	8	24.520	35635.758	15.8	12.4	2.756	22.332	4.054	0.213	0.737357	3.838805	0.055905
214	1	1	8	3	8	24.604	35758.477	10.6	6.4	2.574	22.408	4.068	0.213	0.739896	3.825631	0.055485
215	1	2	7	5	8	24.638	35807.902	0.1	0.1	0.023	22.439	4.074	0.213	0.740919	3.820350	0.055318
216	1	5	5	6	8	24.647	35821.582	2.9	2.2	0.561	22.447	4.075	0.213	0.741202	3.818891	0.055272
217	1	8	5	0	4	24.654	35831.695	0.3	0.2	0.062	22.453	4.076	0.213	0.741411	3.817813	0.055238
218	1	9	0	4	4	24.657	35836.469	5.2	4.1	0.933	22.456	4.077	0.213	0.741510	3.817305	0.055222
219	1	3	1	9	8	24.670	35856.098	0.9	0.8	0.089	22.468	4.079	0.213	0.741916	3.815215	0.055157
220	1	7	4	5	8	24.686	35878.480	0.0	0.0	0.005	22.482	4.082	0.213	0.742379	3.812835	0.055082
221	1	3	8	1	8	24.688	35882.008	22.6	19.7	2.581	22.485	4.082	0.213	0.742452	3.812460	0.055070
222	1	4	3	8	8	24.725	35936.645	0.1	0.1	0.017	22.519	4.088	0.213	0.743583	3.806664	0.054889
223	1	9	3	2	8	24.737	35953.668	6.8	5.5	1.043	22.529	4.090	0.213	0.743935	3.804861	0.054832
224	1	3	6	6	8	24.756	35981.105	28.2	19.8	5.750	22.546	4.093	0.213	0.744503	3.801960	0.054742
225	1	6	5	5	8	24.764	35992.676	2.9	2.0	0.642	22.553	4.095	0.213	0.744742	3.800738	0.054704
226	1	2	2	9	8	24.780	36016.633	31.2	19.8	7.103	22.568	4.097	0.213	0.745238	3.798210	0.054626
227	1	6	4	6	8	24.820	36075.031	0.5	0.5	0.078	22.604	4.104	0.213	0.746446	3.792061	0.054435
228	1	3	0	9	4	24.844	36109.727	1.1	1.1	0.143	22.626	4.108	0.213	0.747164	3.788417	0.054323
229	1	5	7	2	8	24.862	36136.297	15.3	13.3	1.877	22.643	4.111	0.213	0.747714	3.785632	0.054237
230	1	8	2	5	8	24.876	36156.715	0.8	0.6	0.121	22.655	4.113	0.213	0.748136	3.783494	0.054172
231	1	3	5	7	8	24.886	36171.727	5.7	4.6	0.915	22.665	4.115	0.213	0.748447	3.781924	0.054124
232	1	2	8	2	8	24.909	36205.504	0.0	0.0	0.005	22.685	4.119	0.213	0.749146	3.778396	0.054016
233	1	9	2	3	8	24.921	36223.895	26.8	20.8	4.626	22.697	4.121	0.213	0.749526	3.776478	0.053957
234	1	5	1	8	8	24.980	36310.352	19.1	15.6	2.973	22.751	4.131	0.213	0.751315	3.767486	0.053684
235	1	8	4	3	8	24.985	36317.492	0.0	0.0	0.000	22.755	4.132	0.213	0.751463	3.766745	0.053662
236	1	1	7	5	8	25.018	36365.895	0.5	0.4	0.142	22.785	4.137	0.213	0.752464	3.761731	0.053511
237	1	2	4	8	8	25.028	36380.562	1.2	0.6	0.365	22.794	4.139	0.213	0.752768	3.760215	0.053465
238	1	6	6	3	8	25.049	36411.254	1.8	0.9	0.652	22.813	4.142	0.213	0.753403	3.757045	0.053370
239	1	6	2	7	8	25.130	36529.680	23.9	20.7	2.859	22.887	4.156	0.213	0.755853	3.744865	0.053006
240	1	0	7	5	4	25.149	36557.766	3.8	3.1	0.559	22.904	4.159	0.213	0.756435	3.741988	0.052920

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
241	1	9	3	1	8	25.156	36567.797	15.7	12.2	2.681	22.910	4.160	0.213	0.756642	3.740962	0.052890	
242	1	5	0	8	4	25.160	36573.816	19.8	15.0	3.538	22.914	4.161	0.213	0.756767	3.740346	0.052872	
243	1	1	2	9	8	25.168	36584.590	34.8	26.7	6.100	22.921	4.162	0.213	0.756990	3.739244	0.052839	
244	1	3	7	4	8	25.251	36706.406	23.5	17.5	4.379	22.996	4.176	0.213	0.759510	3.726835	0.052474	
245	1	8	3	4	8	25.253	36709.301	9.2	6.8	1.722	22.998	4.176	0.213	0.759570	3.726542	0.052465	
246	1	7	2	6	8	25.277	36744.465	8.9	7.2	1.371	23.020	4.180	0.213	0.760298	3.722975	0.052361	
247	1	5	7	1	8	25.287	36759.992	3.1	2.8	0.300	23.030	4.182	0.213	0.760619	3.721402	0.052315	
248	1	1	8	2	8	25.303	36782.594	19.2	20.6	1.565	23.044	4.184	0.213	0.761087	3.719116	0.052248	
249	1	2	1	9	8	25.318	36804.832	0.8	1.0	0.142	23.058	4.187	0.213	0.761547	3.716869	0.052183	
250	1	4	7	3	8	25.330	36823.270	9.4	10.3	0.904	23.069	4.189	0.213	0.761928	3.715008	0.052129	
251	1	7	5	3	8	25.332	36825.023	35.2	38.3	3.347	23.070	4.189	0.213	0.761964	3.714831	0.052124	
252	1	2	8	1	8	25.337	36832.855	103.2	114.4	12.194	23.075	4.190	0.213	0.762127	3.714041	0.052101	
253	1	4	6	5	8	25.401	36926.828	0.0	0.0	0.003	23.133	4.201	0.213	0.764071	3.704589	0.051828	
254	1	2	6	6	8	25.410	36940.062	1.8	2.4	0.809	23.141	4.202	0.213	0.764345	3.703262	0.051790	
255	1	8	1	5	8	25.420	36954.355	7.0	8.3	1.584	23.150	4.204	0.213	0.764641	3.701829	0.051749	
256	1	1	4	8	8	25.428	36966.199	12.3	13.7	1.519	23.158	4.205	0.213	0.764886	3.700643	0.051714	
257	1	0	8	2	4	25.438	36981.176	88.4	96.6	8.876	23.167	4.207	0.213	0.765195	3.699145	0.051672	
258	1	9	1	3	8	25.469	37026.082	2.7	3.6	1.073	23.195	4.212	0.213	0.766125	3.694659	0.051543	
259	1	2	8	0	4	25.485	37049.332	0.3	0.3	0.095	23.209	4.215	0.213	0.766606	3.692340	0.051477	
260	1	2	0	9	4	25.505	37079.289	16.7	16.2	0.920	23.228	4.218	0.213	0.767226	3.689357	0.051392	
261	1	5	6	4	8	25.505	37080.031	0.2	0.2	0.012	23.228	4.218	0.213	0.767241	3.689283	0.051390	
262	1	2	5	7	8	25.551	37146.430	0.3	0.2	0.033	23.270	4.226	0.213	0.768615	3.682688	0.051203	
263	1	0	4	8	4	25.565	37167.789	10.1	6.6	2.333	23.283	4.228	0.213	0.769057	3.680572	0.051143	
264	1	4	4	7	8	25.603	37223.426	1.8	1.1	0.423	23.317	4.235	0.213	0.770208	3.675071	0.050989	
265	1	8	0	5	4	25.609	37232.199	4.0	2.8	0.827	23.323	4.236	0.213	0.770390	3.674205	0.050964	
266	1	4	2	8	8	25.635	37270.734	71.7	55.8	12.130	23.347	4.240	0.213	0.771187	3.670406	0.050858	
267	1	9	2	2	8	25.648	37289.727	10.7	9.1	1.331	23.358	4.242	0.213	0.771580	3.668537	0.050805	
268	1	3	3	8	8	25.653	37296.000	10.8	9.6	1.047	23.362	4.243	0.213	0.771710	3.667919	0.050788	

269	1	9	0	3	4	25.659	37305.562	6.6	6.4	0.291	23.368	4.244	0.213	0.771908	3.666979	0.050762
270	1	5	3	7	8	25.691	37352.223	0.6	0.7	0.150	23.397	4.249	0.213	0.772873	3.662399	0.050634
271	1	6	1	7	8	25.691	37352.824	0.3	0.3	0.074	23.398	4.249	0.213	0.772886	3.662339	0.050633
272	1	8	4	2	8	25.718	37391.859	29.1	23.1	4.711	23.422	4.254	0.213	0.773693	3.658516	0.050527
273	1	1	1	9	8	25.732	37411.543	29.9	22.6	5.443	23.434	4.256	0.213	0.774100	3.656592	0.050473
274	1	1	8	1	8	25.752	37440.977	7.7	6.5	1.027	23.452	4.259	0.213	0.774709	3.653717	0.050394
275	1	6	6	2	8	25.788	37494.215	0.0	0.0	0.004	23.485	4.265	0.213	0.775811	3.648529	0.050251
276	1	1	6	6	8	25.828	37553.602	2.1	0.9	0.628	23.522	4.272	0.213	0.777040	3.642759	0.050093
277	1	4	5	6	8	25.847	37580.688	0.5	0.3	0.093	23.539	4.275	0.213	0.777600	3.640134	0.050021
278	1	7	1	6	8	25.848	37582.551	0.8	0.6	0.148	23.540	4.275	0.213	0.777639	3.639953	0.050016
279	1	0	1	9	4	25.874	37620.543	61.2	45.6	11.420	23.564	4.280	0.213	0.778425	3.636277	0.049916
280	1	6	0	7	4	25.887	37639.828	25.6	20.3	4.116	23.576	4.282	0.213	0.778824	3.634414	0.049865
281	1	1	0	9	4	25.928	37699.906	1.6	1.9	0.303	23.613	4.289	0.213	0.780067	3.628622	0.049708
282	1	2	7	4	8	25.946	37726.207	99.5	98.8	1.218	23.629	4.292	0.213	0.780611	3.626093	0.049640
283	1	0	6	6	4	25.972	37765.008	14.4	15.6	1.314	23.653	4.296	0.213	0.781414	3.622367	0.049540
284	1	1	5	7	8	25.976	37770.480	18.4	20.2	2.076	23.657	4.297	0.213	0.781527	3.621842	0.049525
285	1	7	3	5	8	25.982	37779.648	4.2	4.8	0.686	23.662	4.298	0.213	0.781717	3.620964	0.049502
286	1	7	4	4	8	26.002	37808.773	0.5	0.7	0.236	23.680	4.301	0.213	0.782320	3.618174	0.049427
287	1	7	0	6	4	26.047	37874.922	0.1	0.1	0.008	23.721	4.309	0.213	0.783688	3.611855	0.049258
288	1	0	8	0	2	26.052	37881.781	8.2	8.5	0.541	23.726	4.309	0.213	0.783830	3.611201	0.049241
289	1	6	5	4	8	26.093	37942.480	113.2	103.6	8.560	23.763	4.316	0.213	0.785086	3.605424	0.049087
290	1	4	7	2	8	26.095	37944.562	0.1	0.1	0.008	23.765	4.317	0.213	0.785129	3.605226	0.049082
291	1	7	5	2	8	26.096	37946.480	14.4	13.1	1.129	23.766	4.317	0.213	0.785169	3.605044	0.049077
292	1	9	2	1	8	26.116	37976.234	49.1	47.3	1.736	23.784	4.320	0.213	0.785785	3.602219	0.049002
293	1	0	5	7	4	26.123	37985.594	25.2	23.9	1.172	23.790	4.321	0.213	0.785978	3.601332	0.048979
294	1	6	3	6	8	26.139	38009.332	303.5	282.0	19.642	23.805	4.324	0.213	0.786470	3.599083	0.048919
295	1	8	4	1	8	26.190	38084.129	0.2	0.3	0.165	23.851	4.333	0.213	0.788017	3.592014	0.048733
296	1	8	2	4	8	26.225	38134.801	147.1	131.8	13.409	23.883	4.338	0.213	0.789066	3.587241	0.048608
297	1	4	1	8	8	26.232	38146.227	1.0	0.9	0.075	23.890	4.340	0.213	0.789302	3.586167	0.048580
298	1	9	1	2	8	26.246	38166.586	3.8	4.0	0.235	23.902	4.342	0.213	0.789723	3.584254	0.048530
299	1	6	6	1	8	26.264	38192.293	18.0	21.6	4.209	23.918	4.345	0.213	0.790255	3.581841	0.048467
300	1	5	5	5	8	26.278	38212.602	4.6	6.0	1.679	23.931	4.347	0.213	0.790676	3.579937	0.048418

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
301	1	3	7	3	8	26.330	38289.953	20.3	19.4	0.830	23.979	4.356	0.213	0.792276	3.572706	0.048231	
302	1	8	3	3	8	26.332	38293.238	59.4	56.4	2.845	23.981	4.356	0.213	0.792344	3.572399	0.048223	
303	1	5	4	6	8	26.345	38311.195	0.6	0.6	0.011	23.992	4.358	0.213	0.792716	3.570724	0.048180	
304	1	8	4	0	4	26.353	38323.570	3.9	4.2	0.324	24.000	4.360	0.213	0.792972	3.569571	0.048150	
305	1	2	3	8	8	26.383	38367.199	97.4	86.5	9.477	24.027	4.365	0.213	0.793874	3.565512	0.048046	
306	1	1	7	4	8	26.392	38380.457	2.2	1.9	0.205	24.035	4.366	0.213	0.794149	3.564281	0.048014	
307	1	3	6	5	8	26.410	38406.426	69.3	64.5	4.409	24.051	4.369	0.213	0.794686	3.561871	0.047952	
308	1	6	6	0	4	26.428	38433.793	3.8	3.8	0.072	24.068	4.372	0.213	0.795252	3.559335	0.047888	
309	1	4	0	8	4	26.441	38452.055	7.2	7.2	0.210	24.079	4.374	0.213	0.795630	3.557644	0.047844	
310	1	9	0	2	4	26.455	38472.914	4.0	4.0	0.161	24.092	4.377	0.213	0.796062	3.555715	0.047795	
311	1	6	4	5	8	26.487	38520.715	34.4	25.2	6.656	24.122	4.382	0.213	0.797051	3.551303	0.047683	
312	1	4	7	1	8	26.588	38668.590	32.1	29.8	2.207	24.214	4.399	0.213	0.800111	3.537722	0.047341	
313	1	7	5	1	8	26.590	38670.617	9.5	8.8	0.694	24.215	4.399	0.213	0.800153	3.537536	0.047336	
314	1	5	6	3	8	26.620	38714.625	31.7	26.3	4.463	24.242	4.404	0.213	0.801063	3.533516	0.047236	
315	1	3	4	7	8	26.637	38740.453	15.5	12.3	2.495	24.258	4.407	0.213	0.801598	3.531160	0.047177	
316	1	3	2	8	8	26.673	38793.793	16.3	10.4	3.744	24.291	4.413	0.213	0.802701	3.526304	0.047056	
317	1	5	2	7	8	26.717	38857.074	0.9	1.2	0.331	24.330	4.420	0.213	0.804011	3.520562	0.046914	
318	1	9	1	1	8	26.748	38903.645	22.4	25.7	3.815	24.359	4.426	0.213	0.804974	3.516347	0.046810	
319	1	4	7	0	4	26.759	38919.297	0.9	1.2	0.426	24.369	4.428	0.213	0.805298	3.514933	0.046775	
320	1	4	6	4	8	26.842	39041.629	6.0	9.7	5.708	24.445	4.441	0.213	0.807829	3.503919	0.046506	
321	1	1	3	8	8	26.852	39055.984	9.2	12.6	4.620	24.454	4.443	0.213	0.808126	3.502632	0.046475	
322	1	8	1	4	8	26.864	39074.164	0.1	0.1	0.035	24.465	4.445	0.213	0.808503	3.501002	0.046435	
323	1	3	5	6	8	26.912	39143.684	32.8	31.4	1.685	24.508	4.453	0.213	0.809941	3.494784	0.046284	
324	1	9	0	1	4	26.969	39228.219	33.3	27.5	4.855	24.560	4.463	0.213	0.811690	3.487253	0.046103	
325	1	7	2	5	8	27.045	39338.957	0.3	0.1	0.157	24.629	4.475	0.213	0.813981	3.477437	0.045869	
326	1	4	3	7	8	27.059	39359.719	1.0	0.1	0.464	24.642	4.478	0.213	0.814411	3.475602	0.045825	
327	1	8	0	4	4	27.088	39403.059	0.5	0.0	0.295	24.669	4.483	0.213	0.815308	3.471779	0.045734	
328	1	2	7	3	8	27.122	39451.828	0.8	0.2	0.451	24.699	4.488	0.213	0.816317	3.467488	0.045633	
329	1	7	4	3	8	27.186	39546.277	23.3	21.0	2.099	24.757	4.499	0.213	0.818271	3.459206	0.045438	
330	1	3	7	2	8	27.192	39555.379	11.1	9.6	1.262	24.763	4.500	0.213	0.818460	3.458410	0.045419	
331	1	8	3	2	8	27.195	39559.008	3.2	2.8	0.382	24.765	4.500	0.213	0.818535	3.458093	0.045412	
332	1	2	6	5	8	27.208	39579.262	32.0	27.5	3.848	24.778	4.503	0.213	0.818954	3.456323	0.045371	
333	1	6	2	6	8	27.221	39598.465	4.7	4.2	0.476	24.790	4.505	0.213	0.819351	3.454647	0.045331	
334	1	6	5	3	8	27.290	39699.348	1.3	0.0	0.568	24.852	4.516	0.214	0.821439	3.445868	0.045127	
335	1	3	1	8	8	27.348	39783.992	0.7	0.5	0.495	24.904	4.526	0.214	0.823190	3.438537	0.044958	
336	1	5	1	7	8	27.394	39852.246	2.1	4.6	5.055	24.947	4.534	0.214	0.824602	3.432648	0.044823	
337	1	8	2	3	8	27.440	39919.801	3.4	4.4	1.194	24.989	4.541	0.214	0.826000	3.426839	0.044690	
338	1	2	4	7	8	27.457	39945.133	67.7	53.9	10.801	25.004	4.544	0.214	0.826524	3.424666	0.044641	
339	1	2	2	8	8	27.497	40003.613	3.0	2.9	0.173	25.040	4.551	0.214	0.827734	3.419659	0.044527	
340	1	5	6	2	8	27.511	40024.094	22.9	22.2	0.911	25.053	4.553	0.214	0.828158	3.417909	0.044488	
341	1	7	3	4	8	27.531	40053.684	11.8	12.8	1.196	25.071	4.557	0.214	0.828770	3.415384	0.044431	
342	1	3	0	8	4	27.584	40131.297	0.1	0.2	0.059	25.120	4.565	0.214	0.830376	3.408779	0.044282	
343	1	5	0	7	4	27.632	40201.355	15.4	14.3	1.125	25.163	4.573	0.214	0.831826	3.402838	0.044149	
344	1	1	7	3	8	27.632	40201.859	23.0	21.3	1.658	25.163	4.573	0.214	0.831836	3.402796	0.044148	
345	1	1	6	5	8	27.724	40336.730	2.7	3.6	1.204	25.247	4.589	0.214	0.834627	3.391418	0.043896	
346	1	4	5	5	8	27.747	40370.305	65.8	65.9	0.476	25.267	4.593	0.214	0.835322	3.388598	0.043834	
347	1	7	1	5	8	27.748	40372.617	0.1	0.1	0.001	25.269	4.593	0.214	0.835369	3.388404	0.043830	
348	1	3	7	1	8	27.752	40377.637	52.5	51.6	0.909	25.272	4.593	0.214	0.835473	3.387982	0.043820	

349	1	8	3	1	8	27.754	40381.496	121.2	119.6	1.703	25.274	4.594	0.214	0.835553	3.387659	0.043813
350	1	2	5	6	8	27.758	40387.598	51.2	51.4	0.361	25.278	4.595	0.214	0.835679	3.387147	0.043802
351	1	0	7	3	4	27.809	40461.543	30.1	40.8	14.119	25.324	4.603	0.214	0.837209	3.380957	0.043666
352	1	4	4	6	8	27.826	40486.613	0.6	0.9	0.505	25.339	4.606	0.214	0.837728	3.378863	0.043620
353	1	5	5	4	8	27.883	40570.730	0.3	0.8	1.003	25.391	4.615	0.214	0.839469	3.371858	0.043468
354	1	5	3	6	8	27.939	40652.492	4.5	4.6	0.090	25.442	4.625	0.214	0.841160	3.365076	0.043321
355	1	6	1	6	8	27.939	40653.277	76.0	76.7	1.358	25.443	4.625	0.214	0.841177	3.365011	0.043320
356	1	8	3	0	4	27.949	40667.277	7.9	8.1	0.249	25.451	4.626	0.214	0.841466	3.363853	0.043295
357	1	1	4	7	8	27.987	40724.223	3.4	5.1	2.569	25.486	4.633	0.214	0.842645	3.359149	0.043194
358	1	7	0	5	4	27.995	40735.707	1.1	1.7	1.047	25.494	4.634	0.214	0.842882	3.358202	0.043173
359	1	1	2	8	8	28.030	40786.191	6.1	8.5	3.293	25.525	4.640	0.214	0.843927	3.354045	0.043084
360	1	3	6	4	8	28.041	40802.922	22.0	28.4	8.102	25.535	4.642	0.214	0.844273	3.352670	0.043055

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
361	1	2	7	2	8	28.066	40840.270	12.9	17.8	6.557	25.558	4.646	0.214	0.845046	3.349604	0.042990	
362	1	5	6	1	8	28.091	40876.566	7.2	10.0	3.743	25.581	4.650	0.214	0.845797	3.346630	0.042927	
363	1	6	3	5	8	28.109	40903.078	2.2	2.9	0.975	25.597	4.653	0.214	0.846345	3.344460	0.042881	
364	1	6	4	4	8	28.134	40940.047	3.7	3.9	0.246	25.620	4.657	0.214	0.847110	3.341440	0.042817	
365	1	7	4	2	8	28.138	40945.078	29.5	31.0	1.687	25.623	4.658	0.214	0.847215	3.341030	0.042808	
366	1	4	6	3	8	28.150	40963.629	4.2	4.7	0.470	25.635	4.660	0.214	0.847598	3.339517	0.042776	
367	1	8	1	3	8	28.176	41001.211	7.7	9.9	2.738	25.658	4.664	0.214	0.848376	3.336456	0.042712	
368	1	6	0	6	4	28.191	41024.066	0.6	0.8	0.385	25.672	4.667	0.214	0.848849	3.334597	0.042673	
369	1	0	2	8	4	28.214	41057.441	0.2	0.4	0.345	25.693	4.671	0.214	0.849540	3.331886	0.042616	
370	1	2	1	8	8	28.238	41092.031	0.0	0.0	0.005	25.714	4.675	0.214	0.850255	3.329082	0.042557	
371	1	6	5	2	8	28.253	41115.047	3.8	6.6	4.777	25.728	4.677	0.214	0.850731	3.327218	0.042518	
372	1	4	2	7	8	28.265	41132.477	0.5	0.7	0.286	25.739	4.679	0.214	0.851092	3.325808	0.042489	
373	1	3	3	7	8	28.288	41166.441	63.2	59.0	4.152	25.760	4.683	0.214	0.851795	3.323064	0.042432	
374	1	1	5	6	8	28.306	41193.387	0.2	0.2	0.033	25.777	4.686	0.214	0.852352	3.320890	0.042387	
375	1	5	4	5	8	28.365	41279.980	0.2	0.6	1.196	25.830	4.696	0.214	0.854144	3.313924	0.042243	
376	1	8	2	2	8	28.420	41360.082	0.0	0.0	0.021	25.880	4.705	0.214	0.855802	3.307506	0.042111	
377	1	8	0	3	4	28.434	41381.691	3.8	3.2	1.181	25.893	4.708	0.214	0.856249	3.305779	0.042076	
378	1	2	0	8	4	28.498	41475.070	0.3	1.0	2.495	25.951	4.718	0.214	0.858181	3.298336	0.041924	
379	1	1	7	2	8	28.633	41674.027	35.2	46.5	14.629	26.074	4.741	0.214	0.862298	3.282589	0.041607	
380	1	2	7	1	8	28.683	41747.168	0.0	0.1	0.082	26.119	4.749	0.214	0.863811	3.276838	0.041492	
381	1	7	4	1	8	28.759	41859.133	6.4	7.4	1.372	26.188	4.762	0.214	0.866128	3.268074	0.041318	
382	1	7	2	4	8	28.805	41926.441	4.5	4.9	0.449	26.230	4.770	0.214	0.867520	3.262827	0.041215	
383	1	1	1	8	8	28.815	41941.629	53.1	53.0	1.209	26.239	4.771	0.214	0.867835	3.261646	0.041191	
384	1	6	5	1	8	28.882	42040.793	3.7	5.2	2.107	26.301	4.783	0.214	0.869887	3.253952	0.041041	
385	1	2	7	0	4	28.898	42063.164	0.4	0.8	0.620	26.314	4.785	0.214	0.870349	3.252221	0.041007	
386	1	7	3	3	8	28.948	42137.273	28.3	35.8	9.362	26.360	4.794	0.214	0.871883	3.246502	0.040896	
387	1	2	6	4	8	29.003	42217.723	0.0	0.0	0.006	26.410	4.803	0.214	0.873547	3.240315	0.040777	
388	1	8	2	1	8	29.060	42302.863	2.4	2.5	0.158	26.463	4.812	0.214	0.875309	3.233794	0.040651	
389	1	4	1	7	8	29.071	42318.465	176.1	163.6	11.349	26.472	4.814	0.214	0.875632	3.232601	0.040629	
390	1	3	5	5	8	29.077	42326.914	136.6	126.5	9.143	26.477	4.815	0.214	0.875807	3.231956	0.040616	
391	1	1	0	8	4	29.092	42349.160	27.0	26.6	0.386	26.491	4.818	0.214	0.876267	3.230258	0.040584	
392	1	6	5	0	4	29.102	42363.555	350.9	362.7	12.021	26.500	4.819	0.214	0.876565	3.229161	0.040563	
393	1	3	4	6	8	29.168	42461.027	32.6	43.2	13.734	26.560	4.830	0.214	0.878582	3.221748	0.040422	
394	1	4	6	2	8	29.211	42524.395	219.5	268.3	58.236	26.599	4.838	0.214	0.879893	3.216947	0.040331	
395	1	8	1	2	8	29.239	42566.449	3.2	4.4	1.624	26.625	4.842	0.214	0.880763	3.213769	0.040272	
396	1	5	2	6	8	29.272	42614.715	5.0	6.1	1.253	26.655	4.848	0.214	0.881762	3.210129	0.040203	
397	1	2	3	7	8	29.276	42620.770	3.9	4.5	0.676	26.659	4.849	0.214	0.881887	3.209673	0.040195	
398	1	8	2	0	4	29.284	42631.746	6.0	6.3	0.341	26.666	4.850	0.214	0.882114	3.208846	0.040179	
399	1	1	7	1	8	29.289	42638.945	10.3	10.4	0.157	26.670	4.851	0.214	0.882263	3.208304	0.040169	
400	1	0	0	8	2	29.298	42653.039	58.1	56.1	2.046	26.679	4.852	0.214	0.882555	3.207245	0.040149	
401	1	4	0	7	4	29.355	42737.188	5.1	4.9	0.204	26.731	4.862	0.214	0.884296	3.200930	0.040032	
402	1	5	5	3	8	29.358	42740.527	31.7	30.6	1.439	26.733	4.862	0.214	0.884365	3.200679	0.040027	
403	1	6	2	5	8	29.468	42903.633	0.1	0.0	0.055	26.834	4.881	0.214	0.887740	3.188512	0.039803	
404	1	0	7	1	4	29.499	42949.152	14.1	15.4	1.451	26.862	4.886	0.214	0.888682	3.185132	0.039741	
405	1	8	0	2	4	29.529	42992.648	144.2	135.4	8.167	26.889	4.891	0.214	0.889582	3.181910	0.039682	
406	1	3	6	3	8	29.542	43012.262	10.0	10.0	0.160	26.901	4.893	0.214	0.889988	3.180459	0.039655	
407	1	1	6	4	8	29.629	43140.676	2.2	2.6	0.537	26.980	4.908	0.214	0.892645	3.170992	0.039484	
408	1	6	4	3	8	29.651	43172.980	26.6	24.7	1.830	27.000	4.911	0.214	0.893313	3.168619	0.039441	
409	1	4	5	4	8	29.657	43181.750	1.1	1.0	0.106	27.005	4.912	0.214	0.893495	3.167975	0.039430	
410	1	7	1	4	8	29.659	43184.578	6.7	5.9	0.700	27.007	4.913	0.214	0.893553	3.167768	0.039426	
411	1	3	2	7	8	29.675	43207.855	42.7	35.9	5.671	27.021	4.915	0.214	0.894035	3.166061	0.039395	
412	1	4	3	6	8	29.724	43280.375	3.4	2.2	0.860	27.066	4.924	0.214	0.895535	3.160757	0.039300	
413	1	0	6	4	4	29.848	43462.039	68.7	81.6	15.119	27.178	4.944	0.214	0.899294	3.147545	0.039065	
414	1	4	6	1	8	29.908	43551.074	1.3	1.3	0.213	27.233	4.954	0.214	0.901137	3.141110	0.038952	
415	1	1	3	7	8	29.921	43571.008	0.9	0.8	0.256	27.246	4.957	0.214	0.901549	3.139673	0.038927	
416	1	8	1	1	8	29.939	43596.254	0.2	0.1	0.093	27.261	4.960	0.214	0.902071	3.137855	0.038895	
417	1	7	0	4	4	29.961	43629.816	0.4	0.2	0.352	27.282	4.963	0.214	0.902766	3.135441	0.038853	
418	1	6	3	4	8	30.101	43835.637	22.9	23.9	1.177	27.409	4.987	0.214	0.907025	3.120719	0.038598	
419	1	7	3	2	8	30.105	43841.812	37.2	39.2	2.149	27.413	4.988	0.214	0.907152	3.120280	0.038590	
420	1	0	3	7	4	30.146	43902.164	42.1	50.4	9.664	27.450	4.994	0.214	0.908401	3.115991	0.038517	

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
421	1	4	6	0	4	30.152	43910.195	46.6	56.7	12.104	27.455	4.995	0.214	0.908567	3.115421	0.038507	
422	1	2	5	5	8	30.153	43912.590	2.4	2.9	0.651	27.456	4.996	0.214	0.908617	3.115251	0.038504	
423	1	5	1	6	8	30.170	43937.828	1.2	1.6	0.621	27.472	4.998	0.214	0.909139	3.113461	0.038474	
424	1	8	1	0	4	30.183	43956.496	0.1	0.2	0.097	27.484	5.001	0.214	0.909525	3.112139	0.038451	
425	1	4	4	5	8	30.240	44039.949	1.4	1.4	0.152	27.535	5.010	0.214	0.911252	3.106242	0.038351	

426	1	8	0	1	4	30.249	44054.480	7.1	6.3	1.054	27.544	5.012	0.214	0.911553	3.105217	0.038333
427	1	2	4	6	8	30.255	44062.402	1.8	1.6	0.294	27.549	5.013	0.214	0.911717	3.104659	0.038324
428	1	5	3	5	8	30.385	44253.688	0.0	0.0	0.001	27.667	5.034	0.214	0.915675	3.091239	0.038098
429	1	6	1	5	8	30.385	44254.703	1.8	1.5	0.642	27.667	5.034	0.214	0.915696	3.091168	0.038097
430	1	5	4	4	8	30.416	44300.520	2.4	2.6	0.422	27.696	5.040	0.214	0.916644	3.087971	0.038044
431	1	7	2	3	8	30.439	44334.480	29.8	28.6	1.557	27.717	5.044	0.214	0.917346	3.085606	0.038004
432	1	5	0	6	4	30.489	44407.023	0.3	0.4	0.028	27.761	5.052	0.214	0.918847	3.080565	0.037921
433	1	8	0	0	2	30.502	44426.301	51.1	51.3	1.173	27.773	5.054	0.214	0.919246	3.079228	0.037898
434	1	5	5	2	8	30.567	44522.492	22.2	25.3	3.565	27.833	5.065	0.214	0.921237	3.072576	0.037789
435	1	3	1	7	8	30.612	44588.812	28.1	27.7	0.961	27.874	5.073	0.214	0.922609	3.068006	0.037714
436	1	2	6	3	8	30.673	44679.316	47.8	59.7	14.647	27.929	5.083	0.214	0.924481	3.061791	0.037613
437	1	6	0	5	4	30.710	44734.238	170.5	153.4	15.113	27.963	5.089	0.214	0.925618	3.058032	0.037552
438	1	3	6	2	8	30.775	44829.898	8.3	9.6	1.554	28.022	5.100	0.214	0.927597	3.051507	0.037446
439	1	2	2	7	8	30.822	44898.668	8.5	7.2	1.241	28.065	5.108	0.214	0.929020	3.046833	0.037372
440	1	1	5	5	8	30.859	44954.039	2.2	1.9	0.211	28.099	5.114	0.214	0.930166	3.043080	0.037312
441	1	7	3	1	8	30.870	44969.488	26.2	23.0	2.895	28.108	5.116	0.214	0.930486	3.042034	0.037295
442	1	6	4	2	8	30.899	45011.949	2.6	2.2	0.384	28.134	5.121	0.214	0.931364	3.039165	0.037249
443	1	3	0	7	4	30.944	45079.410	4.0	1.2	1.106	28.176	5.128	0.214	0.932760	3.034616	0.037177
444	1	1	4	6	8	30.968	45114.805	0.2	0.0	0.072	28.198	5.132	0.214	0.933492	3.032236	0.037140
445	1	0	5	5	4	31.106	45318.008	177.7	184.8	7.560	28.323	5.155	0.214	0.937697	3.018639	0.036926
446	1	0	4	6	4	31.218	45482.723	120.7	136.4	17.443	28.424	5.174	0.214	0.941105	3.007707	0.036757
447	1	3	5	4	8	31.299	45602.078	30.5	35.0	5.124	28.498	5.188	0.214	0.943575	2.999835	0.036636
448	1	4	2	6	8	31.346	45671.762	77.1	76.6	1.201	28.541	5.196	0.214	0.945017	2.995258	0.036567
449	1	5	5	1	8	31.368	45704.953	5.3	5.3	0.097	28.561	5.199	0.214	0.945703	2.993083	0.036534
450	1	3	3	6	8	31.377	45718.277	13.6	13.9	0.392	28.570	5.201	0.214	0.945979	2.992211	0.036520
451	1	1	6	3	8	31.418	45777.656	57.9	64.4	7.109	28.606	5.208	0.214	0.947208	2.988329	0.036462
452	1	4	5	3	8	31.451	45826.750	106.3	114.4	8.636	28.636	5.213	0.214	0.948224	2.985128	0.036413
453	1	7	1	3	8	31.453	45830.129	69.7	75.3	5.961	28.638	5.214	0.214	0.948294	2.984908	0.036410
454	1	1	2	7	8	31.577	46013.676	0.0	0.0	0.019	28.751	5.235	0.214	0.952091	2.973001	0.036232
455	1	3	6	1	8	31.594	46037.699	72.2	95.4	30.004	28.766	5.237	0.214	0.952588	2.971450	0.036209
456	1	6	4	1	8	31.727	46234.934	3.9	5.5	2.426	28.888	5.260	0.214	0.956670	2.958774	0.036022
457	1	6	2	4	8	31.789	46325.684	0.4	0.4	0.020	28.944	5.270	0.214	0.958547	2.952978	0.035937
458	1	7	2	2	8	31.794	46332.969	59.6	60.1	1.251	28.948	5.271	0.214	0.958698	2.952514	0.035930
459	1	7	0	3	4	31.814	46363.359	28.6	28.3	0.817	28.967	5.274	0.214	0.959327	2.950578	0.035902
460	1	2	1	7	8	31.876	46454.180	1.6	0.6	0.464	29.023	5.285	0.214	0.961206	2.944810	0.035819
461	1	6	3	3	8	31.981	46610.562	11.0	9.0	1.625	29.119	5.303	0.214	0.964442	2.934930	0.035676
462	1	3	4	5	8	31.985	46616.328	118.8	96.7	17.671	29.122	5.303	0.214	0.964561	2.934567	0.035671
463	1	6	4	0	4	32.018	46665.293	2.4	2.2	0.184	29.153	5.309	0.214	0.965574	2.931488	0.035627
464	1	2	6	2	8	32.060	46726.996	1.5	0.8	0.448	29.191	5.316	0.214	0.966851	2.927617	0.035572
465	1	5	2	5	8	32.123	46819.926	5.7	1.4	1.378	29.248	5.326	0.214	0.968774	2.921806	0.035490
466	1	2	0	7	4	32.252	47009.754	262.4	211.9	39.941	29.364	5.348	0.214	0.972702	2.910007	0.035324
467	1	5	4	3	8	32.360	47170.602	52.5	46.5	5.470	29.463	5.366	0.214	0.976030	2.900084	0.035187
468	1	4	1	6	8	32.456	47312.020	0.0	0.0	0.013	29.550	5.382	0.214	0.978956	2.891416	0.035068
469	1	2	5	4	8	32.653	47603.383	0.1	0.2	0.108	29.730	5.415	0.214	0.984985	2.873719	0.034828
470	1	7	2	1	8	32.698	47670.094	12.3	16.3	5.217	29.771	5.423	0.214	0.986365	2.869697	0.034774
471	1	1	1	7	8	32.713	47692.422	26.6	30.7	4.581	29.784	5.426	0.214	0.986827	2.868353	0.034756
472	1	4	3	5	8	32.723	47707.059	125.5	138.6	14.180	29.793	5.427	0.214	0.987130	2.867473	0.034744
473	1	2	3	6	8	32.743	47735.605	153.7	169.5	16.983	29.811	5.430	0.214	0.987721	2.865759	0.034721
474	1	4	4	4	8	32.763	47765.754	153.0	177.4	27.671	29.829	5.434	0.214	0.988344	2.863950	0.034697
475	1	4	0	6	4	32.853	47899.340	60.6	55.8	4.494	29.911	5.449	0.214	0.991109	2.855963	0.034591
476	1	1	6	2	8	32.913	47987.781	34.9	39.8	5.457	29.966	5.459	0.214	0.992939	2.850699	0.034522
477	1	5	3	4	8	32.948	48038.805	23.7	23.5	0.329	29.997	5.465	0.214	0.993994	2.847671	0.034483
478	1	6	1	4	8	32.948	48040.102	107.4	106.2	1.525	29.998	5.465	0.214	0.994021	2.847594	0.034482
479	1	4	5	2	8	32.951	48044.340	4.0	3.9	0.049	30.001	5.466	0.214	0.994109	2.847343	0.034478
480	1	7	1	2	8	32.954	48048.234	41.5	41.4	0.382	30.003	5.466	0.214	0.994189	2.847113	0.034475

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
481	1	2	6	1	8	32.989	48099.547	21.7	26.0	4.979	30.035	5.472	0.214	0.995251	2.844075	0.034436	
482	1	0	1	7	4	33.008	48127.703	11.6	14.1	3.078	30.052	5.475	0.214	0.995834	2.842411	0.034414	
483	1	1	0	7	4	33.120	48294.203	17.9	17.6	1.488	30.154	5.494	0.214	0.999279	2.832612	0.034287	
484	1	0	6	2	4	33.213	48431.270	0.1	0.0	0.164	30.238	5.510	0.214	1.002115	2.824595	0.034185	
485	1	3	2	6	8	33.303	48564.828	27.3	25.1	2.293	30.320	5.525	0.214	1.004879	2.816827	0.034086	
486	1	2	6	0	4	33.316	48584.664	0.1	0.1	0.009	30.333	5.527	0.214	1.005289	2.815677	0.034071	
487	1	5	1	5	8	33.321	48591.941	6.0	5.4	0.586	30.337	5.528	0.214	1.005440	2.815255	0.034066	
488	1	6	0	4	4	33.364	48655.309	15.5	13.2	1.953	30.376	5.535	0.214	1.006751	2.811589	0.034020	
489	1	7	0	2	4	33.370	48663.754	21.0	18.5	2.319	30.381	5.536	0.214	1.006925	2.811101	0.034014	
490	1	3	5	3	8	33.429	48751.293	27.0	33.9	8.534	30.435	5.546	0.214	1.008737	2.806053	0.033950	
491	1	2	4	5	8	33.435	48760.602	0.2	0.2	0.064	30.441	5.547	0.214	1.008929	2.805517	0.033944	
492	1	1	5	4	8	33.555	48938.504	0.1	0.1	0.005	30.550	5.567	0.214	1.012610	2.795319	0.033817	
493	1	6	3	2	8	33.563	48949.848	452.7	457.7	5.562	30.557	5.569	0.214	1.012845	2.794671	0.033809	
494	1	1	3	6	8	33.652	49082.207	24.7	24.4	1.056	30.638	5.584	0.214	1.015584	2.787135	0.033716	
495	1	5	0	5	4	33.752	49228.879	2.6	1.1	1.033	30.728	5.600	0.214	1.018619	2.778831	0.033615	
496	1	1	6	1	8	33.920	49478.090	15.6	21.6	8.097	30.881	5.629	0.214	1.023775	2.764835	0.033446	
497	1	4	5	1	8	33.962	49540.086	72.1	91.4	23.979	30.919	5.636	0.214	1.025058	2.761374	0.033405	
498	1	7	1	1	8	33.964	49544.355	29.2	36.8	9.366	30.922	5.636	0.214	1.025146	2.761136	0.033402	
499	1	5	4	2	8	34.002	49599.719	62.6	69.9	7.994	30.956	5.643	0.214	1.026292	2.758054	0.033365	
500	1	6	2	3	8	34.028	49638.438	264.2	258.7	5.689	30.979	5.647	0.214	1.027093	2.755903	0.033340	
501	1	4	5	0	4	34.320	50070.594	0.1	2.1	34.246	31.244	5.696	0.214	1.036035	2.732117	0.033062	
502	1	1	4	5	8	34.406	50198.496	0.4	0.5	0.288	31.323	5.711	0.214	1.038682	2.725156	0.032982	
503	1	7	0	1	4	34.420	50220.016	5.3	4.7	1.490	31.336	5.713	0.214	1.039127	2.723988	0.032968	
504	1	0	6	0	2	34.615	50509.039	298.0	345.4	53.773	31.513	5.746	0.214	1.045107	2.708401	0.032792	
505	1	6	3	1	8	34.633	50534.621	9.4	10.7	1.437	31.529	5.749	0.214	1.045636	2.707030	0.032776	

506	1	3	1	6	8	34.644	50551.113	65.1	74.1	10.045	31.539	5.751	0.214	1.045978	2.706146	0.032766
507	1	4	2	5	8	34.926	50969.164	9.4	9.5	0.724	31.795	5.798	0.214	1.054628	2.683951	0.032520
508	1	2	2	6	8	34.949	51003.980	1.2	1.2	0.086	31.817	5.802	0.214	1.055348	2.682119	0.032500
509	1	3	3	5	8	34.969	51033.832	133.8	133.1	1.626	31.835	5.806	0.214	1.055966	2.680550	0.032483
510	1	6	3	0	4	35.012	51098.094	73.9	81.2	7.931	31.874	5.813	0.214	1.057296	2.677179	0.032446
511	1	3	4	4	8	35.018	51105.695	80.9	90.1	10.125	31.879	5.814	0.214	1.057453	2.676780	0.032442
512	1	2	5	3	8	35.095	51220.094	0.0	0.0	0.003	31.949	5.827	0.214	1.059820	2.670802	0.032377
513	1	5	4	1	8	35.115	51250.625	21.7	22.2	0.602	31.968	5.830	0.214	1.060452	2.669211	0.032360
514	1	3	0	6	4	35.128	51269.406	69.9	66.4	3.418	31.979	5.832	0.214	1.060840	2.668233	0.032350
515	1	5	2	4	8	35.199	51374.312	10.8	13.5	3.486	32.043	5.844	0.214	1.063011	2.662785	0.032291
516	1	4	4	3	8	35.231	51422.523	2.9	4.1	1.538	32.073	5.850	0.214	1.064008	2.660288	0.032265
517	1	3	5	2	8	35.248	51447.332	19.1	28.8	14.386	32.088	5.853	0.214	1.064522	2.659005	0.032251
518	1	5	3	3	8	35.461	51763.676	33.9	35.6	2.809	32.282	5.889	0.214	1.071067	2.642755	0.032080
519	1	6	1	3	8	35.462	51765.301	0.0	0.0	0.003	32.283	5.889	0.214	1.071101	2.642672	0.032079
520	1	6	2	2	8	35.952	52493.215	21.0	14.2	4.728	32.728	5.972	0.214	1.086163	2.606027	0.031704
521	1	6	0	3	4	35.982	52537.410	26.1	21.3	3.957	32.755	5.977	0.214	1.087077	2.603835	0.031682
522	1	4	3	4	8	35.993	52553.219	6.7	5.9	0.780	32.765	5.979	0.214	1.087404	2.603051	0.031674
523	1	1	2	6	8	36.062	52656.547	2.9	4.8	3.239	32.828	5.990	0.214	1.089542	2.597943	0.031623
524	1	1	5	3	8	36.222	52894.461	109.2	134.2	30.131	32.973	6.017	0.214	1.094465	2.586258	0.031508
525	1	0	2	6	4	36.457	53244.156	511.0	539.4	29.402	33.187	6.057	0.214	1.101701	2.569272	0.031344
526	1	4	1	5	8	36.481	53279.895	34.4	37.9	3.806	33.209	6.061	0.214	1.102440	2.567549	0.031327
527	1	3	5	1	8	36.493	53296.762	180.9	205.4	27.147	33.219	6.063	0.214	1.102789	2.566736	0.031319
528	1	2	1	6	8	36.508	53319.664	18.1	21.5	3.845	33.233	6.066	0.214	1.103263	2.565634	0.031309
529	1	0	5	3	4	36.623	53490.164	25.9	45.1	32.775	33.338	6.085	0.214	1.106791	2.557456	0.031231
530	1	5	1	4	8	36.793	53743.199	6.3	16.6	26.564	33.492	6.114	0.214	1.112027	2.545415	0.031118
531	1	2	3	5	8	36.890	53887.035	0.0	0.5	10.339	33.580	6.130	0.214	1.115003	2.538620	0.031055
532	1	2	4	4	8	36.946	53971.656	0.5	6.0	64.005	33.632	6.140	0.214	1.116754	2.534640	0.031018
533	1	4	0	5	4	37.048	54122.906	0.2	1.4	10.917	33.724	6.157	0.214	1.119883	2.527557	0.030953
534	1	2	0	6	4	37.076	54164.594	5.1	8.4	5.331	33.749	6.162	0.214	1.120746	2.525611	0.030935
535	1	2	5	2	8	37.217	54374.520	776.2	1019.9	313.276	33.878	6.186	0.214	1.125090	2.515861	0.030847
536	1	6	2	1	8	37.276	54462.164	201.3	235.3	38.914	33.931	6.196	0.214	1.126903	2.511812	0.030810
537	1	5	0	4	4	37.374	54608.754	0.1	0.1	0.023	34.020	6.212	0.214	1.129936	2.505069	0.030750
538	1	4	4	2	8	37.380	54616.883	165.3	203.2	45.596	34.025	6.213	0.214	1.130105	2.504697	0.030747
539	1	5	3	2	8	37.655	55026.164	97.0	100.8	4.069	34.275	6.260	0.214	1.138573	2.486067	0.030583
540	1	6	1	2	8	37.656	55028.117	29.3	30.3	1.076	34.276	6.260	0.214	1.138614	2.485979	0.030582

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
541	1	3	2	5	8	37.697	55088.555	175.9	168.9	6.821	34.313	6.267	0.214	1.139864	2.483251	0.030558	
542	1	6	2	0	4	37.751	55169.414	0.1	0.1	0.028	34.362	6.276	0.214	1.141537	2.479612	0.030527	
543	1	1	1	6	8	37.782	55216.363	1.7	2.6	1.385	34.391	6.282	0.214	1.142509	2.477503	0.030509	
544	1	3	4	3	8	38.082	55662.254	41.6	50.7	11.120	34.663	6.332	0.214	1.151735	2.457657	0.030340	
545	1	1	3	5	8	38.206	55847.188	11.2	18.6	12.050	34.776	6.353	0.214	1.155561	2.449519	0.030272	
546	1	1	4	4	8	38.269	55941.402	17.7	24.9	10.052	34.833	6.364	0.214	1.157511	2.445393	0.030238	
547	1	6	0	2	4	38.280	55958.344	0.9	1.2	0.389	34.843	6.366	0.214	1.157861	2.444653	0.030232	
548	1	5	2	3	8	38.315	56009.832	73.9	73.4	1.794	34.875	6.372	0.214	1.158927	2.442405	0.030213	
549	1	1	0	6	4	38.413	56156.332	9.3	11.0	2.299	34.964	6.388	0.214	1.161958	2.436034	0.030161	
550	1	1	5	2	8	38.570	56390.375	82.1	113.7	42.940	35.106	6.415	0.215	1.166801	2.425923	0.030079	
551	1	0	3	5	4	38.677	56549.691	3.5	6.0	4.219	35.203	6.433	0.215	1.170097	2.419089	0.030024	
552	1	2	5	1	8	38.692	56571.984	1.9	3.1	1.906	35.217	6.436	0.215	1.170558	2.418136	0.030016	
553	1	0	4	4	4	38.742	56647.516	28.2	36.0	9.884	35.263	6.444	0.215	1.172121	2.414912	0.029990	
554	1	4	4	1	8	38.875	56845.078	0.0	0.0	0.002	35.383	6.467	0.215	1.176209	2.406518	0.029924	
555	1	0	0	6	2	38.892	56870.719	12.4	18.4	8.708	35.399	6.470	0.215	1.176740	2.405434	0.029915	
556	1	4	2	4	8	38.988	57014.000	902.9	921.7	19.034	35.486	6.486	0.215	1.179704	2.399388	0.029868	
557	1	3	3	4	8	39.048	57104.555	167.7	187.9	22.277	35.541	6.496	0.215	1.181578	2.395583	0.029838	
558	1	5	3	1	8	39.184	57306.961	21.0	29.5	11.582	35.664	6.519	0.215	1.185766	2.387122	0.029772	
559	1	6	1	1	8	39.185	57309.172	1.8	2.6	1.037	35.665	6.520	0.215	1.185812	2.387030	0.029772	
560	1	2	5	0	4	39.223	57365.875	249.0	349.5	137.909	35.700	6.526	0.215	1.186985	2.384671	0.029754	
561	1	4	3	3	8	39.345	57547.590	295.5	318.5	24.451	35.810	6.547	0.215	1.190745	2.377141	0.029696	
562	1	4	4	0	4	39.414	57650.691	6.8	7.5	0.824	35.873	6.558	0.215	1.192878	2.372890	0.029664	
563	1	3	1	5	8	39.675	58040.375	393.4	371.6	20.311	36.110	6.603	0.215	1.200942	2.356958	0.029545	
564	1	6	1	0	4	39.738	58134.965	788.2	765.0	22.237	36.167	6.614	0.215	1.202899	2.353123	0.029516	
565	1	6	0	1	4	39.890	58362.207	117.8	110.1	7.362	36.305	6.639	0.215	1.207601	2.343961	0.029449	
566	1	2	2	5	8	40.135	58728.762	190.4	211.6	23.171	36.528	6.681	0.215	1.215185	2.329331	0.029343	
567	1	1	5	1	8	40.218	58852.848	27.0	28.6	2.051	36.603	6.695	0.215	1.217753	2.324420	0.029308	
568	1	5	1	3	8	40.397	59120.828	95.9	91.5	4.225	36.766	6.726	0.215	1.223298	2.313884	0.029234	
569	1	3	0	5	4	40.407	59135.020	211.7	193.5	16.398	36.775	6.727	0.215	1.223591	2.313329	0.029230	
570	1	6	0	0	2	40.474	59235.066	15.3	12.6	2.305	36.835	6.739	0.215	1.225662	2.309421	0.029203	
571	1	2	4	3	8	40.601	59425.363	2.1	16.6	109.187	36.951	6.760	0.215	1.229599	2.302026	0.029152	
572	1	0	5	1	4	40.769	59676.715	124.8	300.0	411.781	37.103	6.789	0.215	1.234800	2.292330	0.029085	
573	1	3	4	2	8	40.838	59781.047	38.7	89.1	113.677	37.166	6.801	0.215	1.236959	2.288329	0.029058	
574	1	5	2	2	8	41.126	60212.254	155.0	160.7	6.086	37.428	6.850	0.215	1.245881	2.271941	0.028948	
575	1	5	0	3	4	41.171	60278.988	103.1	98.0	5.077	37.468	6.857	0.215	1.247262	2.269426	0.028931	
576	1	4	1	4	8	41.188	60305.445	0.2	0.2	0.008	37.484	6.860	0.215	1.247809	2.268431	0.028925	
577	1	2	3	4	8	41.778	61190.086	1372.1	1497.2	133.404	38.020	6.961	0.215	1.266114	2.235636	0.028713	
578	1	1	2	5	8	41.847	61292.781	3.2	3.7	0.560	38.082	6.973	0.215	1.268239	2.231890	0.028689	
579	1	4	0	4	4	42.009	61536.102	0.0	0.0	0.001	38.229	7.000	0.215	1.273273	2.223065	0.028634	
580	1	1	4	3	8	42.375	62085.930	148.9	154.1	6.266	38.562	7.063	0.215	1.284650	2.203377	0.028513	
581	1	4	3	2	8	42.408	62135.223	6.5	6.5	0.265	38.592	7.069	0.215	1.285670	2.201629	0.028502	
582	1	2	1	5	8	42.548	62345.711	5.0	0.0	1.550	38.719	7.093	0.215	1.290025	2.194196	0.028458	
583	1	3	4	1	8	42.810	62739.332	230.8	293.0	77.240	38.957	7.137	0.215	1.298170	2.180430	0.028376	
584	1	3	2	4	8	42.961	62966.656	259.4	269.8	10.985	39.094	7.163	0.215	1.302874	2.172558	0.028330	
585	1	5	2	1	8	43.142	63238.328	59.9	66.1	7.109	39.258	7.194	0.215	1.308495	2.163225	0.028276	

586	1	4	2	3	8	43.357	63562.117	0.1	0.2	0.510	39.453	7.231	0.215	1.315195	2.152205	0.028214
587	1	3	3	3	8	43.441	63687.672	192.0	212.7	22.499	39.529	7.245	0.215	1.317793	2.147962	0.028190
588	1	2	0	5	4	43.455	63708.438	220.5	232.3	12.302	39.541	7.248	0.215	1.318222	2.147262	0.028186
589	1	1	3	4	8	43.719	64106.777	35.1	46.2	14.272	39.782	7.293	0.215	1.326465	2.133920	0.028112
590	1	5	1	2	8	43.734	64129.195	116.2	142.3	31.423	39.795	7.295	0.215	1.326928	2.133174	0.028108
591	1	2	4	2	8	43.993	64518.391	1.3	5.1	14.864	40.030	7.340	0.215	1.334981	2.120306	0.028038
592	1	1	1	5	8	44.604	65439.363	0.7	1.1	0.683	40.584	7.444	0.215	1.354038	2.090465	0.027880
593	1	4	3	1	8	44.629	65477.211	828.4	966.7	157.757	40.607	7.449	0.215	1.354821	2.089257	0.027874
594	1	5	0	2	4	44.720	65615.086	76.4	80.2	4.243	40.690	7.464	0.215	1.357674	2.084867	0.027851
595	1	0	1	5	4	45.358	66577.641	376.1	339.7	32.331	41.268	7.574	0.215	1.377590	2.054725	0.027700
596	1	4	3	0	4	45.450	66717.039	17.6	10.4	4.325	41.352	7.590	0.215	1.380475	2.050432	0.027679
597	1	1	0	5	4	45.651	67020.500	17.2	12.8	3.927	41.534	7.624	0.215	1.386754	2.041147	0.027634
598	1	3	1	4	8	45.961	67488.312	189.1	198.4	10.174	41.815	7.678	0.215	1.396434	2.026999	0.027567
599	1	5	1	1	8	46.182	67823.141	29.3	27.9	2.171	42.016	7.716	0.215	1.403362	2.016992	0.027520
600	1	1	4	2	8	46.276	67965.383	169.6	225.6	72.993	42.101	7.732	0.215	1.406305	2.012770	0.027500

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
601	1	4	1	3	8	46.446	68223.047	79.9	102.7	28.579	42.255	7.761	0.215	1.411636	2.005169	0.027465	
602	1	2	4	1	8	46.487	68284.055	77.5	109.7	44.588	42.292	7.768	0.215	1.412899	2.003377	0.027457	
603	1	2	2	4	8	46.680	68577.414	6.2	6.8	2.261	42.468	7.801	0.215	1.418969	1.994807	0.027418	
604	1	3	0	4	4	47.109	69226.711	73.1	113.2	60.636	42.856	7.875	0.216	1.432404	1.976097	0.027336	
605	1	0	4	2	4	47.120	69243.266	193.9	294.9	150.170	42.866	7.877	0.216	1.432746	1.975625	0.027334	
606	1	2	3	3	8	47.297	69511.859	14.4	12.3	2.176	43.027	7.908	0.216	1.438304	1.967991	0.027300	
607	1	5	0	1	4	47.347	69588.219	27.2	32.3	6.256	43.073	7.916	0.216	1.439884	1.965832	0.027291	
608	1	2	4	0	4	47.417	69693.789	0.1	0.2	0.126	43.136	7.928	0.216	1.442068	1.962854	0.027278	
609	1	4	2	2	8	47.563	69915.844	3.9	6.2	3.881	43.268	7.954	0.216	1.446663	1.956620	0.027252	
610	1	4	0	3	4	47.632	70020.375	25.4	22.8	2.580	43.331	7.966	0.216	1.448826	1.953699	0.027239	
611	1	3	3	2	8	47.674	70083.039	127.1	136.6	10.302	43.368	7.973	0.216	1.450122	1.951952	0.027232	
612	1	3	2	3	8	49.034	72150.062	161.7	178.2	18.144	44.601	8.208	0.216	1.492892	1.896031	0.027007	
613	1	1	4	1	8	49.205	72411.008	83.7	120.0	50.941	44.757	8.238	0.216	1.498291	1.889198	0.026980	
614	1	1	2	4	8	49.435	72761.125	99.2	169.1	116.433	44.965	8.277	0.216	1.505536	1.880107	0.026946	
615	1	1	3	3	8	50.169	73880.125	204.0	214.8	11.915	45.630	8.405	0.216	1.528690	1.851631	0.026841	
616	1	0	2	4	4	50.467	74335.578	35.5	39.8	5.220	45.901	8.457	0.216	1.538114	1.840286	0.026801	
617	1	2	1	4	8	50.602	74541.469	237.5	220.2	15.976	46.023	8.480	0.216	1.542374	1.835203	0.026783	
618	1	4	2	1	8	50.761	74783.719	10.1	8.4	1.838	46.167	8.508	0.216	1.547386	1.829258	0.026762	
619	1	3	3	1	8	50.895	74988.430	576.1	692.9	137.315	46.288	8.531	0.216	1.551622	1.824264	0.026745	
620	1	0	3	3	4	51.249	75530.016	942.4	1082.7	157.505	46.609	8.592	0.216	1.562828	1.811184	0.026701	
621	1	0	4	0	2	51.402	75763.562	739.6	872.4	153.139	46.747	8.619	0.216	1.567661	1.805600	0.026682	
622	1	4	1	2	8	51.732	76269.602	5.7	5.3	1.952	47.047	8.677	0.216	1.578131	1.793621	0.026642	
623	1	4	2	0	4	51.979	76647.141	133.6	169.3	44.410	47.270	8.720	0.216	1.585943	1.784786	0.026614	
624	1	2	0	4	4	52.146	76904.109	0.4	2.1	7.793	47.422	8.749	0.216	1.591260	1.778822	0.026595	
625	1	2	3	2	8	52.915	78083.258	24.9	47.0	41.203	48.118	8.883	0.216	1.615659	1.751960	0.026511	
626	1	4	0	2	4	53.385	78806.117	1801.1	1722.4	73.744	48.544	8.965	0.216	1.630616	1.735890	0.026463	
627	1	3	1	3	8	53.640	79196.930	248.6	283.1	38.522	48.774	9.010	0.217	1.638702	1.727324	0.026438	
628	1	1	1	4	8	54.166	80007.227	4.8	17.1	42.395	49.250	9.102	0.217	1.655468	1.709830	0.026387	
629	1	2	2	3	8	54.793	80973.227	781.7	816.5	35.995	49.818	9.212	0.217	1.675457	1.689431	0.026331	
630	1	3	2	2	8	55.380	81880.094	185.8	236.5	63.154	50.349	9.315	0.217	1.694221	1.670720	0.026280	
631	1	3	0	3	4	55.489	82048.133	52.4	65.7	16.586	50.448	9.334	0.217	1.697698	1.667298	0.026271	
632	1	4	1	1	8	55.923	82720.164	9.5	25.2	40.707	50.841	9.410	0.217	1.711603	1.653753	0.026236	
633	1	1	0	4	4	56.072	82950.141	7.3	17.9	25.403	50.975	9.437	0.217	1.716362	1.649168	0.026225	
634	1	1	3	2	8	57.030	84435.445	648.3	851.7	260.760	51.842	9.606	0.217	1.747095	1.620158	0.026153	
635	1	2	3	1	8	57.425	85048.789	5.7	6.0	1.312	52.199	9.675	0.217	1.759786	1.608474	0.026125	
636	1	4	1	0	4	57.563	85263.492	1.7	2.3	0.792	52.324	9.700	0.217	1.764228	1.604423	0.026116	
637	1	0	0	4	2	57.591	85306.078	778.5	739.6	36.460	52.349	9.705	0.217	1.765110	1.603622	0.026114	
638	1	4	0	1	4	58.027	85985.297	18.6	11.5	5.760	52.744	9.782	0.217	1.779164	1.590955	0.026084	
639	1	2	3	0	4	59.205	87820.391	352.9	491.4	188.204	53.808	9.991	0.217	1.817134	1.557710	0.026011	
640	1	1	2	3	8	59.400	88124.805	430.6	447.0	17.203	53.985	10.025	0.217	1.823433	1.552329	0.026000	
641	1	4	0	0	2	59.865	88852.602	656.8	643.5	13.963	54.405	10.108	0.218	1.838492	1.539614	0.025973	
642	1	3	2	1	8	60.613	90023.898	883.1	1037.3	176.857	55.081	10.241	0.218	1.862728	1.519582	0.025932	
643	1	2	1	3	8	61.454	91343.523	4.4	31.2	188.539	55.841	10.391	0.218	1.890033	1.497629	0.025890	
644	1	3	1	2	8	62.285	92651.367	239.3	310.0	89.452	56.591	10.540	0.218	1.917095	1.476489	0.025850	
645	1	1	3	1	8	62.794	93453.992	254.1	428.5	286.926	57.051	10.631	0.218	1.933702	1.463808	0.025828	
646	1	2	2	2	8	64.107	95531.508	0.0	0.0	0.013	58.236	10.868	0.218	1.976689	1.431975	0.025773	
647	1	2	0	3	4	64.276	95798.680	1032.7	999.5	32.015	58.388	10.898	0.218	1.982217	1.427981	0.025766	
648	1	0	3	1	4	64.946	96862.539	1440.6	1872.2	546.875	58.993	11.019	0.219	2.004230	1.412297	0.025741	
649	1	3	0	2	4	65.228	97310.617	71.2	134.8	117.391	59.247	11.070	0.219	2.013501	1.405794	0.025731	
650	1	1	1	3	8	68.166	102007.961	1189.0	1108.2	73.859	61.896	11.605	0.219	2.110696	1.341059	0.025636	
651	1	3	1	1	8	70.014	104986.430	2422.9	2464.6	42.249	63.560	11.943	0.220	2.172325	1.303013	0.025586	
652	1	0	1	3	4	70.940	106488.312	14.2	66.1	235.309	64.395	12.114	0.220	2.203402	1.284636	0.025563	
653	1	1	2	2	8	71.835	107943.312	1235.3	1426.7	216.054	65.200	12.280	0.220	2.233508	1.267320	0.025543	
654	1	1	0	3	4	72.072	108329.188	935.0	868.4	60.776	65.413	12.324	0.220	2.241492	1.262806	0.025538	
655	1	2	2	1	8	72.626	109233.766	4551.1	5227.0	756.328	65.911	12.427	0.220	2.260209	1.252348	0.025526	
656	1	3	0	1	4	74.262	111916.688	1196.9	1344.6	161.757	67.382	12.732	0.221	2.315723	1.222326	0.025494	
657	1	0	2	2	4	75.099	113295.031	4996.1	5275.3	287.385	68.134	12.889	0.221	2.344243	1.207456	0.025479	
658	1	2	1	2	8	75.542	114028.000	6455.2	6528.0	72.976	68.532	12.972	0.221	2.359409	1.199694	0.025471	

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 BRAGG R-Factors and weight fractions for Pattern #  1
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=> Phase:  1     VOSO4 Nuclear
=> Bragg R-factor:   11.4       Vol:  325.587( 2.991)  Fract(%):  100.00( 1.65)
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=> Rf-factor= 10.5 ATZ: 651.994 Brindley: 1.0000

Pattern# 2 Phase No: 1 Phase name: VOSO4 Nuclear

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
1	1	1	6	5	8	123.103	29078.863	0.0	0.0	0.000	120.385	5.072	0.055	0.835386	3.388336	0.043828	
2	1	4	5	5	8	123.214	29103.881	0.0	0.0	0.000	120.494	5.076	0.055	0.836105	3.385423	0.043764	
3	1	7	1	5	8	123.229	29107.342	0.0	0.0	0.000	120.509	5.077	0.055	0.836204	3.385020	0.043755	
4	1	3	7	1	8	123.232	29108.051	0.0	0.0	0.000	120.512	5.077	0.055	0.836225	3.384938	0.043753	
5	1	8	3	1	8	123.258	29113.818	0.0	0.0	0.000	120.537	5.078	0.055	0.836390	3.384267	0.043739	
6	1	2	5	6	8	123.268	29116.035	0.0	0.0	0.000	120.547	5.078	0.055	0.836454	3.384010	0.043733	
7	1	0	7	3	4	123.499	29168.291	0.0	0.0	0.000	120.773	5.087	0.055	0.837955	3.377947	0.043600	
8	1	4	4	6	8	123.587	29188.084	0.0	0.0	0.000	120.859	5.091	0.055	0.838524	3.375657	0.043550	
9	1	5	5	4	8	123.855	29248.600	0.0	0.0	0.000	121.121	5.101	0.055	0.840263	3.368672	0.043399	
10	1	5	3	6	8	124.119	29308.184	0.0	0.0	0.000	121.380	5.112	0.055	0.841974	3.361824	0.043251	
11	1	6	1	6	8	124.124	29309.361	0.0	0.0	0.000	121.385	5.112	0.055	0.842008	3.361688	0.043248	
12	1	8	3	0	4	124.171	29319.875	0.0	0.0	0.000	121.431	5.114	0.055	0.842310	3.360483	0.043222	
13	1	1	4	7	8	124.344	29358.979	0.0	0.0	0.000	121.600	5.120	0.055	0.843433	3.356007	0.043126	
14	1	7	0	5	4	124.389	29369.182	0.0	0.0	0.000	121.645	5.122	0.055	0.843727	3.354841	0.043101	
15	1	1	2	8	8	124.544	29404.139	0.1	0.1	0.001	121.796	5.128	0.055	0.844731	3.350853	0.043016	
16	1	3	6	4	8	124.593	29415.119	0.7	0.6	0.005	121.844	5.130	0.055	0.845046	3.349602	0.042990	
17	1	2	7	2	8	124.710	29441.383	0.9	0.7	0.015	121.958	5.135	0.055	0.845801	3.346614	0.042926	
18	1	5	6	1	8	124.831	29468.641	1.1	0.8	0.035	122.076	5.140	0.055	0.846584	3.343518	0.042861	
19	1	6	3	5	8	124.921	29489.141	0.5	0.4	0.027	122.165	5.143	0.055	0.847173	3.341194	0.042812	
20	1	6	4	4	8	125.038	29515.512	1.4	1.0	0.116	122.280	5.148	0.055	0.847930	3.338209	0.042749	
21	1	7	4	2	8	125.056	29519.492	11.6	8.7	1.051	122.297	5.148	0.055	0.848045	3.337759	0.042739	
22	1	4	6	3	8	125.108	29531.154	1.9	1.4	0.208	122.348	5.151	0.055	0.848380	3.336441	0.042711	
23	1	8	1	3	8	125.240	29560.984	4.7	3.4	0.684	122.478	5.156	0.055	0.849237	3.333074	0.042641	
24	1	6	0	6	4	125.310	29576.742	0.4	0.3	0.061	122.546	5.158	0.055	0.849689	3.331298	0.042604	
25	1	0	2	8	4	125.412	29599.660	0.2	0.1	0.026	122.646	5.162	0.055	0.850348	3.328719	0.042550	
26	1	2	1	8	8	125.524	29624.832	0.0	0.0	0.000	122.755	5.167	0.055	0.851071	3.325891	0.042491	
27	1	6	5	2	8	125.597	29641.309	3.0	2.4	0.447	122.827	5.170	0.055	0.851544	3.324042	0.042452	
28	1	4	2	7	8	125.654	29654.195	0.4	0.3	0.049	122.883	5.172	0.055	0.851915	3.322597	0.042422	
29	1	3	3	7	8	125.761	29678.283	50.3	47.0	3.136	122.987	5.176	0.055	0.852607	3.319901	0.042366	
30	1	1	5	6	8	125.843	29696.826	0.1	0.2	0.003	123.068	5.179	0.055	0.853139	3.317827	0.042323	
31	1	5	4	5	8	126.125	29760.287	0.1	0.2	0.037	123.344	5.190	0.055	0.854962	3.310753	0.042178	
32	1	8	2	2	8	126.389	29819.627	0.0	0.0	0.006	123.602	5.201	0.055	0.856667	3.304164	0.042043	
33	1	8	0	3	4	126.459	29835.377	3.1	4.0	1.281	123.670	5.204	0.055	0.857120	3.302420	0.042007	
34	1	2	0	8	4	126.750	29901.021	0.2	0.4	0.220	123.956	5.215	0.055	0.859006	3.295170	0.041860	
35	1	1	7	2	8	127.378	30042.268	28.1	36.1	10.056	124.571	5.240	0.055	0.863063	3.279677	0.041548	
36	1	2	7	1	8	127.613	30095.074	0.0	0.0	0.006	124.801	5.249	0.055	0.864580	3.273923	0.041434	
37	1	7	4	1	8	127.984	30178.514	5.1	4.8	0.331	125.164	5.263	0.055	0.866977	3.264871	0.041255	
38	1	7	2	4	8	128.203	30227.568	3.6	3.0	0.467	125.378	5.272	0.055	0.868387	3.259572	0.041151	
39	1	1	1	8	8	128.246	30237.258	42.5	35.3	5.900	125.420	5.274	0.055	0.868665	3.258528	0.041130	
40	1	6	5	1	8	128.564	30308.709	3.0	2.2	0.537	125.731	5.286	0.055	0.870718	3.250846	0.040980	
41	1	2	7	0	4	128.627	30322.838	0.3	0.3	0.063	125.793	5.289	0.055	0.871124	3.249331	0.040951	
42	1	7	3	3	8	128.879	30379.363	22.6	16.6	4.341	126.040	5.298	0.055	0.872747	3.243286	0.040834	
43	1	2	6	4	8	129.126	30434.826	0.0	0.0	0.001	126.281	5.308	0.055	0.874341	3.237375	0.040720	
44	1	8	2	1	8	129.414	30499.422	1.9	1.6	0.257	126.563	5.319	0.055	0.876197	3.230519	0.040589	
45	1	4	1	7	8	129.458	30509.375	140.8	119.1	18.009	126.607	5.321	0.055	0.876482	3.229465	0.040569	
46	1	3	5	5	8	129.479	30514.178	109.2	92.9	13.576	126.628	5.322	0.055	0.876620	3.228956	0.040559	
47	1	1	0	8	4	129.555	30531.104	21.6	18.8	2.427	126.701	5.325	0.055	0.877107	3.227166	0.040525	
48	1	6	5	0	4	129.601	30541.400	281.0	246.6	29.579	126.746	5.327	0.055	0.877402	3.226078	0.040504	
49	1	3	4	6	8	129.912	30611.266	26.1	24.3	1.612	127.051	5.339	0.055	0.879410	3.218715	0.040365	
50	1	4	6	2	8	130.113	30656.250	175.6	167.0	8.091	127.248	5.347	0.055	0.880702	3.213992	0.040276	
51	1	8	1	2	8	130.262	30689.621	2.5	2.4	0.133	127.394	5.353	0.055	0.881661	3.210497	0.040210	
52	1	5	2	6	8	130.411	30723.098	4.0	3.7	0.299	127.540	5.358	0.055	0.882622	3.206999	0.040145	
53	1	2	3	7	8	130.427	30726.592	3.1	2.8	0.242	127.555	5.359	0.055	0.882723	3.206634	0.040138	
54	1	8	2	0	4	130.471	30736.568	4.8	4.3	0.418	127.599	5.361	0.055	0.883009	3.205594	0.040119	
55	1	1	7	1	8	130.476	30737.770	8.3	7.4	0.728	127.604	5.361	0.055	0.883044	3.205468	0.040116	
56	1	0	0	8	2	130.532	30750.148	46.5	41.1	4.658	127.658	5.363	0.055	0.883399	3.204178	0.040092	
57	1	4	0	7	4	130.805	30811.307	4.0	3.2	0.627	127.925	5.374	0.055	0.885156	3.197818	0.039974	
58	1	5	5	3	8	130.811	30812.834	25.3	20.3	3.958	127.932	5.374	0.055	0.885200	3.197659	0.039971	
59	1	6	2	5	8	131.342	30931.740	0.1	0.1	0.021	128.451	5.395	0.055	0.888616	3.185367	0.039745	
60	1	0	7	1	4	131.474	30961.324	11.3	8.5	2.069	128.581	5.400	0.055	0.889466	3.182323	0.039689	

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
61	1	8	0	2	4	131.634	30996.990	115.3	85.9	21.488	128.737	5.406	0.055	0.890491	3.178662	0.039623	
62	1	3	6	3	8	131.682	31007.705	8.0	5.9	1.507	128.784	5.408	0.055	0.890799	3.177563	0.039603	
63	1	1	6	4	8	132.094	31100.018	1.8	1.2	0.386	129.188	5.424	0.055	0.893451	3.168131	0.039432	
64	1	6	4	3	8	132.207	31125.369	21.3	13.7	4.778	129.298	5.429	0.055	0.894179	3.165551	0.039386	
65	1	4	5	4	8	132.231	31130.629	0.9	0.6	0.197	129.322	5.429	0.055	0.894330	3.165016	0.039376	
66	1	7	1	4	8	132.250	31134.867	5.4	3.4	1.215	129.340	5.430	0.055	0.894452	3.164585	0.039369	
67	1	3	2	7	8	132.319	31150.236	34.2	21.6	7.804	129.407	5.433	0.055	0.894893	3.163024	0.039341	
68	1	4	3	6	8	132.552	31202.500	2.7	1.7	0.630	129.636	5.442	0.055	0.896395	3.157726	0.039246	
69	1	0	6	4	4	133.130	31331.633	54.9	39.7	10.822	130.202	5.465	0.055	0.900105	3.144711	0.039015	
70	1	4	6	1	8	133.419	31396.336	1.0	0.7	0.227	130.485	5.476	0.055	0.901963	3.138231	0.038902	
71	1	1	3	7	8	133.487	31411.539	0.7	0.5	0.170	130.552	5.478	0.055	0.902400	3.136712	0.038875	
72	1	8	1	1	8	133.580	31432.188	0.2	0.1	0.038	130.642	5.482	0.055	0.902993	3.134651	0.038839	

73	1	7	0	4	4	133.686	31455.951	0.4	0.2	0.086	130.746	5.486	0.055	0.903676	3.132283	0.038798
74	1	6	3	4	8	134.347	31603.473	18.3	16.1	1.909	131.393	5.512	0.055	0.907914	3.117662	0.038546
75	1	7	3	2	8	134.369	31608.357	29.8	26.3	2.986	131.415	5.513	0.055	0.908054	3.117180	0.038537
76	1	0	3	7	4	134.556	31650.238	33.8	30.4	3.010	131.598	5.520	0.055	0.909258	3.113055	0.038467
77	1	4	6	0	4	134.579	31655.203	37.3	33.5	3.399	131.620	5.521	0.055	0.909400	3.112567	0.038458
78	1	2	5	5	8	134.587	31657.084	1.9	1.7	0.175	131.628	5.521	0.055	0.909454	3.112382	0.038455
79	1	5	1	6	8	134.677	31677.188	0.9	0.8	0.101	131.717	5.525	0.055	0.910032	3.110407	0.038422
80	1	8	1	0	4	134.743	31691.951	0.1	0.1	0.013	131.781	5.527	0.055	0.910456	3.108958	0.038397
81	1	4	4	5	8	135.002	31749.754	1.1	0.8	0.229	132.035	5.537	0.055	0.912116	3.103298	0.038301
82	1	8	0	1	4	135.060	31762.656	5.7	3.8	1.247	132.092	5.540	0.055	0.912487	3.102037	0.038280
83	1	2	4	6	8	135.073	31765.535	1.5	1.0	0.324	132.104	5.540	0.055	0.912570	3.101756	0.038275
84	1	5	3	5	8	135.696	31904.508	0.0	0.0	0.000	132.715	5.564	0.055	0.916562	3.088245	0.038048
85	1	6	1	5	8	135.703	31906.025	1.4	0.8	0.339	132.721	5.565	0.055	0.916606	3.088098	0.038046
86	1	5	4	4	8	135.846	31937.912	1.9	1.2	0.421	132.861	5.570	0.055	0.917522	3.085015	0.037994
87	1	7	2	3	8	135.963	31963.838	23.9	16.9	4.848	132.975	5.575	0.055	0.918267	3.082513	0.037953
88	1	5	0	6	4	136.195	32015.527	0.3	0.2	0.046	133.203	5.584	0.055	0.919752	3.077536	0.037870
89	1	8	0	0	2	136.263	32030.771	40.9	32.6	6.551	133.270	5.586	0.055	0.920190	3.076072	0.037846
90	1	5	5	2	8	136.563	32097.467	17.8	14.8	2.450	133.563	5.598	0.055	0.922106	3.069680	0.037741
91	1	3	1	7	8	136.780	32145.982	22.5	18.8	2.998	133.776	5.607	0.055	0.923499	3.065047	0.037666
92	1	2	6	3	8	137.064	32209.199	38.2	31.8	5.247	134.054	5.618	0.055	0.925315	3.059031	0.037568
93	1	6	0	5	4	137.256	32251.834	136.4	111.5	19.979	134.242	5.625	0.055	0.926540	3.054987	0.037503
94	1	3	6	2	8	137.553	32317.922	6.6	5.1	1.117	134.533	5.637	0.055	0.928439	3.048740	0.037402
95	1	2	2	7	8	137.783	32369.033	6.8	5.0	1.313	134.758	5.645	0.055	0.929907	3.043926	0.037325
96	1	1	5	5	8	137.957	32407.715	1.7	1.2	0.366	134.928	5.652	0.055	0.931019	3.040293	0.037267
97	1	7	3	1	8	138.018	32421.438	21.0	14.0	4.564	134.988	5.655	0.055	0.931413	3.039006	0.037247
98	1	6	4	2	8	138.152	32451.205	2.1	1.3	0.469	135.120	5.660	0.055	0.932268	3.036218	0.037202
99	1	3	0	7	4	138.371	32499.740	3.2	1.9	0.740	135.333	5.668	0.055	0.933662	3.031684	0.037131
100	1	1	4	6	8	138.480	32524.092	0.1	0.1	0.034	135.441	5.673	0.055	0.934362	3.029414	0.037095
101	1	0	5	5	4	139.137	32670.045	142.2	113.6	22.459	136.084	5.698	0.055	0.938555	3.015880	0.036884
102	1	0	4	6	4	139.674	32789.281	96.6	84.2	10.624	136.610	5.719	0.055	0.941980	3.004913	0.036714
103	1	3	5	4	8	140.061	32875.152	24.4	21.4	2.547	136.989	5.734	0.055	0.944447	2.997065	0.036594
104	1	4	2	6	8	140.294	32926.840	61.7	53.9	6.715	137.217	5.743	0.055	0.945932	2.992360	0.036523
105	1	5	5	1	8	140.398	32949.914	4.2	3.7	0.466	137.319	5.747	0.055	0.946595	2.990264	0.036491
106	1	3	3	6	8	140.443	32959.824	10.9	9.5	1.210	137.363	5.749	0.055	0.946880	2.989365	0.036477
107	1	1	6	3	8	140.628	33000.793	46.3	40.3	5.108	137.544	5.756	0.055	0.948057	2.985654	0.036421
108	1	4	5	3	8	140.793	33037.371	85.1	74.7	8.980	137.705	5.762	0.055	0.949108	2.982348	0.036372
109	1	7	1	3	8	140.816	33042.434	55.7	49.0	5.820	137.728	5.763	0.055	0.949253	2.981891	0.036365
110	1	1	2	7	8	141.404	33172.766	0.0	0.0	0.001	138.304	5.786	0.055	0.952997	2.970176	0.036190
111	1	3	6	1	8	141.475	33188.535	57.8	54.7	2.989	138.373	5.788	0.055	0.953450	2.968765	0.036169
112	1	6	4	1	8	142.127	33332.930	3.1	2.9	0.187	139.012	5.814	0.055	0.957598	2.955904	0.035980
113	1	6	2	4	8	142.426	33399.066	0.3	0.3	0.026	139.305	5.825	0.055	0.959498	2.950051	0.035894
114	1	7	2	2	8	142.452	33404.836	47.7	42.6	4.542	139.330	5.826	0.055	0.959664	2.949542	0.035887
115	1	7	0	3	4	142.552	33426.980	22.9	20.1	2.437	139.428	5.830	0.055	0.960300	2.947587	0.035859
116	1	2	1	7	8	142.840	33490.633	1.2	1.0	0.179	139.710	5.841	0.055	0.962129	2.941985	0.035778
117	1	6	3	3	8	143.353	33604.168	8.8	6.3	1.757	140.213	5.861	0.055	0.965391	2.932045	0.035635
118	1	3	4	5	8	143.365	33606.828	95.1	68.2	18.948	140.225	5.861	0.055	0.965467	2.931813	0.035632
119	1	6	4	0	4	143.530	33643.207	1.9	1.4	0.388	140.386	5.868	0.055	0.966512	2.928643	0.035587
120	1	2	6	2	8	143.720	33685.195	1.2	0.9	0.246	140.572	5.875	0.055	0.967718	2.924992	0.035535

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
121	1	5	2	5	8	144.036	33754.980	4.5	3.4	0.854	140.881	5.887	0.055	0.969723	2.918945	0.035450	
122	1	2	0	7	4	144.653	33891.230	210.1	149.7	42.197	141.486	5.911	0.055	0.973637	2.907211	0.035285	
123	1	5	4	3	8	145.178	34007.066	42.0	28.7	8.932	142.000	5.931	0.055	0.976965	2.897308	0.035148	
124	1	4	1	6	8	145.643	34109.590	0.0	0.0	0.002	142.455	5.949	0.055	0.979910	2.888600	0.035029	
125	1	2	5	4	8	146.587	34317.605	0.1	0.1	0.003	143.379	5.985	0.055	0.985886	2.871090	0.034792	
126	1	7	2	1	8	146.820	34368.965	9.9	9.4	0.394	143.608	5.994	0.055	0.987362	2.866800	0.034735	
127	1	1	1	7	8	146.885	34383.207	21.3	20.3	0.993	143.671	5.997	0.055	0.987771	2.865613	0.034719	
128	1	4	3	5	8	146.933	34393.891	100.4	94.9	5.133	143.719	5.999	0.055	0.988078	2.864722	0.034707	
129	1	2	3	6	8	147.024	34413.949	123.1	115.3	7.163	143.808	6.002	0.055	0.988654	2.863052	0.034685	
130	1	4	4	4	8	147.123	34435.746	122.4	113.9	7.771	143.905	6.006	0.055	0.989280	2.861240	0.034661	
131	1	4	0	6	4	147.566	34533.102	48.5	44.0	4.044	144.338	6.023	0.055	0.992077	2.853174	0.034555	
132	1	1	6	2	8	147.842	34593.840	28.0	24.5	2.991	144.609	6.033	0.055	0.993822	2.848164	0.034489	
133	1	5	3	4	8	148.022	34633.449	19.0	16.3	2.269	144.785	6.040	0.055	0.994960	2.844907	0.034446	
134	1	6	1	4	8	148.031	34635.387	85.9	73.7	10.316	144.794	6.041	0.055	0.995016	2.844748	0.034444	
135	1	4	5	2	8	148.033	34635.988	3.2	2.7	0.382	144.796	6.041	0.055	0.995033	2.844699	0.034444	
136	1	7	1	2	8	148.060	34641.820	33.3	28.4	4.053	144.822	6.042	0.055	0.995201	2.844219	0.034437	
137	1	2	6	1	8	148.209	34674.535	17.4	14.7	2.231	144.968	6.048	0.055	0.996140	2.841536	0.034403	
138	1	0	1	7	4	148.311	34696.973	9.2	7.8	1.225	145.068	6.051	0.055	0.996785	2.839699	0.034379	
139	1	1	0	7	4	148.857	34817.117	14.3	11.0	2.576	145.603	6.072	0.055	1.000237	2.829900	0.034252	
140	1	0	6	2	4	149.296	34913.465	0.1	0.1	0.024	146.033	6.089	0.055	1.003004	2.822090	0.034153	
141	1	3	2	6	8	149.746	35012.309	21.8	17.0	3.702	146.474	6.106	0.055	1.005844	2.814123	0.034052	
142	1	2	6	0	4	149.800	35024.207	0.1	0.1	0.012	146.527	6.109	0.055	1.006186	2.813167	0.034040	
143	1	5	1	5	8	149.840	35032.789	4.8	3.8	0.748	146.565	6.110	0.055	1.006432	2.812478	0.034031	
144	1	6	0	4	4	150.050	35079.043	12.4	10.7	1.478	146.772	6.118	0.055	1.007761	2.808769	0.033984	
145	1	7	0	2	4	150.081	35085.723	16.8	14.6	1.909	146.802	6.119	0.055	1.007953	2.808235	0.033978	
146	1	3	5	3	8	150.352	35145.297	21.6	19.9	1.525	147.068	6.130	0.055	1.009665	2.803475	0.033918	
147	1	2	4	5	8	150.385	35152.402	0.1	0.1	0.010	147.099	6.131	0.055	1.009869	2.802908	0.033911	
148	1	1	5	4	8	150.966	35279.879	0.1	0.0	0.006	147.669	6.153	0.055	1.013531	2.792780	0.033786	
149	1	6	3	2	8	151.016	35290.785	362.5	310.6	43.592	147.718	6.155	0.055	1.013844	2.791917	0.033775	
150	1	1	3	6	8	151.444	35384.594	19.8	16.8	2.504	148.137	6.171	0.055	1.016539	2.784515	0.033684	
151	1	5	0	5	4	151.935	35492.094	2.1	2.0	0.130	148.618	6.190	0.055	1.019627	2.776082	0.033582	
152	1	1	6	1	8	152.739	35668.039	12.5	12.8	0.361	149.405	6.221	0.055	1.024682	2.762388	0.033417	

153	1	4	5	1	8	152.950	35714.238	57.7	54.8	2.714	149.612	6.229	0.055	1.026009	2.758814	0.033374
154	1	7	1	1	8	152.979	35720.633	23.4	22.0	1.301	149.641	6.230	0.055	1.026193	2.758320	0.033369
155	1	5	4	2	8	153.152	35758.316	50.2	44.7	4.771	149.810	6.237	0.055	1.027276	2.755414	0.033334
156	1	6	2	3	8	153.286	35787.621	211.4	182.9	24.205	149.941	6.242	0.055	1.028118	2.753157	0.033307
157	1	4	5	0	4	154.701	36096.668	0.1	0.0	0.024	151.327	6.296	0.055	1.036996	2.729586	0.033033
158	1	1	4	5	8	155.123	36188.797	0.4	0.2	0.098	151.741	6.312	0.055	1.039643	2.722637	0.032953
159	1	7	0	1	4	155.210	36207.910	4.3	3.4	0.873	151.827	6.315	0.055	1.040192	2.721200	0.032936
160	1	0	6	0	2	156.142	36411.078	238.6	245.6	7.284	152.739	6.350	0.055	1.046028	2.706016	0.032765
161	1	6	3	1	8	156.245	36433.410	7.5	7.6	0.114	152.840	6.354	0.055	1.046670	2.704357	0.032746
162	1	3	1	6	8	156.296	36444.551	52.1	52.7	0.644	152.890	6.356	0.055	1.046990	2.703531	0.032737
163	1	4	2	5	8	157.681	36746.070	7.5	7.2	0.275	154.247	6.409	0.055	1.055652	2.681346	0.032492
164	1	2	2	6	8	157.794	36770.547	0.9	0.9	0.054	154.357	6.413	0.055	1.056355	2.679562	0.032472
165	1	3	3	5	8	157.892	36791.934	107.2	98.8	7.693	154.454	6.417	0.055	1.056970	2.678004	0.032455
166	1	6	3	0	4	158.112	36839.676	59.2	53.9	4.793	154.669	6.425	0.055	1.058341	2.674533	0.032418
167	1	3	4	4	8	158.128	36843.188	64.8	58.9	5.232	154.685	6.426	0.055	1.058442	2.674279	0.032415
168	1	2	5	3	8	158.503	36924.676	0.0	0.0	0.000	155.052	6.440	0.055	1.060783	2.668377	0.032351
169	1	5	4	1	8	158.613	36948.512	17.4	16.4	0.972	155.159	6.444	0.055	1.061468	2.666655	0.032333
170	1	3	0	6	4	158.677	36962.488	55.9	52.8	2.866	155.222	6.447	0.055	1.061869	2.665647	0.032322
171	1	5	2	4	8	159.028	37038.652	8.6	8.5	0.212	155.566	6.460	0.055	1.064057	2.660166	0.032263
172	1	4	4	3	8	159.181	37071.965	2.4	2.4	0.060	155.716	6.466	0.055	1.065014	2.657775	0.032238
173	1	3	5	2	8	159.258	37088.742	15.3	15.4	0.478	155.792	6.469	0.055	1.065496	2.656573	0.032225
174	1	5	3	3	8	160.319	37318.969	27.1	17.4	6.297	156.831	6.509	0.055	1.072111	2.640184	0.032053
175	1	6	1	3	8	160.330	37321.402	0.0	0.0	0.007	156.842	6.509	0.055	1.072180	2.640012	0.032051
176	1	6	2	2	8	162.753	37846.000	16.8	7.3	4.120	159.216	6.601	0.055	1.087251	2.603418	0.031678
177	1	6	0	3	4	162.902	37878.215	20.9	11.5	5.095	159.362	6.606	0.055	1.088177	2.601203	0.031656
178	1	4	3	4	8	162.946	37887.699	5.4	3.1	1.297	159.405	6.608	0.055	1.088449	2.600553	0.031649
179	1	1	2	6	8	163.289	37961.762	2.3	1.9	0.366	159.741	6.621	0.055	1.090577	2.595479	0.031599
180	1	1	5	3	8	164.074	38131.434	87.4	90.7	3.579	160.511	6.650	0.055	1.095451	2.583930	0.031485

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
181	1	0	2	6	4	165.251	38385.324	409.3	392.9	15.509	161.664	6.695	0.055	1.102745	2.566839	0.031320	
182	1	4	1	5	8	165.376	38412.309	27.5	26.4	1.024	161.786	6.699	0.055	1.103520	2.565036	0.031303	
183	1	3	5	1	8	165.421	38421.895	144.9	139.9	4.721	161.830	6.701	0.055	1.103796	2.564396	0.031297	
184	1	2	1	6	8	165.506	38440.266	14.5	14.3	0.254	161.913	6.704	0.055	1.104324	2.563170	0.031285	
185	1	0	5	3	4	166.065	38560.766	20.7	25.1	5.188	162.461	6.725	0.055	1.107785	2.555161	0.031209	
186	1	5	1	4	8	166.930	38746.895	5.0	5.5	0.818	163.309	6.758	0.055	1.113132	2.542886	0.031094	
187	1	2	3	5	8	167.403	38848.566	0.0	0.0	0.007	163.772	6.776	0.055	1.116053	2.536231	0.031032	
188	1	2	4	4	8	167.683	38908.914	0.4	0.6	0.377	164.047	6.786	0.055	1.117787	2.532298	0.030996	
189	1	4	0	5	4	168.201	39020.199	0.1	0.2	0.194	164.554	6.805	0.054	1.120984	2.525075	0.030930	
190	1	2	0	6	4	168.338	39049.508	4.1	7.1	5.227	164.688	6.811	0.054	1.121826	2.523180	0.030913	
191	1	2	5	2	8	169.031	39198.469	621.0	704.8	93.186	165.368	6.837	0.054	1.126105	2.513592	0.030826	
192	1	6	2	1	8	169.345	39265.688	161.3	174.0	13.493	165.675	6.848	0.054	1.128036	2.509289	0.030788	
193	1	5	0	4	4	169.836	39371.070	0.1	0.1	0.009	166.156	6.867	0.054	1.131064	2.502572	0.030728	
194	1	4	4	2	8	169.853	39374.801	132.4	150.2	19.725	166.173	6.867	0.054	1.131171	2.502335	0.030726	
195	1	5	3	2	8	171.237	39671.141	77.8	72.7	4.649	167.529	6.919	0.054	1.139684	2.483643	0.030562	
196	1	6	1	2	8	171.250	39674.062	23.5	21.9	1.480	167.542	6.920	0.054	1.139768	2.483460	0.030560	
197	1	3	2	5	8	171.444	39715.570	140.9	127.6	11.852	167.732	6.927	0.054	1.140961	2.480864	0.030538	
198	1	6	2	0	4	171.725	39775.645	0.1	0.1	0.002	168.007	6.937	0.054	1.142687	2.477118	0.030505	
199	1	1	1	6	8	171.874	39807.484	1.3	1.4	0.059	168.153	6.943	0.054	1.143601	2.475136	0.030488	
200	1	3	4	3	8	173.373	40127.949	33.3	37.4	4.688	169.623	6.999	0.054	1.152808	2.455369	0.030321	
201	1	1	3	5	8	173.999	40261.438	9.0	10.0	1.145	170.236	7.022	0.054	1.156643	2.447229	0.030253	
202	1	1	4	4	8	174.314	40328.629	14.2	15.0	0.869	170.545	7.034	0.054	1.158573	2.443151	0.030219	
203	1	6	0	2	4	174.390	40344.914	0.8	0.8	0.037	170.619	7.037	0.054	1.159041	2.442165	0.030211	
204	1	5	2	3	8	174.559	40380.871	59.2	61.2	2.253	170.785	7.043	0.054	1.160074	2.439991	0.030193	
205	1	1	0	6	4	175.048	40485.242	7.5	8.3	0.949	171.265	7.061	0.054	1.163072	2.433700	0.030142	
206	1	1	5	2	8	175.828	40651.312	65.7	74.8	10.193	172.029	7.090	0.054	1.167843	2.423758	0.030061	
207	1	0	3	5	4	176.375	40767.797	2.8	3.6	0.951	172.565	7.110	0.054	1.171189	2.416833	0.030005	
208	1	2	5	1	8	176.444	40782.426	1.5	2.0	0.580	172.633	7.113	0.054	1.171610	2.415966	0.029999	
209	1	0	4	4	4	176.703	40837.555	22.6	31.8	12.622	172.887	7.122	0.054	1.173193	2.412704	0.029973	
210	1	4	4	1	8	177.379	40981.133	0.0	0.0	0.001	173.549	7.147	0.054	1.177318	2.404252	0.029906	
211	1	0	0	6	2	177.469	41000.199	10.0	12.0	2.414	173.637	7.151	0.054	1.177866	2.403133	0.029897	
212	1	4	2	4	8	177.958	41104.227	722.5	718.8	4.197	174.117	7.169	0.054	1.180855	2.397052	0.029849	
213	1	3	3	4	8	178.261	41168.445	134.3	138.4	4.162	174.413	7.180	0.054	1.182699	2.393312	0.029820	
214	1	5	3	1	8	178.954	41315.551	16.8	19.9	3.494	175.093	7.206	0.054	1.186926	2.384791	0.029755	
215	1	6	1	1	8	178.970	41318.852	1.5	1.7	0.305	175.108	7.206	0.054	1.187020	2.384600	0.029753	
216	1	2	5	0	4	179.139	41354.668	199.5	231.7	36.702	175.274	7.213	0.054	1.188049	2.382535	0.029737	
217	1	4	3	3	8	179.770	41488.367	236.6	260.0	25.258	175.892	7.236	0.054	1.191890	2.374857	0.029679	
218	1	4	4	0	4	180.117	41561.902	5.4	6.6	1.318	176.232	7.249	0.054	1.194003	2.370656	0.029647	
219	1	3	1	5	8	181.450	41844.023	315.2	305.1	9.685	177.539	7.298	0.054	1.202108	2.354672	0.029528	
220	1	6	1	0	4	181.782	41914.305	631.6	581.6	45.156	177.865	7.310	0.054	1.204127	2.350724	0.029499	
221	1	6	0	1	4	182.559	42078.289	94.4	107.9	15.152	178.626	7.339	0.054	1.208838	2.341563	0.029432	
222	1	2	2	5	8	183.797	42339.570	152.6	174.4	24.473	179.840	7.384	0.054	1.216344	2.327112	0.029328	
223	1	1	5	1	8	184.208	42426.242	21.7	24.9	3.679	180.243	7.400	0.054	1.218834	2.322358	0.029294	
224	1	5	1	3	8	185.149	42624.297	76.8	75.4	1.476	181.165	7.434	0.054	1.224524	2.311568	0.029218	
225	1	3	0	5	4	185.192	42633.355	169.7	167.0	2.867	181.207	7.436	0.054	1.224784	2.311077	0.029214	
226	1	6	0	0	2	185.545	42707.691	12.3	14.0	1.871	181.553	7.449	0.054	1.226919	2.307054	0.029186	
227	1	2	4	3	8	186.175	42840.277	1.7	3.0	2.088	182.171	7.472	0.054	1.230728	2.299914	0.029137	
228	1	0	5	1	4	187.031	43019.992	99.9	151.1	75.789	183.010	7.503	0.054	1.235891	2.290306	0.029071	
229	1	3	4	2	8	187.398	43097.094	31.0	46.8	23.466	183.370	7.517	0.054	1.238106	2.286209	0.029043	
230	1	5	2	2	8	188.894	43410.871	124.2	125.5	1.799	184.837	7.571	0.054	1.247120	2.269684	0.028933	
231	1	5	0	3	4	189.127	43459.504	82.6	83.0	1.051	185.065	7.580	0.054	1.248518	2.267144	0.028916	
232	1	4	1	4	8	189.213	43477.672	0.1	0.2	0.006	185.150	7.583	0.054	1.249040	2.266196	0.028910	

233	1	2	3	4	8	192.254	44113.328	1099.5	1140.0	41.221	188.131	7.694	0.054	1.267301	2.233541	0.028699
234	1	1	2	5	8	192.611	44187.773	2.6	2.9	0.348	188.481	7.707	0.054	1.269440	2.229778	0.028676
235	1	4	0	4	4	193.462	44365.113	0.0	0.0	0.001	189.315	7.738	0.054	1.274534	2.220865	0.028620
236	1	1	4	3	8	195.349	44757.859	119.2	125.8	7.040	191.166	7.806	0.054	1.285817	2.201378	0.028501
237	1	4	3	2	8	195.532	44795.805	5.2	5.5	0.342	191.345	7.813	0.054	1.286907	2.199513	0.028490
238	1	2	1	5	8	196.263	44947.562	4.0	6.4	3.717	192.062	7.839	0.054	1.291267	2.192086	0.028445
239	1	3	4	1	8	197.623	45229.633	184.8	212.3	30.911	193.395	7.888	0.054	1.299370	2.178416	0.028364
240	1	3	2	4	8	198.422	45395.277	207.7	215.0	7.556	194.179	7.917	0.054	1.304129	2.170467	0.028318

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
241	1	5	2	1	8	199.377	45592.730	48.0	63.4	20.010	195.115	7.952	0.054	1.309802	2.161067	0.028264	
242	1	4	2	3	8	200.502	45825.285	0.1	0.1	0.013	196.219	7.992	0.054	1.316483	2.150100	0.028202	
243	1	3	3	3	8	200.933	45914.328	153.8	158.0	4.390	196.642	8.008	0.054	1.319041	2.145930	0.028179	
244	1	2	0	5	4	201.010	45930.180	176.6	180.4	4.008	196.717	8.011	0.054	1.319496	2.145190	0.028174	
245	1	1	3	4	8	202.395	46215.637	28.1	33.6	6.489	198.075	8.060	0.054	1.327697	2.131939	0.028101	
246	1	5	1	2	8	202.491	46235.539	93.0	112.9	23.691	198.170	8.064	0.054	1.328268	2.131022	0.028096	
247	1	2	4	2	8	203.832	46511.562	1.0	5.2	20.134	199.485	8.112	0.054	1.336198	2.118375	0.028027	
248	1	1	1	5	8	207.078	47177.605	0.6	0.6	0.083	202.669	8.228	0.054	1.355332	2.088469	0.027870	
249	1	4	3	1	8	207.213	47205.203	663.7	718.2	57.737	202.801	8.233	0.054	1.356125	2.087248	0.027864	
250	1	5	0	2	4	207.711	47307.121	61.2	71.0	11.058	203.289	8.251	0.054	1.359053	2.082751	0.027840	
251	1	0	1	5	4	211.095	47998.105	301.4	274.4	24.210	206.609	8.371	0.053	1.378904	2.052767	0.027690	
252	1	4	3	0	4	211.590	48099.055	14.1	13.9	0.308	207.095	8.389	0.053	1.381804	2.048459	0.027669	
253	1	1	0	5	4	212.665	48317.676	13.7	19.0	7.205	208.149	8.427	0.053	1.388085	2.039191	0.027625	
254	1	3	1	4	8	214.329	48655.727	151.5	163.9	13.240	209.781	8.486	0.053	1.397796	2.025023	0.027557	
255	1	5	1	1	8	215.529	48899.094	23.5	28.8	6.444	210.959	8.528	0.053	1.404788	2.014944	0.027510	
256	1	1	4	2	8	216.007	48995.898	135.9	161.0	29.114	211.428	8.545	0.053	1.407569	2.010963	0.027492	
257	1	4	1	3	8	216.948	49186.328	64.1	78.4	17.244	212.351	8.579	0.053	1.413040	2.003178	0.027456	
258	1	2	4	1	8	217.144	49225.965	62.1	78.2	19.922	212.543	8.585	0.053	1.414178	2.001565	0.027449	
259	1	2	2	4	8	218.203	49439.738	5.0	10.0	9.987	213.581	8.623	0.053	1.420320	1.992910	0.027410	
260	1	3	0	4	4	220.531	49909.266	58.6	72.7	17.098	215.866	8.705	0.053	1.433808	1.974161	0.027327	
261	1	0	4	2	4	220.569	49916.871	155.4	190.7	42.519	215.904	8.706	0.053	1.434027	1.973861	0.027326	
262	1	2	3	3	8	221.541	50112.402	11.5	15.6	5.352	216.857	8.740	0.053	1.439644	1.966159	0.027293	
263	1	5	0	1	4	221.838	50172.031	21.8	31.1	13.039	217.148	8.750	0.053	1.441357	1.963822	0.027282	
264	1	2	4	0	4	222.187	50242.133	0.1	0.2	0.079	217.491	8.763	0.053	1.443371	1.961082	0.027271	
265	1	4	2	2	8	223.004	50406.254	3.1	3.9	1.018	218.293	8.791	0.053	1.448086	1.954697	0.027244	
266	1	4	0	3	4	223.384	50482.434	20.4	23.0	2.906	218.665	8.805	0.053	1.450274	1.951747	0.027231	
267	1	3	3	2	8	223.595	50524.828	101.9	114.6	14.127	218.873	8.812	0.053	1.451492	1.950109	0.027224	
268	1	3	2	3	8	231.068	52016.078	129.6	159.2	35.730	226.206	9.072	0.053	1.494334	1.894202	0.027000	
269	1	1	4	1	8	231.996	52200.309	67.1	85.8	23.493	227.117	9.104	0.053	1.499626	1.887517	0.026974	
270	1	1	2	4	8	233.283	52455.422	79.5	114.7	49.602	228.380	9.149	0.053	1.506955	1.878337	0.026939	
271	1	1	3	3	8	237.361	53260.918	163.6	182.8	21.222	232.383	9.289	0.053	1.530096	1.849930	0.026835	
272	1	0	2	4	4	239.035	53590.289	28.5	34.0	6.508	234.026	9.347	0.053	1.539558	1.838560	0.026795	
273	1	2	1	4	8	239.798	53740.105	190.3	203.1	13.452	234.774	9.373	0.053	1.543862	1.833434	0.026777	
274	1	4	2	1	8	240.694	53915.980	8.1	9.3	1.360	235.654	9.403	0.053	1.548914	1.827453	0.026756	
275	1	3	3	1	8	241.434	54061.168	461.4	526.1	72.123	236.381	9.429	0.053	1.553085	1.822546	0.026739	
276	1	0	3	3	4	243.421	54450.074	755.1	854.7	110.277	238.332	9.497	0.053	1.564258	1.809528	0.026695	
277	1	0	4	0	2	244.274	54616.613	592.9	696.9	119.610	239.169	9.526	0.053	1.569042	1.804010	0.026677	
278	1	4	1	2	8	246.179	54988.098	4.5	9.0	8.668	241.039	9.590	0.052	1.579715	1.791823	0.026637	
279	1	4	2	0	4	247.573	55259.520	107.0	139.1	40.972	242.408	9.638	0.052	1.587512	1.783022	0.026608	
280	1	2	0	4	4	248.522	55443.730	0.4	1.3	3.432	243.339	9.670	0.052	1.592804	1.777098	0.026589	
281	1	2	3	2	8	252.899	56291.312	19.9	42.2	46.323	247.637	9.818	0.052	1.617154	1.750340	0.026506	
282	1	4	0	2	4	255.628	56817.324	1443.7	1436.5	8.049	250.317	9.909	0.052	1.632265	1.734136	0.026458	
283	1	3	1	3	8	257.085	57097.461	199.1	264.3	84.505	251.748	9.958	0.052	1.640313	1.725627	0.026433	
284	1	1	1	4	8	260.125	57680.059	3.9	18.2	65.920	254.733	10.060	0.052	1.657050	1.708198	0.026383	
285	1	2	2	3	8	263.773	58376.168	626.3	661.4	36.474	258.316	10.181	0.052	1.677048	1.687828	0.026326	
286	1	3	2	2	8	267.220	59031.023	148.9	171.1	25.057	261.702	10.296	0.052	1.695861	1.669104	0.026276	
287	1	3	0	3	4	267.866	59153.484	42.0	53.5	14.343	262.337	10.317	0.052	1.699379	1.665649	0.026267	
288	1	4	1	1	8	270.435	59639.254	7.6	20.0	31.902	264.861	10.402	0.052	1.713334	1.652082	0.026232	
289	1	1	0	4	4	271.298	59802.043	5.9	17.5	34.237	265.708	10.430	0.052	1.718011	1.647585	0.026221	
290	1	1	3	2	8	276.981	60869.652	519.9	640.6	145.358	271.291	10.616	0.052	1.748682	1.618688	0.026149	
291	1	2	3	1	8	279.351	61312.500	4.6	6.2	2.134	273.620	10.693	0.052	1.761404	1.606996	0.026122	
292	1	4	1	0	4	280.212	61473.137	1.4	1.4	0.014	274.466	10.721	0.052	1.766019	1.602797	0.026112	
293	1	0	0	4	2	280.358	61500.297	623.4	612.7	10.888	274.609	10.726	0.052	1.766799	1.602089	0.026110	
294	1	4	0	1	4	283.011	61993.980	14.9	26.5	20.369	277.216	10.812	0.051	1.780982	1.589331	0.026081	
295	1	2	3	0	4	290.132	63310.406	283.0	354.6	87.673	284.214	11.042	0.051	1.818800	1.556284	0.026008	
296	1	1	2	3	8	291.332	63531.070	345.2	381.9	39.777	285.393	11.080	0.051	1.825140	1.550878	0.025997	
297	1	4	0	0	2	294.224	64061.543	526.8	553.3	27.406	288.235	11.173	0.051	1.840379	1.538036	0.025970	
298	1	3	2	1	8	298.830	64902.410	708.0	836.5	148.275	292.763	11.320	0.051	1.864536	1.518109	0.025930	
299	1	2	1	3	8	304.074	65853.680	3.5	27.5	184.997	297.918	11.486	0.051	1.891864	1.496180	0.025887	
300	1	3	1	2	8	309.315	66798.133	191.8	261.4	92.597	303.071	11.650	0.051	1.918997	1.475026	0.025848	

No.	Code	H	K	L	Mult	Hw	2theta/TOF	Icalc	Iobs	Sigma	HwG	HwL	ETA	d-hkl	TOF_alpha	TOF_beta	CORR
301	1	1	3	1	8	312.508	67370.391	203.6	299.9	138.387	306.210	11.750	0.051	1.935437	1.462496	0.025825	
302	1	2	2	2	8	320.944	68871.492	0.0	0.0	0.019	314.506	12.012	0.050	1.978561	1.430620	0.025771	
303	1	2	0	3	4	322.045	69066.203	828.6	898.9	74.561	315.588	12.046	0.050	1.984154	1.426587	0.025764	
304	1	0	3	1	4	326.360	69826.930	1155.7	1518.5	465.066	319.833	12.178	0.050	2.006009	1.411045	0.025739	
305	1	3	0	2	4	328.246	70158.086	57.1	128.7	157.732	321.688	12.236	0.050	2.015522	1.404385	0.025728	
306	1	1	1	3	8	347.769	73541.094	952.9	1081.5	142.370	340.894	12.826	0.050	2.112710	1.339781	0.025634	
307	1	3	1	1	8	360.429	75692.000	1942.7	2207.8	293.675	353.353	13.201	0.049	2.174502	1.301709	0.025584	
308	1	0	1	3	4	366.852	76770.648	11.4	22.7	22.156	359.674	13.390	0.049	2.205490	1.283419	0.025562	
309	1	1	2	2	8	373.135	77817.828	988.6	1097.6	117.925	365.859	13.572	0.049	2.235574	1.266149	0.025542	

310	1	1	0	3	4	374.830	78099.016	747.9	830.0	88.767	367.528	13.621	0.049	2.243652	1.261590	0.025536
311	1	2	2	1	8	378.765	78749.602	3650.4	4222.6	644.607	371.403	13.735	0.049	2.262342	1.251167	0.025525
312	1	3	0	1	4	390.611	80689.828	960.3	1158.3	232.523	383.067	14.073	0.049	2.318082	1.221083	0.025493
313	1	0	2	2	4	396.689	81675.109	4005.9	4465.8	499.008	389.053	14.245	0.048	2.346387	1.206352	0.025478
314	1	2	1	2	8	399.998	82208.453	5158.2	5631.5	502.714	392.312	14.338	0.048	2.361709	1.198526	0.025470
315	1	2	2	0	4	405.706	83123.805	10.7	56.5	234.117	397.934	14.498	0.048	2.388005	1.185328	0.025457
316	1	2	0	2	4	441.495	88730.227	39.8	92.9	120.433	433.198	15.475	0.047	2.549068	1.110433	0.025393
317	1	1	2	1	8	469.884	93023.125	736.3	940.4	252.998	461.186	16.224	0.047	2.672396	1.059188	0.025356
318	1	1	1	2	8	510.032	98879.477	2411.7	2673.8	281.850	500.786	17.246	0.046	2.840639	0.996455	0.025317
319	1	2	1	1	8	523.651	100812.508	11.4	121.4	1132.962	514.224	17.583	0.045	2.896172	0.977348	0.025307
320	1	0	2	0	2	585.155	109233.227	2920.3	3918.5	1295.927	574.940	19.051	0.044	3.138085	0.902005	0.025272
321	1	2	1	0	4	594.863	110519.039	2741.2	3220.5	544.633	584.527	19.276	0.044	3.175024	0.891511	0.025267
322	1	1	0	2	4	597.661	110887.461	1171.8	1385.6	244.508	587.290	19.340	0.044	3.185608	0.888549	0.025266
323	1	2	0	1	4	618.741	113634.648	2868.3	3271.4	444.402	608.113	19.819	0.043	3.264530	0.867068	0.025258
324	1	0	0	2	2	693.578	123000.594	287.5	568.9	537.394	682.073	21.452	0.042	3.533598	0.801044	0.025236
325	1	2	0	0	2	736.486	128123.086	15.7	257.0	3818.320	724.502	22.346	0.041	3.680758	0.769018	0.025227

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 BRAGG R-Factors and weight fractions for Pattern #  2
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=> Phase:  1     VOSO4 Nuclear
=> Bragg R-factor:   14.0       Vol:  326.520( 0.000)  Fract(%):  100.00( 0.00)
=> Rf-factor=  8.28             ATZ:         651.994   Brindley:  1.0000

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Pattern#  3 Phase No:   1 Phase name: VOSO4 Nuclear
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No.	Code	H	K	L	Mult	Hw	ETA/M	2theta/TOF	Icalc	Iobs	Sigma	StrFactor^2	d-hkl	CORR
1	1	1	0	1	4	0.134834	0.000000	17.419	613.5	762.4	185.293	1708.4188	5.098137	1.000000
2	1	0	1	1	4	0.130248	0.000000	18.937	439.0	862.0	830.413	1450.8103	4.692774	1.000000
3	1	1	1	1	8	0.119794	0.000000	22.500	408.9	485.6	91.510	965.0206	3.957122	1.000000
4	1	2	0	0	2	0.114953	0.000000	24.214	107.4	355.8	822.104	1181.8676	3.680758	1.000000
5	1	0	0	2	2	0.112129	0.000000	25.238	689.5	706.1	18.770	8270.8066	3.533598	1.000000
6	1	2	0	1	4	0.106483	0.000000	27.357	2320.4	2159.3	150.090	16491.5312	3.264530	1.000000
7	1	1	0	2	4	0.104704	0.000000	28.049	475.4	359.0	87.905	3561.0671	3.185608	1.000000
8	1	2	1	0	4	0.104462	0.000000	28.144	8.0	4.2	2.004	60.3759	3.175024	1.000000
9	1	0	2	0	2	0.103606	0.000000	28.482	1746.5	1696.9	48.595	27025.6875	3.138085	1.000000
10	1	2	1	1	8	0.097721	0.000000	30.919	277.6	248.2	26.796	1279.0918	2.896172	1.000000
11	1	1	1	2	8	0.096308	0.000000	31.539	449.7	468.6	20.447	2161.4563	2.840639	1.000000
12	1	1	2	1	8	0.091939	0.000000	33.581	243.0	444.8	369.195	1336.5267	2.672396	1.000000
13	1	2	0	2	4	0.088724	0.000000	35.258	59.3	207.3	517.171	725.0848	2.549068	1.000000
14	1	2	2	0	4	0.084719	0.000000	37.722	89.9	295.8	677.329	1272.9370	2.388005	1.000000
15	1	2	1	2	8	0.084111	0.000000	38.158	17.8	64.7	170.884	128.9409	2.361709	1.000000
16	1	0	2	2	4	0.083765	0.000000	38.417	5.7	41.5	262.317	83.3219	2.346387	1.000000
17	1	3	0	1	4	0.083145	0.000000	38.905	5.6	11.3	12.010	85.1833	2.318082	1.000000
18	1	2	2	1	8	0.082012	0.000000	39.904	189.1	317.5	215.563	1514.4487	2.262342	1.000000
19	1	1	0	3	4	0.081663	0.000000	40.251	1.2	2.7	3.042	20.2191	2.243652	1.000000
20	1	1	2	2	8	0.081517	0.000000	40.402	379.0	507.6	172.318	3118.6741	2.235574	1.000000
21	1	0	1	3	4	0.081007	0.000000	40.978	488.4	622.2	170.525	8292.5078	2.205490	1.000000
22	1	3	1	1	8	0.080539	0.000000	41.589	38.9	68.0	50.850	341.4664	2.174503	1.000000
23	1	1	1	3	8	0.079817	0.000000	42.864	48.0	84.8	65.092	450.3593	2.112710	1.000000
24	1	3	0	2	4	0.079420	0.000000	45.042	47.3	99.2	108.947	990.3688	2.015522	1.000000
25	1	0	3	1	4	0.079442	0.000000	45.267	315.6	512.6	320.064	6679.8301	2.006009	1.000000
26	1	2	0	3	4	0.079539	0.000000	45.794	209.9	198.7	10.928	4561.2671	1.984154	1.000000
27	1	2	2	2	8	0.079575	0.000000	45.931	78.5	65.9	10.903	858.7982	1.978561	1.000000
28	1	1	3	1	8	0.080018	0.000000	47.015	49.6	42.1	7.215	571.0631	1.935437	1.000000
29	1	3	1	2	8	0.080270	0.000000	47.442	52.6	43.7	7.954	618.1785	1.918997	1.000000
30	1	2	1	3	8	0.080796	0.000000	48.165	58.5	59.3	3.774	710.7715	1.891864	1.000000
31	1	3	2	1	8	0.081475	0.000000	48.917	1.7	13.2	91.966	20.7892	1.864536	1.000000
32	1	4	0	0	2	0.082211	0.000000	49.602	222.2	288.1	85.387	11542.8174	1.840379	1.000000
33	1	1	2	3	8	0.082746	0.000000	50.045	2.2	5.0	6.124	29.5690	1.825140	1.000000
34	1	2	3	0	4	0.082985	0.000000	50.231	78.2	216.8	384.115	2088.1670	1.818800	1.000000
35	1	4	0	1	4	0.084626	0.000000	51.375	70.8	71.7	3.429	1989.1326	1.780982	1.000000
36	1	0	0	4	2	0.085342	0.000000	51.818	98.6	119.5	25.263	5649.1660	1.766799	1.000000
37	1	4	1	0	4	0.085383	0.000000	51.842	76.8	88.0	12.903	2201.8342	1.766019	1.000000
38	1	2	3	1	8	0.085629	0.000000	51.988	44.7	68.4	36.413	644.2196	1.761404	1.000000
39	1	1	3	2	8	0.086341	0.000000	52.395	101.3	118.8	20.781	1486.7444	1.748681	1.000000
40	1	1	0	4	4	0.088261	0.000000	53.404	12.3	35.9	68.676	378.0764	1.718011	1.000000
41	1	4	1	1	8	0.088580	0.000000	53.561	5.8	2.9	2.103	89.4394	1.713334	1.000000
42	1	3	0	3	4	0.089577	0.000000	54.037	46.1	71.0	38.347	1450.5143	1.699379	1.000000
43	1	3	2	2	8	0.089838	0.000000	54.158	70.3	65.4	5.136	1110.2814	1.695861	1.000000
44	1	2	2	3	8	0.091311	0.000000	54.816	2.6	3.0	2.593	41.4319	1.677048	1.000000
45	1	1	1	4	8	0.093018	0.000000	55.534	2.7	27.0	243.627	44.8639	1.657050	1.000000
46	1	3	1	3	8	0.094564	0.000000	56.151	47.6	87.9	74.617	814.6120	1.640313	1.000000
47	1	4	0	2	4	0.095347	0.000000	56.452	225.7	260.0	39.530	7823.8931	1.632265	1.000000
48	1	2	3	2	8	0.096887	0.000000	57.028	163.5	326.7	325.912	2897.8904	1.617154	1.000000
49	1	2	0	4	4	0.099574	0.000000	57.982	15.2	47.9	102.869	559.6502	1.592804	1.000000
50	1	4	2	0	4	0.100192	0.000000	58.194	53.7	55.9	2.950	1989.9320	1.587512	1.000000
51	1	4	1	2	8	0.101127	0.000000	58.509	121.8	250.5	264.644	2284.0901	1.579715	1.000000
52	1	0	4	0	2	0.102451	0.000000	58.946	246.7	205.7	34.236	18806.0879	1.569043	1.000000

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    53   1      0   3   3     4  0.103062  0.000000      59.144      351.2      546.7    304.279      13488.0898  1.564258      1.000000
    54   1      3   3   1     8  0.104532  0.000000      59.612        5.2        7.2      2.794        101.7405  1.553085      1.000000
    55   1      4   2   1     8  0.105097  0.000000      59.789      121.5      130.1      9.279       2397.0217  1.548915      1.000000
    56   1      2   1   4     8  0.105792  0.000000      60.005      384.5      612.3    341.873       8080.6782  1.543862      1.000000

    ------------------------------------------------------
    BRAGG R-Factors and weight fractions for Pattern #  3
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=> Phase:  1     VOSO4 Nuclear
=> Bragg R-factor:   25.4       Vol:  326.520( 0.000)  Fract(%):  100.00( 0.00)
=> Rf-factor=  17.7             ATZ:         651.994   Brindley:  1.0000

    ---------------------------------------------------------------
     SYMBOLIC NAMES AND FINAL VALUES AND SIGMA OF REFINED PARAMETERS:
    ---------------------------------------------------------------

     ->  Parameter number    1 :      Cell_A_ph1_pat1     7.3539782    ( +/-    0.39001860E-01 )
     ->  Parameter number    2 :             X_V1_ph1    0.16364004    ( +/-    0.12658078E-02 )
     ->  Parameter number    3 :            Zero_pat1    -1.9953272    ( +/-     2.1815798     )
     ->  Parameter number    4 :             Z_V1_ph1    0.23747978    ( +/-    0.14008972E-02 )
     ->  Parameter number    5 :             X_S1_ph1    0.87405801    ( +/-    0.12579196E-02 )
     ->  Parameter number    6 :            Dtt1_pat1     48329.039    ( +/-     256.27936     )
     ->  Parameter number    7 :             Z_S1_ph1    0.87407881    ( +/-    0.92349324E-03 )
     ->  Parameter number    8 :             X_O1_ph1    0.71441048    ( +/-    0.52903622E-03 )
     ->  Parameter number    9 :            Dtt2_pat1    -3.2745945    ( +/-     1.0731602     )
     ->  Parameter number   10 :             Z_O1_ph1    0.98820972    ( +/-    0.69793494E-03 )
     ->  Parameter number   11 :             X_O2_ph1    0.44627253E-01( +/-    0.54321694E-03 )
     ->  Parameter number   12 :            Zero_pat2    -5.3567719    ( +/-     8.9365711     )
     ->  Parameter number   13 :             Z_O2_ph1    0.97938156    ( +/-    0.67112118E-03 )
     ->  Parameter number   14 :             X_O3_ph1    0.37422553    ( +/-    0.78570709E-03 )
     ->  Parameter number   15 :            Dtt1_pat2     34808.738    ( +/-     10.998049     )
     ->  Parameter number   16 :             Z_O3_ph1    0.16945940    ( +/-    0.48556097E-03 )
     ->  Parameter number   17 :             X_O4_ph1    0.11908086    ( +/-    0.86413400E-03 )
     ->  Parameter number   18 :             Y_O4_ph1    0.56241012    ( +/-    0.36183369E-03 )
     ->  Parameter number   19 :             Z_O4_ph1    0.25823894    ( +/-    0.39830123E-03 )
     ->  Parameter number   20 :            Dtt2_pat2    -3.1474333    ( +/-     3.0181901     )
     ->  Parameter number   21 :       Scale_ph1_pat1     1.1250159    ( +/-    0.80381203E-02 )
     ->  Parameter number   22 :      Cell_B_ph1_pat1     6.2706499    ( +/-    0.33256516E-01 )
     ->  Parameter number   23 :      Cell_C_ph1_pat1     7.0604458    ( +/-    0.37445270E-01 )

-----------------------------------------------------------------
=> Number of bytes for floating point variables: 4
=> Dimensions of dynamic allocated arrays in this run of FullProf:
-----------------------------------------------------------------

=> Total approximate array memory (dynamic + static): 121369011 bytes

   MaxPOINT=    70000 Max.num. of points(+int. Inten.)/diffraction pattern
   MaxREFLT=    20000 Max.num. of reflections/diffraction pattern
   MaxPARAM=      500 Max.num. of refinable parameters
   MaxOVERL=     2024 Max.num. of overlapping reflections

-----------------------------------------------------------
=> Number of bytes for floating point arrays: 4
=> Dimensions of fixed arrays in this release of FullProf:
-----------------------------------------------------------

   NPATT   =       80 Max.num. of powder diffraction patterns
   NATS    =      830 Max.num. of atoms (all kind) in asymmetric unit
   MPAR    =     1800 Max.num. of non atomic parameters/phase
   IEXCL   =       30 Max.num. of excluded regions
   IBACP   =      277 Max.num. of background points for interpolation
   NPHT    =       16 Max.num. of phases
   NMAGM   =        8 Max.num. of rotation-matrices sets for magnetic structure
   NBASIS  =       12 Max.num. of basis functions associated to a single atom
   NIREPS  =        9 Max.num. of irreducible representations to be combined
   N_EQ    =      384 Max.num. of user-supplied symmetry operators/propagation vectors
   NGL     =      300 Max.num. of global parameters/diffraction pattern
   N_LINC  =       30 Max.num. of global linear restraints
   NAT_P   =       64 Max.num. of atomic parameters per atom
   NCONST  =      500 Max.num. of slack constraints per phase
   N_SPE   =       30 Max.num. of different chemical species
   N_FORM  =       60 Max.num. of scattering factor values in a table
   NPR     =      150 Max.num. of points defining a numerical profile
   INPR    =       25 Max.num. of different numerical peak shapes
   NPRC    =      150 Max.num. of terms in the table for correcting intensities
   NSOL    =       10 Max.num. of solutions to be stored in Montecarlo searchs


              CPU Time:    25.656 seconds
                            0.428 minutes
```

```
=> Run finished at:     Date: 10/06/2021  Time: 17:15:45.419
```

end of pcr out file pdf.pdf

Appendix:C Python Code

appendix C1

In [1]:

```
import pandas as pd
import numpy as np
from scipy.optimize import curve_fit
from matplotlib import pyplot as plt
```

In [2]:

```
df=pd.read_csv('sample.txt')
df2=pd.read_csv('sampleset2.txt')
df3=pd.read_csv('sampleset3.txt')
```

In [3]:

```
#creating a data frame Q that has the mag moment and tempfor data set1 and the dc err
Q = df[['Temperature_K','DC_Moment_Free_Ctr_emu','DC_Moment_Err_Free_Ctr_emu']]

#survey_sub = surveys_df.head(10)
Q1=Q.DC_Moment_Free_Ctr_emu
#declearing err in sub
Ea=Q.DC_Moment_Err_Free_Ctr_emu*4.643
#taking the inverse of the err
E1=1/Ea
#Q1
```

In [4]:

```
#creating a data frame Q that has the mag moment and tempfor data set2
Q21=df2[['Temperature2_K','DC_Moment_FreeCtr2_emu','DC_Moment_Err_Free_Ctr2_emu']]
Q2=sum([Q21.DC_Moment_FreeCtr2_emu]+[Q21.DC_Moment_Err_Free_Ctr2_emu])
Q2=Q21.DC_Moment_FreeCtr2_emu
Eb=Q21.DC_Moment_Err_Free_Ctr2_emu
#taking the inverse of the err
E2=1/Eb
#Q2
```

In [5]:

```
Q31=df3[['Temperature3_K','DC_Moment_FreeCtr3_emu','DC_Moment_Err_Free_Ctr3_emu']]
#Q3=sum([Q31.DC_Moment_FreeCtr3_emu]+[Q31.DC_Moment_Err_Free_Ctr3_emu])
Q3=Q31.DC_Moment_FreeCtr3_emu
Ec=Q31.DC_Moment_Err_Free_Ctr3_emu*4.643
E3=1/Ec
#Q3
```

In [6]:

```
#assigning T T2 M M2 to the tep mag colom in the new data frams
T=Q.Temperature_K
T2=Q21.Temperature2_K
T3=Q31.Temperature3_K
M13=Q3
M12=Q2
M1=Q1
#converting to mol/cm3 to revert to former format remove the 1 infront of all the Ms ab
ove thend delete the decleration below
M=M1*4.643
M
M2=M12*4.643
M3=M13*4.643
R12=max(M12)
R1=max(M1)
R13=max(M13)



#extract the maximum value of magnetic susceptibility and temperature
Zz= Q[Q.DC_Moment_Free_Ctr_emu>=R1]
Zz2=Q21[Q21.DC_Moment_FreeCtr2_emu>=R12]
Zz3=Q31[Q31.DC_Moment_FreeCtr3_emu>=R13]
#P1=Q[Q.DC_Moment_Free_Ctr_emu=0.00103661367255475]
#maximum susceptibility
R=max(M)
R2=max(M2)
R3=max(M3)
#printing curve maximums
print('curve max are:', R,R2,R3)
```

```
curve max are: 0.004812997281671704 0.00476551917912033 0.0048496865042160
25
```

In [7]:

```
#M=e+M
```

In [8]:

```
Zz
```

Out[8]:

	Temperature_K	DC_Moment_Free_Ctr_emu	DC_Moment_Err_Free_Ctr_emu
28	29.101299	0.001037	0.00005

In [9]:

```
Zz2
```

Out[9]:

	Temperature2_K	DC_Moment_FreeCtr2_emu	DC_Moment_Err_Free_Ctr2_emu
27	28.112946	0.001026	0.00005

In [10]:

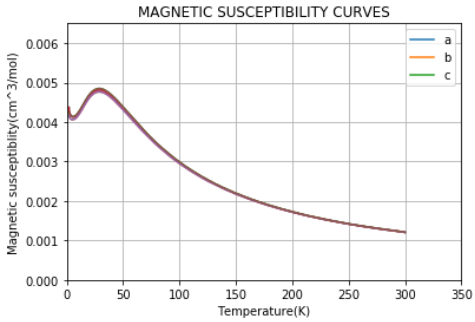
```
Zz3
```

Out[10]:

	Temperature3_K	DC_Moment_FreeCtr3_emu	DC_Moment_Err_Free_Ctr3_emu
28	29.121679	0.001045	0.000051

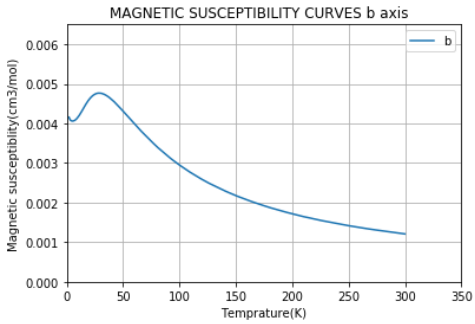
In [11]:

```
plt.plot(T,M,label='a')
plt.plot(T2,M2,label='b')
plt.plot(T3,M3,label='c')
plt.title('MAGNETIC SUSCEPTIBILITY CURVES')
#plt.errorbar(T, M, yerr=e, fmt="none")
plt.plot(T,M,T2,M2,T3,M3)
plt.axis([0,350,0,0.0065])
plt.xlabel('Temperature(K)')
plt.ylabel('Magnetic susceptiblity(cm^3/mol)')
plt.legend()
plt.grid()
```



In [12]:

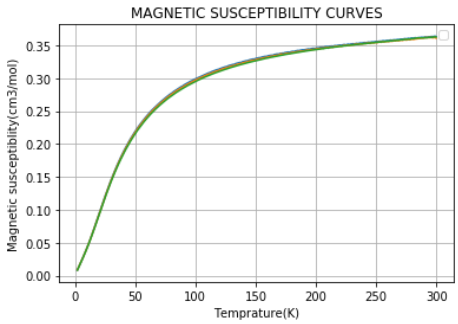
```
plt.title('MAGNETIC SUSCEPTIBILITY CURVES b axis  ')
plt.plot(T2,M2,label='b')
plt.xlabel('Temprature(K)')
plt.ylabel('Magnetic susceptiblity(cm3/mol)')
plt.legend()
plt.axis([0,350,0,0.0065])
plt.grid()
```



In [13]:

```
K3=M3*T3
K=M*T
K2=M2*T2
plt.plot(T3,K3,T,K,T2,K2)
plt.title('MAGNETIC SUSCEPTIBILITY CURVES')
#plt.plot(T3,M3,label='c')
plt.xlabel('Temprature(K)')
plt.ylabel('Magnetic susceptiblity(cm3/mol)')
plt.legend()
#plt.axis([0,350,0,0.0065])
plt.grid()
```

```
No handles with labels found to put in legend.
```

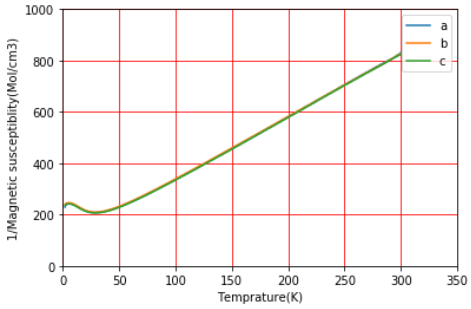


In [14]:

```
plt.plot(T,1/M,label='a')
plt.plot(T2,1/M2,label='b')
plt.plot(T3,1/M3,label='c')
plt.legend()
plt.axis([0,350,0,1000])
plt.grid(color='red')
plt.xlabel('Temprature(K)')
plt.ylabel('1/Magnetic susceptiblity(Mol/cm3)')
```

Out[14]:

```
Text(0, 0.5, '1/Magnetic susceptiblity(Mol/cm3)')
```



In [15]:

```
#creating a data frame that have only higher temperature from 150
Z= Q[Q.Temperature_K>200]
Z2=Q21[Q21.Temperature2_K>200]
Z3=Q31[Q31.Temperature3_K>200]

#Z2
#Z
```

In [16]:

```
temp=Z.Temperature_K
temp2=Z2.Temperature2_K
temp3=Z3.Temperature3_K
#temp2
#temp
```

In [17]:

```
u=1/M
u2=1/M2
u3=1/M3
#u2
```

In [18]:

```
#adding the err to the subs
meg1=Z.DC_Moment_Free_Ctr_emu
meg12=Z2.DC_Moment_FreeCtr2_emu
meg13=Z3.DC_Moment_FreeCtr3_emu
#meg2
#meg
meg=meg1*4.643
meg2=meg12*4.643

meg3=meg13*4.643
meg
E11=Z.DC_Moment_Err_Free_Ctr_emu*4.643
E22=Z2.DC_Moment_Err_Free_Ctr2_emu*4.643
E33=Z3.DC_Moment_Err_Free_Ctr3_emu*4.643
```

In [19]:

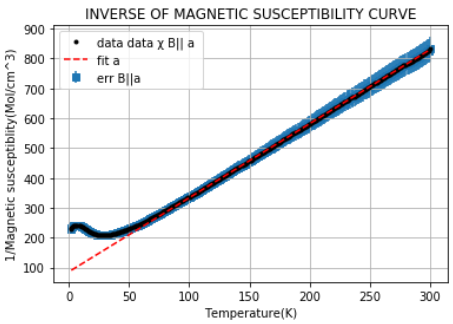
```
U=1/meg
U
U2=1/meg2
U3=1/meg3
#U2
#E11=1/E11
#E2=1/E22
#E3=1/E33
```

In [20]:

```
#fitting the curve to curie wiess law using only temperatyres above 150k m=1/curiewiess
constant
def objective(temp,m,C):
    return m*(temp + C)
popt,pcov = curve_fit(objective, temp, U,sigma=(E11/meg**2), maxfev=1500000)#,method='d
ogbox',bounds=([0, 0], [25.0459917,0.00860, 25,]))#,p0=(30,0.4,4,20,0.002) )
m, C = popt
print('U=%5f*temp + %.5f' %(m, C))
#plt.axis([200,350,200,1200])
plt.plot(T,u,'.' ,color='black',label='data data χ B|| a ')
x_line = sorted(T,key=lambda T:float(T) )
y_line = objective(x_line, m,C)

perr=np.sqrt(np.diag(pcov))
plt.grid()
plt.plot(x_line, y_line,'--',color='red', label='fit a')
plt.errorbar(T,u,yerr=(Ea/M**2),fmt='s',zorder=0,label='err B||a')
#plt.plot(x2_line, y2_line,'--', color='green',label='b')
#plt.plot(x2_line, y2_line,'--', color='black',label='c')
plt.legend()
plt.xlabel('Temperature(K)')
plt.ylabel('1/Magnetic susceptiblity(Mol/cm^3)')
plt.title('INVERSE OF MAGNETIC SUSCEPTIBILITY CURVE')
print(perr)
print('err in m =', perr[0],'err in C =',perr[1])
print('m =',m, 'C3 =',-C)
# cal culating the curre constant m= 1/C, C = curie wiess temperature
CW = 1/m
print('curie weiss constant =',CW)
print('err in CW =',perr[0]/m**2)
```

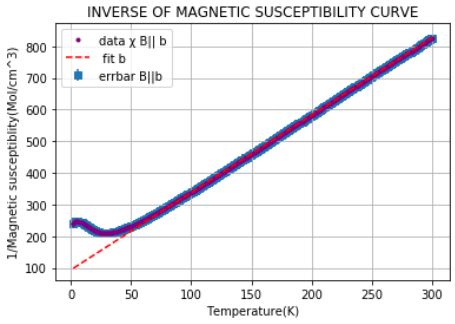
```
U=2.476631*temp + 34.75929
[0.00271953 0.30786438]
err in m = 0.0027195294492701493 err in C = 0.30786437636765707
m = 2.476630788822832 C3 = -34.75928619049622
curie weiss constant = 0.40377435527049643
err in CW = 0.0004433750298889362
```



In [24]:

```
#fitting the curve to curie wiess law using only temperatyres above 150k m=1/curiewiess
constant
def objective(temp2,m2,C2):
    return m2*(temp2 + C2) #Curie weiss law =1/x = 1/C(T+)
popt,pcov = curve_fit(objective, temp2, U2,sigma=(E22/meg2**2), maxfev=1500000)
m2, C2 = popt
print('U=%5f*temp  %.5f' %(m2, C2))
#plt.axis([0,150,0.0,1200])
plt.plot(T2,u2,'.' ,color='purple',label='data χ B|| b')
x2_line = sorted(T2,key=lambda T:float(T) )
y2_line = objective(x2_line, m2,C2)
perr2=np.sqrt(np.diag(pcov))
plt.grid()
plt.plot(x2_line, y2_line,'--',color='red', label=' fit b')
plt.errorbar(T2,u2,yerr=(Eb/M2**2),fmt='s',zorder=0,label='errbar B||b')
#plt.plot(x2_line, y2_line,'--', color='green',label='b')
#plt.plot(x2_line, y2_line,'--', color='black',label='c')
plt.legend()
plt.xlabel('Temperature(K)')
plt.ylabel('1/Magnetic susceptiblity(Mol/cm^3)')
plt.title('INVERSE OF MAGNETIC SUSCEPTIBILITY CURVE')
print(perr2)
print('err in m =', perr2[0],'err in C =',perr2[1])
print('m =',m2, 'C =',-C2)
# cal culating the curre constant m= 1/C, C = curie wiess temperature
CW2 = 1/m2
print('curie weiss constant =',CW2)
print('err in CW =',perr2[0]/m3**2)
print ('Tcw=',-C2)
```

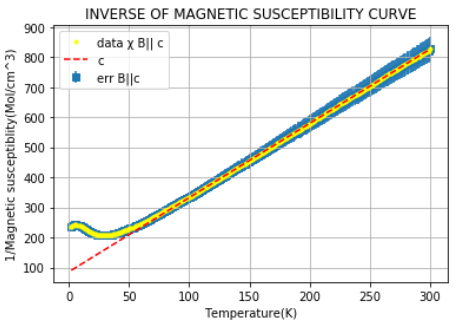
```
U=2.443846*temp  38.48262
[0.00165529 0.19215436]
err in m = 0.0016552936256537323 err in C = 0.19215436201401304
m = 2.44384602266463 C = -38.48261651651336
curie weiss constant = 0.40919108271381893
err in CW = 0.0002718132101373695
Tcw= -38.48261651651336
```



In [22]:

```
#fitting the curve to curie wiess law using only temperatyres above 150k m=1/curiewiess
constant
def objective(temp3,m3,C3):
    return m3*(temp3 + C3)
popt,_ = curve_fit(objective, temp3, U3,sigma=(E33/meg3**2), maxfev=1500000)
m3, C3 = popt
print('U=%5f*temp + %.5f' %(m3, C3))
#plt.axis([0,350,0,1200])
plt.plot(T3,u3,'.' ,color='yellow',label='data χ B|| c')
x3_line = sorted(T3,key=lambda T:float(T) )
y3_line = objective(x3_line, m3,C3)
perr3=np.sqrt(np.diag(pcov))
plt.grid()
plt.plot(x3_line, y3_line,'--',color='red', label='c')
plt.errorbar(T3,u3,yerr=(Ec/M3**2),fmt='s',zorder=0,label='err B||c')
#plt.plot(x2_line, y2_line,'--', color='green',label='b')
#plt.plot(x2_line, y2_line,'--', color='black',label='c')
plt.legend()
plt.xlabel('Temperature(K)')
plt.ylabel('1/Magnetic susceptiblity(Mol/cm^3)')
plt.title('INVERSE OF MAGNETIC SUSCEPTIBILITY CURVE')
print(perr3)
print('err in m =', perr3[0],'err in C3 =',perr3[1])
print('m =',m3, 'C3 =',-C3)
# cal culating the curre constant m= 1/C, C = curie wiess temperature
CW3 = 1/m3
print('curie weiss constant =',CW3)
print('err in CW =',perr3[0]/m3**2)
print ('Tcw=',-C3)
```

```
U=2.467756*temp + 34.68685
[0.00165529 0.19215436]
err in m = 0.0016552936256537323 err in C3 = 0.19215436201401304
m = 2.467756141992745 C3 = -34.686849275924736
curie weiss constant = 0.4052264253276205
err in CW = 0.0002718132101373695
Tcw= -34.686849275924736
```



In [23]:

```
#fitting the curve to curie wiess law using only temperatyres above 150k m=1/curiewiess
constant
def objective(x,m3,C3):
    return m3*(x + C3)
x=np.random.uniform(-50, 350., 101)
popt,_ = curve_fit(objective, temp3, U3,sigma=(E33/meg3**2), maxfev=1500000)
m3, C3 = popt
print('U=%5f*temp + %.5f' %(m3, C3))
#plt.axis([0,350,0,1200])
plt.plot(T3,u3,'.' ,color='yellow',label='c')
x3_line = sorted(x,key=lambda x:float(x) )
y3_line = objective(x3_line, m3,C3)
perr3=np.sqrt(np.diag(pcov))
plt.grid()
plt.plot(x3_line, y3_line,'--',color='red', label='c')
plt.errorbar(T3,u3,yerr=(Ec/M3**2),fmt='s',zorder=0)
#plt.plot(x2_line, y2_line,'--', color='green',label='b')
#plt.plot(x2_line, y2_line,'--', color='black',label='c')
plt.legend()
plt.xlabel('Temperature(K)')
plt.ylabel('1/Magnetic susceptiblity(Mol/cm^3)')
plt.title('INVERSE OF MAGNETIC SUSCEPTIBILITY CURVE')
print(perr3)
print('err in m =', perr3[0],'err in C3 =',perr3[1])
print('m =',m3, 'C3 =',C3)
# cal culating the curre constant m= 1/C, C = curie wiess temperature
CW3 = 1/m3
print('curie weiss constant =',CW3)
print('err in CW =',perr3[0]/m3**2)
x=T3
y=u3

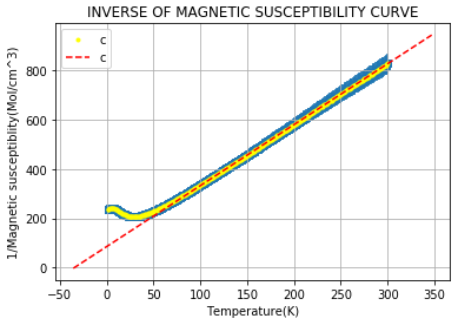
#x=np.random.uniform(1.8, 200., 1000)
fig, ax = plt.subplots()
ax.plot(x, y,x3_line, y3_line,'--',color='red', label='c')
ax.scatter(x,y)
#ax.plot(x, np.log(x))
#ax.set_aspect('equal')
ax.grid(True, which='both',color='g')

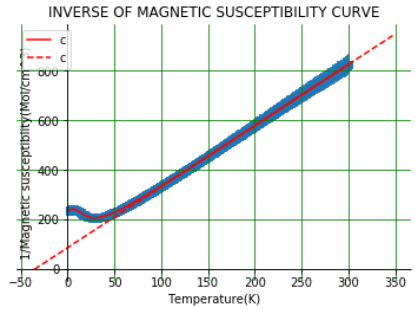
# set the x-spine (see below for more info on `set_position`)
ax.spines['left'].set_position('zero')

# turn off the right spine/ticks
ax.spines['right'].set_color('none')
#ax.yaxis.tick_left()

# set the y-spine
ax.spines['bottom'].set_position('zero')
ax.errorbar(T3,u3,yerr=(Ec/M3**2),fmt='s',zorder=0)
# turn off the top spine/ticks
ax.spines['top'].set_color('none')
ax.xaxis.tick_bottom()
plt.legend()
plt.xlabel('Temperature(K)')
plt.ylabel('1/Magnetic susceptiblity(Mol/cm^3)')
plt.title('INVERSE OF MAGNETIC SUSCEPTIBILITY CURVE')
print(perr3)
```

```
U=2.467756*temp + 34.68685
[0.00165529 0.19215436]
err in m = 0.0016552936256537323 err in C3 = 0.19215436201401304
m = 2.467756141992745 C3 = 34.686849275924736
curie weiss constant = 0.4052264253276205
err in CW = 0.0002718132101373695
[0.00165529 0.19215436]
```





In [1]:

```
import pandas as pd
import numpy as np
from numpy import arange
from scipy.optimize import curve_fit
from scipy import constants
from scipy.constants import find
from matplotlib import pyplot as plt
import math
from scipy import special
```

In [2]:

```
df=pd.read_csv('sample.txt')
df2=pd.read_csv('sampleset2.txt')
df3=pd.read_csv('sampleset3.txt')
```

In [3]:

```
#creating a data frame Q that has the mag moment and tempfor data set1 and the dc err
Q = df[['Temperature_K','DC_Moment_Free_Ctr_emu','DC_Moment_Err_Free_Ctr_emu']]
#Q
#e=df[['DC_Moment_Err_Free_Ctr_emu']]
#e=e*4.643
#adding the err to the mag sub data.
#Q1=sum([Q.DC_Moment_Free_Ctr_emu]+[Q.DC_Moment_Err_Free_Ctr_emu])
#Q2=[[Q.DC_Moment_Free_Ctr_emu,e.DC_Moment_Err_Free_Ctr_emu,Q1]]
#Q1
Q1=Q.DC_Moment_Free_Ctr_emu
#declearing err values
E1=Q.DC_Moment_Err_Free_Ctr_emu*4.643
```

In [4]:

```
#creating a data frame Q that has the mag moment and tempfor data set2
Q21=df2[['Temperature2_K','DC_Moment_FreeCtr2_emu','DC_Moment_Err_Free_Ctr2_emu']]
#Q2=sum([Q21.DC_Moment_FreeCtr2_emu]+[Q21.DC_Moment_Err_Free_Ctr2_emu])
#Q2
Q2=Q21.DC_Moment_FreeCtr2_emu
#declearing err values
E2=Q21.DC_Moment_Err_Free_Ctr2_emu*4.643
```

In [5]:

```
Q31=df3[['Temperature3_K','DC_Moment_FreeCtr3_emu','DC_Moment_Err_Free_Ctr3_emu']]
#Q3=sum([Q31.DC_Moment_FreeCtr3_emu]+[Q31.DC_Moment_Err_Free_Ctr3_emu])
#Q3
Q3=Q31.DC_Moment_FreeCtr3_emu
#declearing err values
E3=Q31.DC_Moment_Err_Free_Ctr3_emu*4.643
```

In [6]:

```
#assigning T T2 M M2 to the tep mag colom in the new data frams
T=Q.Temperature_K
T2=Q21.Temperature2_K
T3=Q31.Temperature3_K
#M12=Q2.DC_Moment_FreeCtr2_emu
#M13=Q3.DC_Moment_FreeCtr3_emu
#M1=Q.DC_Moment_Free_Ctr_emu
M13=Q3
M12=Q2
M1=Q1
#converting to mol/cm3 to revert to former format remove the 1 infront of all the Ms ab
ove thend delete the decleration below
M=M1*4.643
#M
M2=M12*4.643
M3=M13*4.643
R2=max(M2)
R=max(M)
R3=max(M3)
#printing curve maximums
print('curve max are:', R,R2,R3)
#extract the maximum value of magnetic susceptibility and temperature
#Zz= Q[Q.DC_Moment_Free_Ctr_emu>=0.00103661367255475]
#Zz2=Q21[Q21.DC_Moment_FreeCtr2_emu>=0.00102638793433563]
#Zz3=Q31[Q31.DC_Moment_FreeCtr3_emu>=0.00104451572350119]
#P1=Q[Q.DC_Moment_Free_Ctr_emu=0.00103661367255475]
print(M)
#maxima
Zz= Q[Q.DC_Moment_Free_Ctr_emu>=R]
Zz2=Q21[Q21.DC_Moment_FreeCtr2_emu>=R2]
Zz3=Q31[Q31.DC_Moment_FreeCtr3_emu>=R3]
```

```
curve max are: 0.004812997281671704 0.00476551917912033 0.0048496865042160
25
0      0.004371
1      0.004286
2      0.004195
3      0.004153
4      0.004133
         ...
295    0.001222
296    0.001216
297    0.001213
298    0.001210
299    0.001203
Name: DC_Moment_Free_Ctr_emu, Length: 300, dtype: float64
```

In [7]:

```
#creating a data frame that have only  temperature from 0 to 50
Z= Q[Q.Temperature_K<80]
Z2=Q21[Q21.Temperature2_K<200]
Z3=Q31[Q31.Temperature3_K<200]
#this i can use to fit only the peak
#Z2
#Z
```

In [8]:

```
#creating a data frame that have only  temperature from 4 to 50
Z=Z[Z.Temperature_K>8]
Z2=Z2[Z2.Temperature2_K>4]
Z3=Z3[Z3.Temperature3_K>4]
Z4=Z[Z.Temperature_K>200]
```

In [9]:

```
#temp is data set of temperatures form from 4  to  50K
temp=Z.Temperature_K
temp2=Z2.Temperature2_K
temp3=Z3.Temperature3_K
#temp2
#temp
x1=Z4
```

In [10]:

```
#adding the err to the subs
#meg1=sum([Z.DC_Moment_Free_Ctr_emu] + [Z.DC_Moment_Err_Free_Ctr_emu])
#meg12=sum([Z2.DC_Moment_FreeCtr2_emu]+ [Z2.DC_Moment_Err_Free_Ctr2_emu])
#meg13=sum([Z3.DC_Moment_FreeCtr3_emu]+ [Z3.DC_Moment_Err_Free_Ctr3_emu])

meg1=Z.DC_Moment_Free_Ctr_emu
meg12=Z2.DC_Moment_FreeCtr2_emu
meg13=Z3.DC_Moment_FreeCtr3_emu
E11=Z.DC_Moment_Err_Free_Ctr_emu*4.643
E22=Z2.DC_Moment_Err_Free_Ctr2_emu*4.643
E33=Z3.DC_Moment_Err_Free_Ctr3_emu*4.643

#meg2

#meg2
#meg
#converting to mol/cm3
meg=meg1*4.643
meg2=meg12*4.643

meg3=meg13*4.643
#meg
```

In [11]:

```
#U1,U2 is the magnetic susceptibilty for 4 to 50
U=meg
U
U2=meg2
U3=meg3
#U2
```

In [12]:

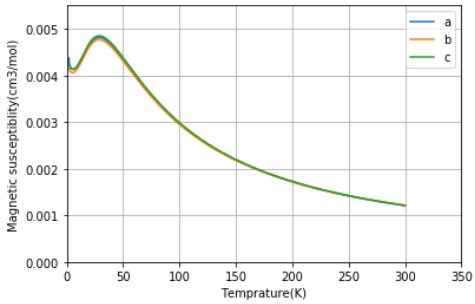
```
#plt.plot(temp,U)
```

In [13]:

```
#  b(((g**2)*(B**2)*N)*(math.exp((-J)/(K*T))*(1-(-tanh(K))**N)))/((4kT)*(1+(-tanh(K))**
N))
#J=45.4
#G=5
#J2=43.9
#J3=45.4
```

In [14]:

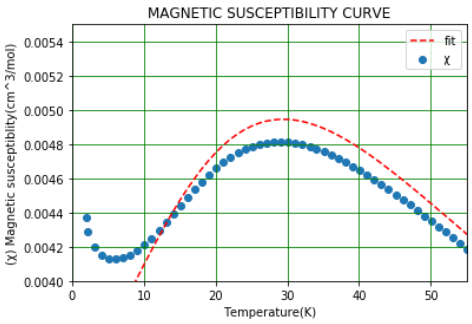
```
plt.plot(T,M,label='a')
plt.plot(T2,M2,label='b')
plt.plot(T3,M3,label='c')
#plt.plot(T,M,T2,M2,T3,M3)
plt.axis([0,350,0,0.0055])
plt.xlabel('Temprature(K)')
plt.ylabel('Magnetic susceptiblity(cm3/mol)')
plt.legend()
plt.grid()
```



In [15]:

```
#fit only the peak for J and C,Tn as P
def objective2(x,J):
    return (1.530518/x)*((0.25+((0.14995*(J/x)+(0.30094*(J/x)**2))))/(1+1.9862*(J/x)+0.
68854*(J/x)**2+6.0626*(J/x)**3 ))
#set J value to calculated value
#J=44.5
x=T
y=M
#remove the # to observe the fit of only the peak data
#x=temp
#y=U
#feeding in intial guess values of j=41 and c=0.4
popt, _ = curve_fit(objective2, x, y,maxfev=10000,bounds=(0.0044,69), p0=(20))
J=popt
print(popt,'J,''C,''Tn')
plt.scatter(T, M,label='χ')
x_line = arange(min(x), max(x), 1)
y_line = objective2(x_line,J)
plt.plot(x_line, y_line, '--', color='red',label ='fit')
plt.axis([0,55,0.004,0.0055])
plt.title('MAGNETIC SUSCEPTIBILITY CURVE')
plt.xlabel('Temperature(K)')
plt.ylabel('(χ) Magnetic susceptiblity(cm^3/mol)')
plt.legend()
plt.grid(color='green')
plt.show()
```

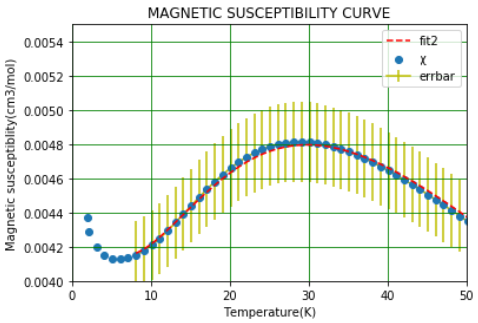
```
[22.71742219] J,C,Tn
```



In [16]:

```
#fit only the peak for J and C,Tn as P
def objective2(x,J,C,P):
    return (1.530518/x)*((0.25+((0.14995*(J/x)+(0.30094*(J/x)**2))))/(1+1.9862*(J/x)+0.
68854*(J/x)**2+6.0626*(J/x)**3 )) +C/(x+P)#work on the u nt and make sure the are in th
e right unit that crospond
#set J value to calculated value
#J=44.5
#x=T
#y=M
#remove the # to observe the fit of only the peak data
x=temp
y=U
#feeding in intial guess values of j=41 and c=0.4
popt, pcov = curve_fit(objective2, x, y,sigma=E11,maxfev=15000,bounds=(0.0044,69), p0=(
41,0.4,5),method='dogbox')
J,C,P= popt
print(popt,'J,''C,''Tn')
plt.scatter(T, M,label='χ')
x_line = arange(min(x), max(x), 1)
y_line = objective2(x_line,J,C,P)
plt.plot(x_line, y_line, '--', color='red',label='fit2',zorder=2)
plt.errorbar(x,y,E11,color='y',label='errbar',zorder=0)
perr = np.sqrt(np.diag(pcov))
plt.axis([0,50,0.004,0.0055])
plt.title('MAGNETIC SUSCEPTIBILITY CURVE')
plt.xlabel('Temperature(K)')
plt.ylabel('Magnetic susceptiblity(cm3/mol)')
plt.legend()
plt.grid(color='green')
plt.show()
print(perr)
```

```
[2.41295617e+01 4.40000000e-03 8.73792245e-01] J,C,Tn
```



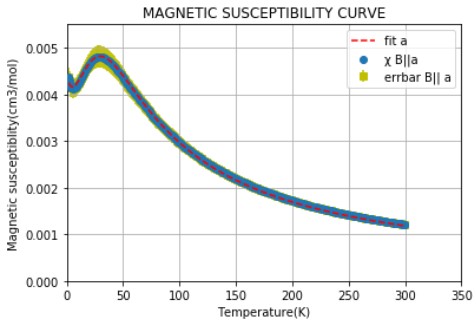

```
[9.68322461e-02 6.64331215e-04 1.14593298e+00]
```

In [ ]:

In [46]:

```
def objective2(x,J,C,K,):
    return (1.5307/x)*((0.25+((0.14995*(J/x)+(0.30094*(J/x)**2))))/(1+1.9862*(J/x)+0.68
854*(J/x)**2+6.0626*(J/x)**3 ))+(C)/(x+K)#(C)/(x+K)
#work on the u nt and make sure the are in the right unit that crospond
#J=43.50
x=T
y=M
#x=temp
#y=U
#method{‘lm’, ‘trf’, ‘dogbox’}, optional
popt, pcov = curve_fit(objective2, x, y,sigma=E1, maxfev=1500000,method='dogbox',bounds
=([23.05, 0 ,-12], [25.0459917,0.00860, 25,]))#,p0=(30,0.4,4,20,0.002))
J,C,K,= popt
print(popt)
plt.scatter(T, M,label='χ B||a',zorder=10)
x_line = arange(min(x), max(x), 1)
y_line = objective2(x_line, J,C,K,)
plt.plot(x_line, y_line, '--', color='red',label='fit a',zorder=15)
plt.errorbar(x,y,E1,zorder=0,fmt='s',color='y',label= 'errbar B|| a')
perr = np.sqrt(np.diag(pcov))
plt.axis([0,350,0.00,0.0055])
plt.title('MAGNETIC SUSCEPTIBILITY CURVE')
plt.xlabel('Temperature(K)')
plt.ylabel('Magnetic susceptiblity(cm3/mol)')
plt.legend()
plt.grid()
plt.show()
#print('err =',perr)
print('J,err =',perr[0],',', 'Cerr=',perr[1],',', 'curie-weiss temp err',perr[2])
```

```
[2.45103379e+01 8.60000000e-03 6.23868443e+00]
```




```
J,err = 0.09967493087286954 , Cerr= 0.0004974860511615364 , curie-weiss te
mp err 0.49101765597375263
```

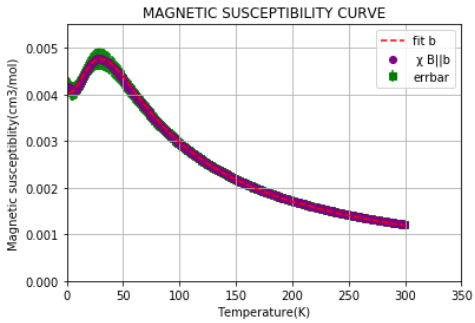
In [18]:

```
Q=Q[Q.Temperature_K>50]
#print(Q)
Tt=Q.Temperature_K
Mt=sum([Q.DC_Moment_Free_Ctr_emu ]+[Q.DC_Moment_Err_Free_Ctr_emu])
#Mt
#plt.plot(Mt,Tt)
```

In [22]:

```
def objective2(x,J,C,K):
    return (1.5307/x)*((0.25+((0.14995*(J/x)+(0.30094*(J/x)**2))))/(1+1.9862*(J/x)+0.68
854*(J/x)**2+6.0626*(J/x)**3 ))+(C)/(x+K)
#work on the u nt and make sure the are in the right unit that crospond
#J=43.50
x=T2
y=M2
#x=temp
#y=U
#method{‘lm’, ‘trf’, ‘dogbox’}, optional
popt, pcov = curve_fit(objective2, x, y,sigma=E2, maxfev=15000,p0=(10,0.4,4),method='do
gbox',bounds=(0.0045, 25.1660920)  )
J,C,K= popt
print(popt)
plt.scatter(T2, M2,color='purple',label=' χ B||b')
x_line = arange(min(x), max(x), 1)
y_line = objective2(x_line, J,C,K)
plt.errorbar(T2,M2,E2, label='errbar', zorder=0,fmt='sg',)
perr = np.sqrt(np.diag(pcov))
plt.plot(x_line, y_line, '--', color='r',label='fit b')
plt.axis([0,350,0.00,0.0055])
plt.title('MAGNETIC SUSCEPTIBILITY CURVE')
plt.xlabel('Temperature(K)')
plt.ylabel('Magnetic susceptiblity(cm3/mol)')
plt.legend()
plt.grid()
plt.show()
print(perr)
print('J,err =',perr[0],',', 'Cerr=',perr[1],',', 'curie-weiss temp err',perr[2])
```

```
[2.51660920e+01 1.28153523e-02 1.18044027e+01]
```



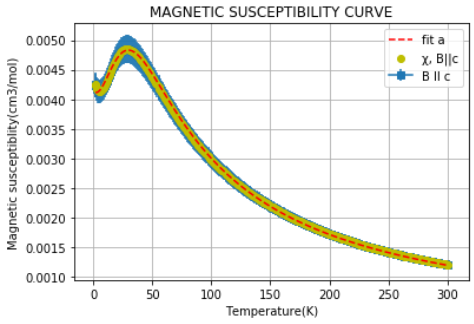

```
[7.25343557e-02 3.76747571e-04 4.48032850e-01]
J,err = 0.07253435568190307 , Cerr= 0.0003767475711328806 , curie-weiss te
mp err 0.44803284959266765
```

In [23]:

```
E1=Q.DC_Moment_Err_Free_Ctr_emu*4.643
def objective2(x,J,C,K):
    return (1.5307/x)*((0.25+((0.14995*(J/x)+(0.30094*(J/x)**2))))/(1+1.9862*(J/x)+0.68
854*(J/x)**2+6.0626*(J/x)**3 ))+(C)/(x+K)
#work on the u nt and make sure the are in the right unit that crospond
#J=43.50
x=T3
y=M3
#x=temp
#y=U
#method{‘lm’, ‘trf’, ‘dogbox’}, optional
popt, pcov = curve_fit(objective2, T3, M3, sigma=E3 , maxfev=150000, method='dogbox',bo
unds=([23.05, 0 ,-12], [25.0967846,1, 25]))
J,C,K= popt
print(popt)
plt.errorbar (T3,M3,yerr=E3, label='B II c',marker='s')
plt.scatter(T3, M3,label='χ, B||c',color='y',zorder=10)
x_line = arange(min(x), max(x), 1)
y_line = objective2(x_line, J,C,K)
plt.plot(x_line, y_line, '--', color='red',label='fit a',zorder=15)

perr = np.sqrt(np.diag(pcov))
#print('err =',perr)
#plt.errorbar (T,M,E1, label='B II a', marker='s')
#plt.errorbar(T, M, yerr=E1, fmt='.k',label='err bar',zorder=0)
#plt.axis([0,200,0,35])
#plt.axis([0,50,0.004,0.0055])
plt.title('MAGNETIC SUSCEPTIBILITY CURVE')
plt.xlabel('Temperature(K)')
plt.ylabel('Magnetic susceptiblity(cm3/mol)')
plt.legend()
plt.grid()
print('J,err =',perr[0],',', 'Cerr=',perr[1],',', 'curie-weiss temp err',perr[2])
```

```
[2.50967846e+01 1.60221721e-02 1.41974977e+01]
J,err = 0.05000624659043914 , Cerr= 0.00026233829978965846 , curie-weiss t
emp err 0.3155850291955115
```



In [ ]:

In [1]:

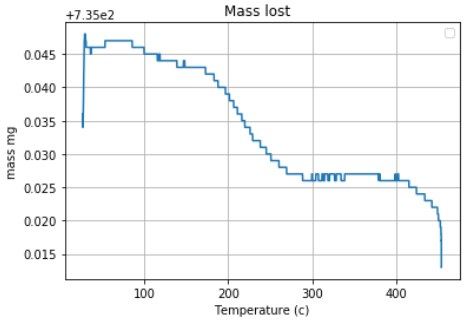
```
import pandas as pd
import numpy as np
from numpy import arange
from scipy.optimize import curve_fit
from scipy import constants
from scipy.constants import find
from matplotlib import pyplot as plt
import math
from scipy import special
```

In [2]:

```
df=pd.read_csv('CPN.txt',delimiter='\s+')
df
HF=df.HF_mW
Tep =df.Ts_C
W11=df.Weight_mg
Wr=(W11/735.048)
time=df.t_s
HF=np.abs([HF])
print(W11,Wr)
#X=df.wave
#y=df.intensity
max(W11)
df
plt.plot(Tep,W11)
plt.title('Mass lost  ')
plt.xlabel('Temperature (c)')
plt.ylabel('mass mg')
plt.legend()
plt.grid()
plt.show()
```

```
No handles with labels found to put in legend.
```

```
0       735.036
1       735.035
2       735.035
3       735.035
4       735.034
         ...
3175    735.013
3176    735.013
3177    735.013
3178    735.013
3179    735.013
Name: Weight_mg, Length: 3180, dtype: float64 0       0.999984
1       0.999982
2       0.999982
3       0.999982
4       0.999981
          ...
3175    0.999952
3176    0.999952
3177    0.999952
3178    0.999952
3179    0.999952
Name: Weight_mg, Length: 3180, dtype: float64
```



In [ ]:

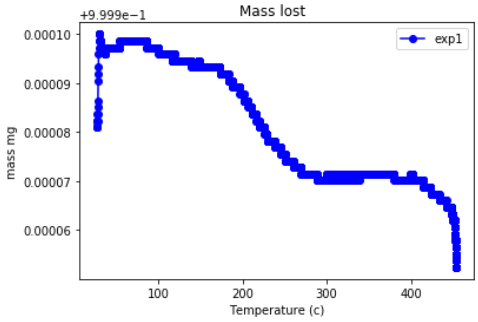
In [3]:

```
#HF
```

plt.plot(Tep,W,'bo-') plt.grid()

In [4]:

```
plt.plot(Tep,Wr,'bo-',label='exp1')
plt.grid()
#plt.axis([0,453,99.9948,100.001])
plt.title('Mass lost  ')
plt.xlabel('Temperature (c)')
plt.ylabel('mass mg')
plt.legend()
plt.grid()
plt.show()
```



In [5]:

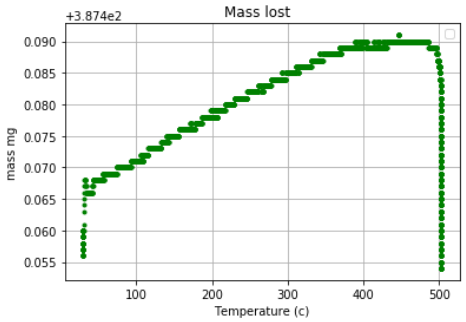
```
min(W11)
MM=max(W11)
ML=max(W11)- min(W11)
ML
print('MM=', max(W11),'mg','ML= ',ML,'mg')
x=(162980/18015)*(ML/(max(W11)-ML))
Y=(MM-ML)/162980
print('x=',x,'Y= ',Y)
print(ML/MM)
x/Y
print(max(W11))
```

```
MM= 735.048 mg ML=  0.03499999999996817 mg
x= 0.000430797397437005 Y=  0.004509835562645724
4.761593800672632e-05
735.048
```

In [6]:

```
df=pd.read_csv('B_VOSO4c.txt',delimiter='\s+')
dg=pd.read_csv('VOSO4a.txt',delimiter='\s+')
dh=pd.read_csv('VOSO4B.txt',delimiter='\s+')
#dh.
HF=df.HF
W2=dg.Weight
Tep2=dg.Ts
Tep11 =df.Ts
W22=df.W
Wr=(W22/735.048)
time=df.t
HF=np.abs([HF])
#print(W,Wr)
plt.plot(Tep11,W22,'.g',)
max(W2)
#Wc is weight of crucible
WC=336.52
W2=W2-WC
W2=(W22-353.63)/735.048
#W=W-Wc
#WL=max(W)-min(w)
plt.title('Mass lost  ')
plt.xlabel('Temperature (c)')
plt.ylabel('mass mg')
plt.legend()
plt.grid()
plt.show()
```

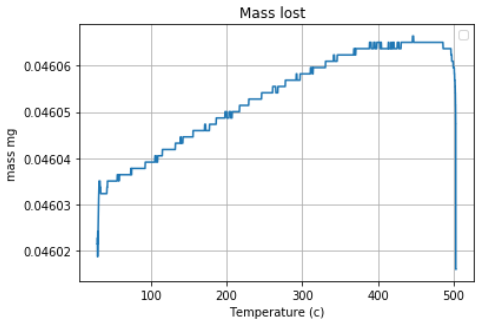
```
No handles with labels found to put in legend.
```



In [7]:

```
plt.plot(Tep2,W2)
plt.title('Mass lost  ')
plt.xlabel('Temperature (c)')
plt.ylabel('mass mg')
plt.legend()
plt.grid()
plt.show()
```

```
No handles with labels found to put in legend.
```



In [8]:

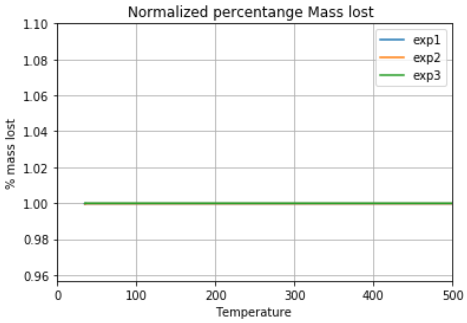
```
df1=pd.read_csv('BVOSO4air1.txt',delimiter='\s+')
df2=pd.read_csv('BVOSO4air2.txt',delimiter='\s+')
df3=pd.read_csv('BVOSO4air3.txt',delimiter='\s+')
df1
HF1=df1.HF
T1 =df1.Ts
W1=df1.Weight
#W1=W1-347.258
Wr1=(W1/2.44705e+002)
t1=df1.t
HF=np.abs([HF])
#print(W1,Wr1)
#X=df.wave
#y=df.intensity
max(W1)
HF2=df2.HF
T2 =df2.Ts
W2=df2.Weight
Wr2=(W2/2.44705e+002)
t2=df2.t
HF3=df3.HF
T3 =df3.Ts
W3=df3.Weight
Wr3=(W3/235.13099999999997)
t1=df1.t
W1
max(W3)
```

Out[8]:

```
235.13099999999997
```

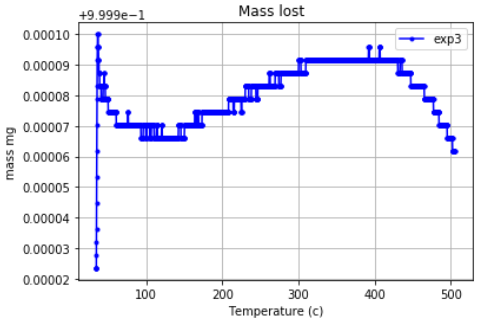
In [9]:

```
#Last set of data
plt.plot(T1,Wr2,label ='exp1')
plt.plot(T2,Wr2,label ='exp2')
plt.plot(T3,Wr3,label ='exp3')
plt.legend()
plt.axis([0,500,0.9568,1.1])
plt.title('Normalized percentange Mass lost  ')
plt.xlabel('Temperature ')
plt.ylabel('% mass lost')
plt.grid()
plt.show()
```



In [10]:

```
plt.plot(T3,Wr3,'.-b',label='exp3')
plt.title('Mass lost  ')
plt.xlabel('Temperature (c)')
plt.ylabel('mass mg')
plt.legend()
plt.grid()
plt.show()
```



In [11]:

```
#water of crystalization mass analysis
min(W1)
MM1=max(W1)
ML1=max(W1)- min(W1)
ML
print('MM=', max(W1),'mg','ML= ',ML1,'mg')
x=(162980/18015)*(ML1/(max(W1)-ML1))
Y=(MM1-ML1)/162980
print('x=',x,'Y= ',Y)
print(ML1/MM1)
x/Y
print(max(W1))
print(ML)
```

```
MM= 244.705 mg ML=  0.05099999999998772 mg
x= 0.0018858967079585784 Y=  0.001501128972880108
0.00020841421303196796
244.705
0.05099999999996817
```

In [12]:

```
df1
```

Out[12]:

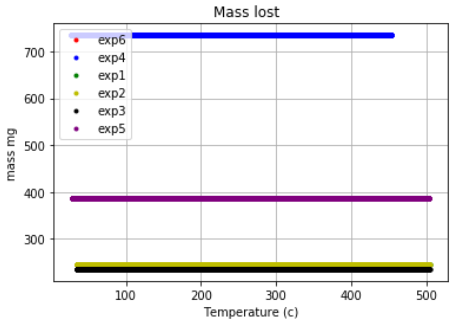
	Index	Ts	t	HF	Weight	Tr
0	0	34.0762	0.0	-1.60275	244.690	25.0000
1	1	34.0228	1.0	-1.61987	244.689	25.1667
2	2	34.0027	2.0	-1.64299	244.689	25.3333
3	3	33.9873	3.0	-1.66798	244.689	25.5000
4	4	34.0040	4.0	-2.03566	244.689	25.6667
...	...	...	...	...	...	...
2846	2846	504.2420	2846.0	-23.75100	244.654	499.3330
2847	2847	504.4090	2847.0	-23.75810	244.654	499.5000
2848	2848	504.5820	2848.0	-23.76420	244.654	499.6670
2849	2849	504.7390	2849.0	-23.76990	244.654	499.8330
2850	2850	504.9020	2850.0	-23.77480	244.654	500.0000

2851 rows × 6 columns

In [23]:

```
plt.plot(Tep11,W22, '.r',label='exp6',)
plt.plot(Tep,W11,'.b',label='exp4',)
plt.plot(T1,W1,'.g',label ='exp1',)
plt.plot(T2,W2,'.y',label ='exp2',)
plt.plot(T3,W3,'.k',label ='exp3',)

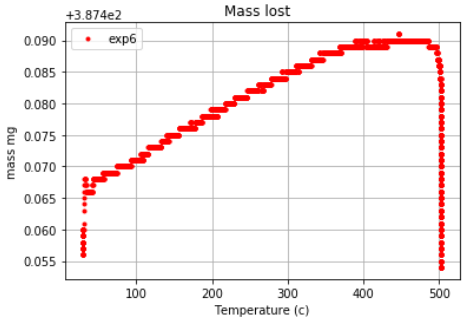
plt.plot(Tep2,W22,'.',color='purple',label='exp5')
plt.title('Mass lost  ')
plt.xlabel('Temperature (c)')
plt.ylabel('mass mg')
plt.legend()
plt.grid()
plt.show()
```



In [29]:

```
plt.plot(Tep11,W22, '.r',label='exp6',)

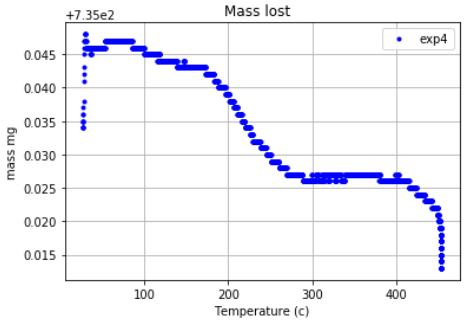
plt.title('Mass lost  ')
plt.xlabel('Temperature (c)')
plt.ylabel('mass mg')
plt.legend()
plt.grid()
plt.show()
```



In [30]:

```
plt.plot(Tep,W11,'.b',label='exp4',)

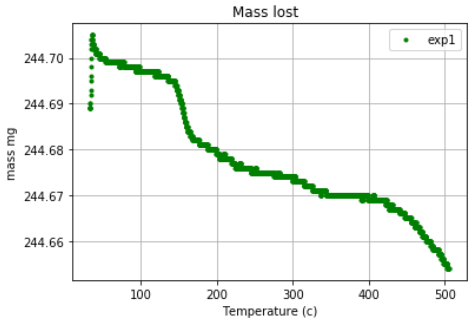
plt.title('Mass lost  ')
plt.xlabel('Temperature (c)')
plt.ylabel('mass mg')
plt.legend()
plt.grid()
plt.show()
```



In [28]:

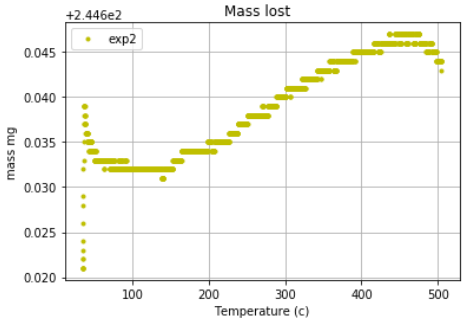
```
plt.plot(T1,W1,'.g',label ='exp1',)

plt.title('Mass lost  ')
plt.xlabel('Temperature (c)')
plt.ylabel('mass mg')
plt.legend()
plt.grid()
plt.show()
```



In [32]:

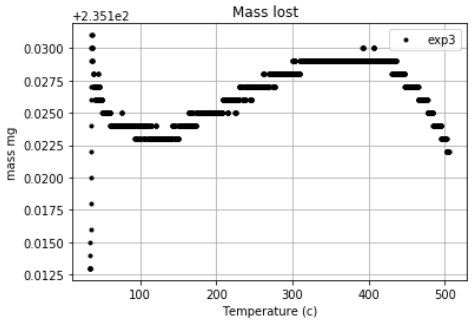
```
plt.plot(T2,W2,'.y',label ='exp2',)
plt.title('Mass lost  ')
plt.xlabel('Temperature (c)')
plt.ylabel('mass mg')
plt.legend()
plt.grid()
plt.show()
```



In [26]:

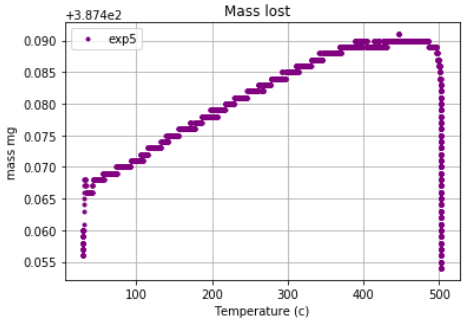
```
plt.plot(T3,W3,'.k',label ='exp3',)

#plt.plot(Tep2,W22,'.',color='purple',label='exp5')
plt.title('Mass lost  ')
plt.xlabel('Temperature (c)')
plt.ylabel('mass mg')
plt.legend()
plt.grid()
plt.show()
```



In [27]:

```
plt.plot(Tep2,W22,'.',color='purple',label='exp5')
plt.title('Mass lost  ')
plt.xlabel('Temperature (c)')
plt.ylabel('mass mg')
plt.legend()
plt.grid()
plt.show()
```



In [ ]:

In [1]:

```
import pandas as pd
import numpy as np
from numpy import arange
from scipy.optimize import curve_fit
from scipy import constants
from scipy.constants import find
from matplotlib import pyplot as plt
import math
from scipy import special
```

In [2]:

```
df=pd.read_csv('VOSO4_532nm_10P_10accum_Acq1_Copy.txt',delimiter='\t')
df
X=df.wave
y=df.intensity
#print(df)
```

In [3]:

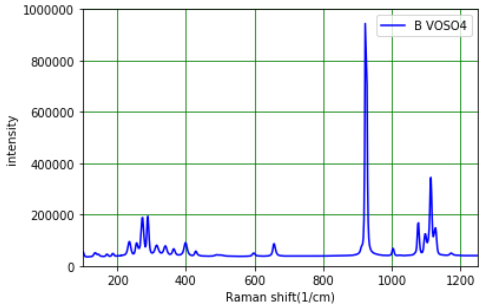
```
Q=df[['wave','intensity']]
Xp=Q[Q.wave>900]
Xp=Xp[Xp.wave<940]
xi=Xp.wave
yi=Xp.intensity
#Xp
```

In [4]:

```
#plt.plot(xi,yi)
```

In [5]:

```
X=df.wave
Y=df.intensity
plt.plot(X,Y,'b-',label='B VOSO4')
plt.grid(color='green')
plt.axis([100,1250,0,1000000])
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
#plt.grid()
plt.show()
```

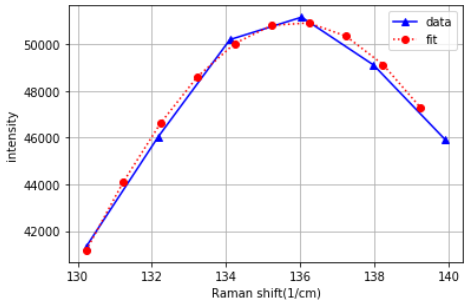


In [6]:

```
Xp=Q[Q.wave>130]
Xp=Xp[Xp.wave<140]
xi=Xp.wave
yi=Xp.intensity
def ampi(x,a,b,c):
    return a*np.exp(-0.5*((x-b)/c)**2)
#x=np.random.uniform(120, 140., 100)
    #a=1/(c*np.sqrt(2*np.pi))
x=xi
y=yi

popt, pcov = curve_fit(ampi,xi , yi, maxfev=1500000 ,p0=(30000,10000,35000),bounds=(0,5
00000))
a,b,c= popt
print(popt)
plt.plot(xi, yi, 'b^-',label='data')
x_line =arange(min(x), max(x), 1)
y_line = ampi(x_line,a,b,c)
#plt.plot(x,amp(x,*popt),'ro:',label='fit')
plt.plot(x_line, y_line, 'ro:', color='red',label='fit')
#plt.axis([1000,1200,0.00,1000009])
#plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
plt.grid()
plt.show()
#print(pcov)
perr=np.sqrt(np.diag(pcov))
print(perr)
```

```
[5.09617918e+04 1.35887633e+02 8.66037997e+00]
```




```
[2.67520662e+02 9.77754382e-02 2.61165704e-01]
```

In [7]:

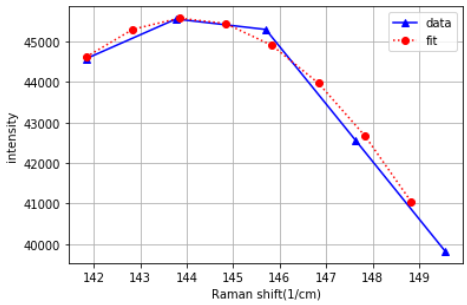
```
#I(J)=CSjNg/Qr*exp(-BJ(J+1)hc/KT)
#I=CNI0
```

In [8]:

```
Xp=Q[Q.wave>140]
Xp=Xp[Xp.wave<150]
x2=Xp.wave
y2=Xp.intensity
def amp2(x,a2,b2,c2):
    return a2*np.exp(-0.5*((x-b2)/c2)**2)
    #a2=1/(c2*np.sqrt(2*np.pi))
#x=np.random.uniform(120, 140., 100)
x=x2
y=y2

popt,pcov2= curve_fit(amp2,x2 , y2, maxfev=1500000 ,p0=(30000,10000,35000),bounds=(0,50
000))
a2,b2,c2= popt
print(popt)
plt.plot(x2, y2, 'b^-',label='data')
x2_line =arange(min(x), max(x), 1)
y2_line = amp2(x2_line,a2,b2,c2)
#plt.plot(x,amp(x,*popt),'ro:',label='fit')
plt.plot(x2_line, y2_line, 'ro:', color='red',label='fit')
#plt.axis([1000,1200,0.00,1000009])
#plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
plt.grid()
plt.show()
perr2=np.sqrt(np.diag(pcov2))
print(perr2)
```

```
[4.55880715e+04 1.44011365e+02 1.05177650e+01]
```



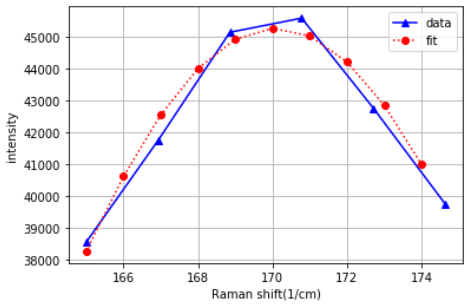

```
[236.40906582   0.27111661   0.71932368]
```

In [9]:

```
Xp=Q[Q.wave>165]
Xp=Xp[Xp.wave<175]
x3=Xp.wave
y3=Xp.intensity
def amp3(x,a3,b3,c3):
    return a3*np.exp(-0.5*((x-b3)/c3)**2)
    #a3=1/(c3*np.sqrt(2*np.pi))
#x=np.random.uniform(120, 140., 100)
x=x3
y=y3

popt,pcov3= curve_fit(amp3,x3 , y3, maxfev=1500000 ,p0=(30000,10000,35000),bounds=(0,50
000))
a3,b3,c3= popt
print(popt)
plt.plot(x3, y3, 'b^-',label='data')
x3_line =arange(min(x), max(x), 1)
y3_line = amp3(x3_line,a3,b3,c3)
#plt.plot(x,amp(x,*popt),'ro:',label='fit')
plt.plot(x3_line, y3_line, 'ro:', color='red',label='fit')
#plt.axis([1000,1200,0.00,1000009])
#plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
plt.grid()
plt.show()
perr3=np.sqrt(np.diag(pcov3))
print(perr3)
```

```
[4.52547357e+04 1.70089874e+02 8.78177585e+00]
```



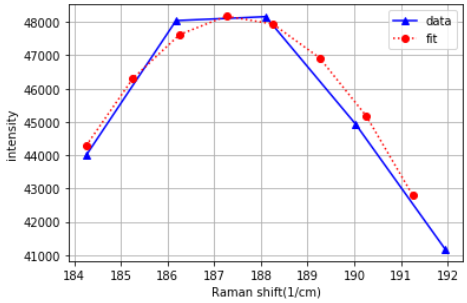

```
[4.01587167e+02 1.51176883e-01 4.54272393e-01]
```

In [10]:

```
Xp=Q[Q.wave>183]
Xp=Xp[Xp.wave<192]
x4=Xp.wave
y4=Xp.intensity
def amp4(x,a4,b4,c4):
    return a4*np.exp(-0.5*((x-b4)/c4)**2)
    #a4=1/(c4*np.sqrt(2*np.pi))
#x=np.random.uniform(120, 140., 100)
x=x4
y=y4

popt,pcov4= curve_fit(amp4,x4 , y4, maxfev=1500000 ,p0=(30000,10000,35000),)
a4,b4,c4= popt
print(popt)
plt.plot(x4, y4, 'b^-',label='data')
x4_line =arange(min(x), max(x), 1)
y4_line = amp4(x4_line,a4,b4,c4)
#plt.plot(x,amp(x,*popt),'ro:',label='fit')
plt.plot(x4_line, y4_line, 'ro:', color='red',label='fit')
#plt.axis([1000,1200,0.00,1000009])
#plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
plt.grid()
plt.show()
perr4=np.sqrt(np.diag(pcov4))
print(perr4)
```

```
[4.81935707e+04 1.87458416e+02 7.78518980e+00]
```



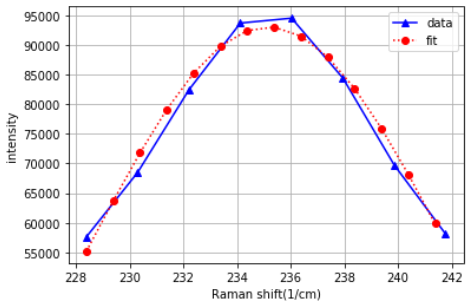

```
[4.86905040e+02 1.79521076e-01 5.34615376e-01]
```

In [11]:

```
Xp=Q[Q.wave>228]
Xp=Xp[Xp.wave<242]
x5=Xp.wave
y5=Xp.intensity
def amp5(x,a5,b5,c5):
    return a5*np.exp(-0.5*((x-b5)/c5)**2)
    #a5=1/(c5*np.sqrt(2*np.pi))
#x=np.random.uniform(120, 140., 100)
x=x5
y=y5

popt,pcov5= curve_fit(amp5,x5 , y5, maxfev=1500000 ,p0=(30000,10000,35000))
a5,b5,c5= popt
print(popt)
plt.plot(x5, y5, 'b^-',label='data')
x5_line =arange(min(x), max(x), 1)
y5_line = amp5(x5_line,a5,b5,c5)
#plt.plot(x,amp(x,*popt),'ro:',label='fit')
plt.plot(x5_line, y5_line, 'ro:', color='red',label='fit')
#plt.axis([1000,1200,0.00,1000009])
#plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
plt.grid()
plt.show()
perr5=np.sqrt(np.diag(pcov5))
print(perr5)
```

```
[9.30311502e+04 2.35158753e+02 6.62788382e+00]
```



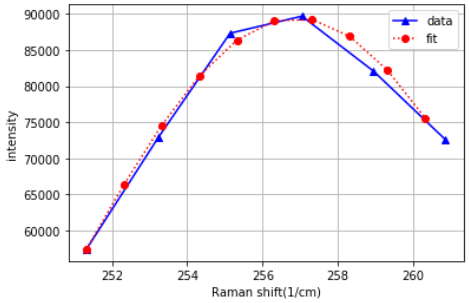

```
[1.51984529e+03 1.42591852e-01 2.39427715e-01]
```

In [12]:

```
Xp=Q[Q.wave>250]
Xp=Xp[Xp.wave<262]
x6=Xp.wave
y6=Xp.intensity
def amp6(x,a6,b6,c6):
    return a6*np.exp(-0.5*((x-b6)/c6)**2)
    #a6=1/(c6*np.sqrt(2*np.pi))
#x=np.random.uniform(120, 140., 100)
x=x6
y=y6

popt, pcov6 = curve_fit(amp6,x6 , y6, maxfev=1500000 ,p0=(30000,10000,35000))
a6,b6,c6= popt
print(popt)
plt.plot(x6, y6, 'b^-',label='data')
x6_line =arange(min(x), max(x), 1)
y6_line = amp6(x6_line,a6,b6,c6)
#plt.plot(x,amp(x,*popt),'ro:',label='fit')
plt.plot(x6_line, y6_line, 'ro:', color='red',label='fit')
#plt.axis([1000,1200,0.00,1000009])
#plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
plt.grid()
plt.show()
perr6=np.sqrt(np.diag(pcov6))
print(perr6)
```

```
[8.94787182e+04 2.56885187e+02 5.90947808e+00]
```




```
[1.18358571e+03 1.24708620e-01 2.34479500e-01]
```

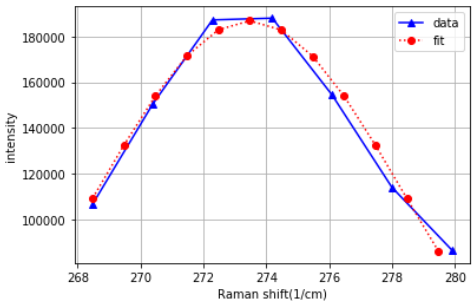
In [13]:

```
Xp=Q[Q.wave>267]
Xp=Xp[Xp.wave<280]
x61=Xp.wave
y61=Xp.intensity
def amp61(x,a61,b61,c61):
    return a61*np.exp(-0.5*((x-b61)/c61)**2)
    #a61=1/(c61*np.sqrt(2*np.pi))

#x=np.random.uniform(120, 140., 100)
x=x61
y=y61

popt, pcov61= curve_fit(amp61,x61 , y61, maxfev=1500000 ,p0=(30000,10000,35000))
a61,b61,c61= popt
print(popt)
plt.plot(x61, y61, 'b^-',label='data')
x61_line =arange(min(x), max(x), 1)
y61_line = amp6(x61_line,a61,b61,c61)
#plt.plot(x,amp(x,*popt),'ro:',label='fit')
plt.plot(x61_line, y61_line, 'ro:', color='red',label='fit')
#plt.axis([1000,1200,0.00,1000009])
#plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
plt.grid()
plt.show()
perr61=np.sqrt(np.diag(pcov61))
print(perr61)
```

```
[1.86883223e+05 2.73471410e+02 4.81930954e+00]
```



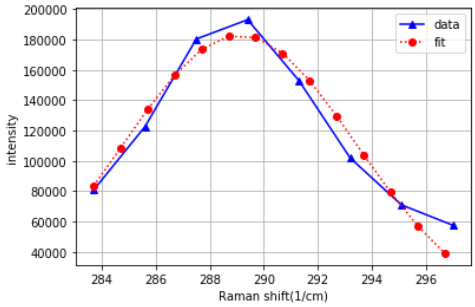

```
[4.93267417e+03 1.60479456e-01 2.23226833e-01]
```

In [14]:

```
Xp=Q[Q.wave>282]
Xp=Xp[Xp.wave<298]
x7=Xp.wave
y7=Xp.intensity
def amp7(x,a7,b7,c7):
    return a7*np.exp(-0.5*((x-b7)/c7)**2)
    #a7=1/(c7*np.sqrt(2*np.pi))
#x=np.random.uniform(120, 140., 100)
x=x7
y=y7

popt, pcov7 = curve_fit(amp7,x7 , y7, maxfev=1500000 ,p0=(30000,10000,35000))
a7,b7,c7= popt
print(popt)
plt.plot(x7, y7, 'b^-',label='data')
x7_line =arange(min(x), max(x), 1)
y7_line = amp7(x7_line,a7,b7,c7)
plt.plot(x7_line, y7_line, 'ro:', color='red',label='fit')
#plt.axis([1000,1200,0.00,1000009])
#plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
plt.grid()
plt.show()
perr7=np.sqrt(np.diag(pcov7))
print(perr7)
```

```
[1.83025075e+05 2.89113289e+02 4.31925099e+00]
```



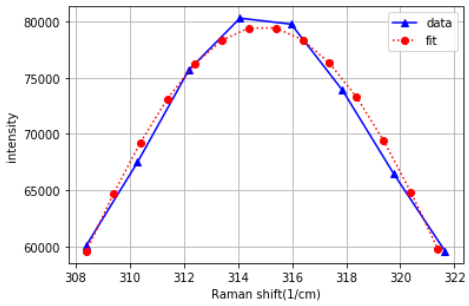

```
[9.52650329e+03 2.69905335e-01 3.14911198e-01]
```

In [15]:

```
Xp=Q[Q.wave>308]
Xp=Xp[Xp.wave<322]
x8=Xp.wave
y8=Xp.intensity
def amp8(x,a8,b8,c8):
    return a8*np.exp(-0.5*((x-b8)/c8)**2)
    #a8=1/(c8*np.sqrt(2*np.pi))
#x=np.random.uniform(120, 140., 100)
x=x8
y=y8

popt, pcov8= curve_fit(amp8,x8 , y8, maxfev=1500000 ,p0=(30000,10000,35000))
a8,b8,c8= popt
print(popt)
plt.plot(x8, y8, 'b^-',label='data')
x8_line =arange(min(x), max(x), 1)
y8_line = amp8(x8_line,a8,b8,c8)
#plt.plot(x,amp(x,*popt),'ro:',label='fit')
plt.plot(x8_line, y8_line, 'ro:', color='red',label='fit')
#plt.axis([1000,1200,0.00,1000009])
#plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
plt.grid()
plt.show()
perr8=np.sqrt(np.diag(pcov8))
print(perr8)
```

```
[7.95422498e+04 3.14904493e+02 8.57353083e+00]
```



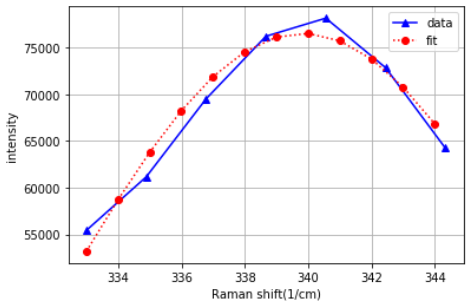

```
[7.23084593e+02 1.20117508e-01 2.64088470e-01]
```

In [16]:

```
Xp=Q[Q.wave>332]
Xp=Xp[Xp.wave<346]
x9=Xp.wave
y9=Xp.intensity
def amp9(x,a9,b9,c9):
    return a9*np.exp(-0.5*((x-b9)/c9)**2)
    #a9=1/(c9*np.sqrt(2*np.pi))
#x=np.random.uniform(120, 140., 100)
x=x9
y=y9

popt, pcov9 = curve_fit(amp9,x9 , y9, maxfev=1500000 ,p0=(30000,10000,35000))
a9,b9,c9= popt
print(popt)
plt.plot(x9, y9, 'b^-',label='data')
x9_line =arange(min(x), max(x), 1)
y9_line = amp9(x9_line,a9,b9,c9)
#plt.plot(x,amp(x,*popt),'ro:',label='fit')
plt.plot(x9_line, y9_line, 'ro:', color='red',label='fit')
#plt.axis([1000,1200,0.00,1000009])
#plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
plt.grid()
plt.show()
perr9=np.sqrt(np.diag(pcov9))
print(perr9)
```

```
[7.65399481e+04 3.39827481e+02 8.00755748e+00]
```



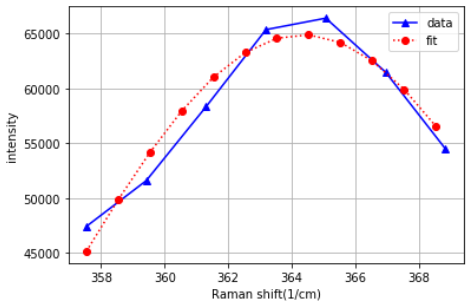

```
[1.23058408e+03 2.46181527e-01 5.08960000e-01]
```

In [17]:

```
Xp=Q[Q.wave>356]
Xp=Xp[Xp.wave<370]
x10=Xp.wave
y10=Xp.intensity
def amp10(x,a10,b10,c10):
    return a10*np.exp(-0.5*((x-b10)/c10)**2)
    #a10=1/(c10*np.sqrt(2*np.pi))
#x=np.random.uniform(120, 140., 100)
x=x10
y=y10

popt, pcov10 = curve_fit(amp10,x10 , y10, maxfev=1500000 ,p0=(300000,1000000,350000))
a10,b10,c10= popt
print(popt)
plt.plot(x10, y10, 'b^-',label='data')
x10_line =arange(min(x), max(x), 1)
y10_line = amp10(x10_line,a10,b10,c10)
#plt.plot(x,amp(x,*popt),'ro:',label='fit')
plt.plot(x10_line, y10_line, 'ro:', color='red',label='fit')
#plt.axis([1000,1200,0.00,1000009])
#plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
plt.grid()
plt.show()
perr10=np.sqrt(np.diag(pcov10))
print(perr10)
```

```
[6.49213839e+04 3.64342251e+02 7.99131558e+00]
```



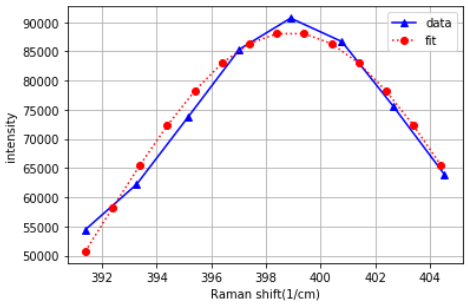

```
[1.27990997e+03 3.01106194e-01 6.23504416e-01]
```

In [18]:

```
Xp=Q[Q.wave>391]
Xp=Xp[Xp.wave<406]
x11=Xp.wave
y11=Xp.intensity
def amp11(x,a11,b11,c11):
    return a11*np.exp(-0.5*((x-b11)/c11)**2)
    #a11=1/(c11*np.sqrt(2*np.pi))
#x=np.random.uniform(120, 140., 100)
x=x11
y=y11

popt, pcov11 = curve_fit(amp11,x11 , y11, maxfev=1500000 ,p0=(80000,100000,35000))
a11,b11,c11= popt
print(popt)
plt.plot(x11, y11, 'b^-',label='data')
x11_line =arange(min(x), max(x), 1)
y11_line = amp11(x11_line,a11,b11,c11)
#plt.plot(x,amp(x,*popt),'ro:',label='fit')
plt.plot(x11_line, y11_line, 'ro:', color='red',label='fit')
#plt.axis([1000,1200,0.00,1000009])
#plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
plt.grid()
plt.show()
perr11=np.sqrt(np.diag(pcov11))
print(perr11)
```

```
[8.82580598e+04 3.98898434e+02 7.12752601e+00]
```



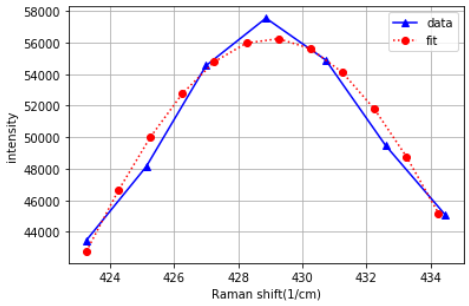

```
[1.60136112e+03 1.91660499e-01 3.34332835e-01]
```

In [19]:

```
Xp=Q[Q.wave>423]
Xp=Xp[Xp.wave<435]
x12=Xp.wave
y12=Xp.intensity
def amp12(x,a12,b12,c12):
    return a12*np.exp(-0.5*((x-b12)/c12)**2)
    #a12=1/(c12*np.sqrt(2*np.pi))
#x=np.random.uniform(120, 140., 100)
x=x12
y=y12

popt, pcov12 = curve_fit(amp12,x12 , y12, maxfev=1500000 ,p0=(300000,1000000,350000),bo
unds=(0,5000000))
a12,b12,c12= popt
print(popt)
plt.plot(x12, y12, 'b^-',label='data')
x12_line =arange(min(x), max(x), 1)
y12_line = amp12(x12_line,a12,b12,c12)
#plt.plot(x,amp(x,*popt),'ro:',label='fit')
plt.plot(x12_line, y12_line, 'ro:', color='red',label='fit')
#plt.axis([1000,1200,0.00,1000009])
#plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
plt.grid()
plt.show()
perr12=np.sqrt(np.diag(pcov12))
print(perr12)
```

```
[5.62665929e+04 4.29061960e+02 7.83872932e+00]
```



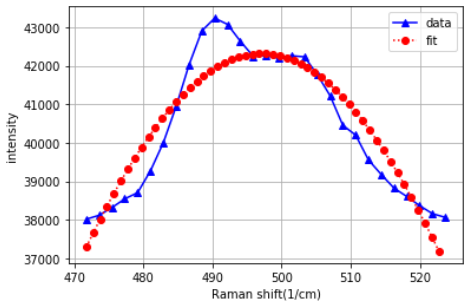

```
[7.76188316e+02 1.73776062e-01 4.06685877e-01]
```

In [20]:

```
Xp=Q[Q.wave>470]
Xp=Xp[Xp.wave<525]
x13=Xp.wave
y13=Xp.intensity
def amp13(x,a13,b13,c13):
    return a13*np.exp(-0.5*((x-b13)/c13)**2)
    #a13=1/(c13*np.sqrt(2*np.pi))
#x=np.random.uniform(120, 140., 100)
x=x13
y=y13

popt, pcov13= curve_fit(amp13,x13 , y13, maxfev=1500000 ,p0=(300000,1000000,350000))
a13,b13,c13= popt
print(popt)
plt.plot(x13, y13, 'b^-',label='data')
x13_line =arange(min(x), max(x), 1)
y13_line = amp13(x13_line,a13,b13,c13)
#plt.plot(x,amp(x,*popt),'ro:',label='fit')
plt.plot(x13_line, y13_line, 'ro:', color='red',label='fit')
#plt.axis([1000,1200,0.00,1000009])
#plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
plt.grid()
plt.show()
perr13=np.sqrt(np.diag(pcov13))
print(perr13)
```

```
[42316.50033808   497.10520185    50.41512429]
```



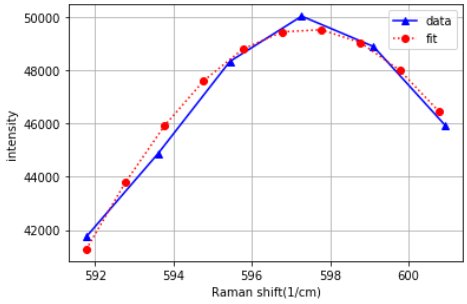

```
[197.59781192   0.54521818   1.95987977]
```

In [21]:

```
Xp=Q[Q.wave>590]
Xp=Xp[Xp.wave<602]
x14=Xp.wave
y14=Xp.intensity
def amp14(x,a14,b14,c14):
    return a14*np.exp(-0.5*((x-b14)/c14)**2)
    #a14=1/(c14*np.sqrt(2*np.pi))
#x=np.random.uniform(120, 140., 100)
x=x14
y=y14

popt, pcov14= curve_fit(amp14,x14 , y14, maxfev=1500000 ,p0=(300000,1000000,350000))
a14,b14,c14= popt
print(popt)
plt.plot(x14, y14, 'b^-',label='data')
x14_line =arange(min(x), max(x), 1)
y14_line = amp14(x14_line,a14,b14,c14)
#plt.plot(x,amp(x,*popt),'ro:',label='fit')
plt.plot(x14_line, y14_line, 'ro:', color='red',label='fit')
#plt.axis([1000,1200,0.00,1000009])
#plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
plt.grid()
plt.show()
perr14=np.sqrt(np.diag(pcov14))
print(perr14)
```

```
[4.95540631e+04 5.97416719e+02 9.33612025e+00]
```



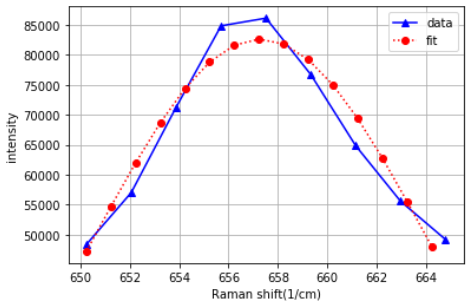

```
[3.67858025e+02 1.85247815e-01 5.16116806e-01]
```

In [22]:

```
Xp=Q[Q.wave>650]
Xp=Xp[Xp.wave<665]
x15=Xp.wave
y15=Xp.intensity
def amp15(x,a15,b15,c15):
    return a15*np.exp(-0.5*((x-b15)/c15)**2)
    #a15=1/(c15*np.sqrt(2*np.pi))
#x=np.random.uniform(120, 140., 100)
x=x15
y=y15

popt, pcov15 = curve_fit(amp15,x15 , y15, maxfev=1500000 ,p0=(300000,1000000,350000))
a15,b15,c15= popt
print(popt)
plt.plot(x15, y15, 'b^-',label='data')
x15_line =arange(min(x), max(x), 1)
y15_line = amp15(x15_line,a15,b15,c15)
#plt.plot(x,amp(x,*popt),'ro:',label='fit')
plt.plot(x15_line, y15_line, 'ro:', color='red',label='fit')
#plt.axis([1000,1200,0.00,1000009])
#plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
plt.grid()
plt.show()
perr15=np.sqrt(np.diag(pcov15))
print(perr15)
```

```
[8.26237588e+04 6.57292880e+02 6.67276646e+00]
```



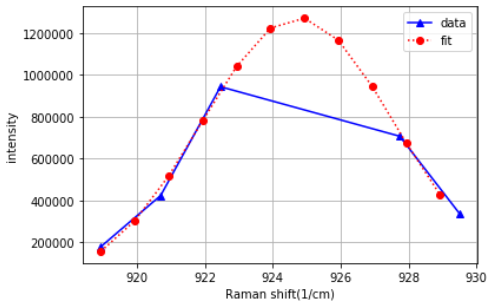

```
[2.37862469e+03 2.46895252e-01 3.88827193e-01]
```

In [23]:

```
Xp=Q[Q.wave>918]
Xp=Xp[Xp.wave<930]
x16=Xp.wave
y16=Xp.intensity
def amp16(x,a16,b16,c16):
    return a16*np.exp(-0.5*((x-b16)/c16)**2)
    #a16=1/(c16*np.sqrt(2*np.pi))
#x=np.random.uniform(120, 140., 100)
x=x16
y=y16

popt, pcov16= curve_fit(amp16,x16 , y16, maxfev=1500000 ,p0=(12000000,100000,35000))
a16,b16,c16= popt
print(popt)
plt.plot(x16, y16, 'b^-',label='data')
x16_line =arange(min(x), max(x), 1)
y16_line = amp16(x16_line,a16,b16,c16)
#plt.plot(x,amp(x,*popt),'ro:',label='fit')
plt.plot(x16_line, y16_line, 'ro:', color='red',label='fit')
#plt.axis([1000,1200,0.00,1000009])
#plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
plt.grid()
plt.show()
perr16=np.sqrt(np.diag(pcov16))
print(perr16)
```

```
[1.27541469e+06 9.24737284e+02 2.83341429e+00]
```



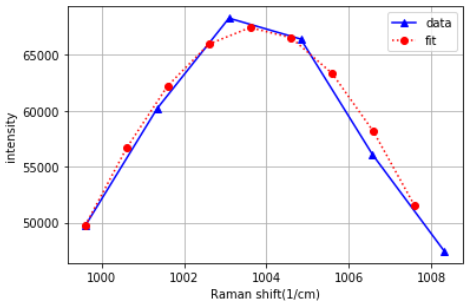

```
[7.84337479e+04 8.70879740e-02 1.27844153e-01]
```

In [24]:

```
Xp=Q[Q.wave>999]
Xp=Xp[Xp.wave<1010]
x17=Xp.wave
y17=Xp.intensity
def amp17(x,a17,b17,c17):
    return a17*np.exp(-0.5*((x-b17)/c17)**2)
    #a17=1/(c17*np.sqrt(2*np.pi))
#x=np.random.uniform(120, 140., 100)
x=x17
y=y17

popt,pcov17= curve_fit(amp17,x17 , y17, maxfev=1500000 ,p0=(3000000,100000,35000))
a17,b17,c17= popt
print(popt)
plt.plot(x17, y17, 'b^-',label='data')
x17_line =arange(min(x), max(x), 1)
y17_line = amp17(x17_line,a17,b17,c17)
#plt.plot(x,amp(x,*popt),'ro:',label='fit')
plt.plot(x17_line, y17_line, 'ro:', color='red',label='fit')
#plt.axis([1000,1200,0.00,1000009])
#plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
plt.grid()
plt.show()
perr17=np.sqrt(np.diag(pcov17))
print(perr17)
```

```
[6.74497162e+04 1.00372310e+03 5.28147602e+00]
```



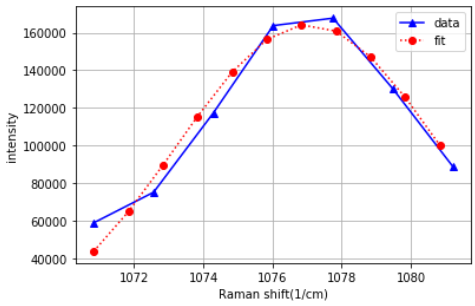

```
[1.14261221e+03 1.28702410e-01 2.53580384e-01]
```

In [41]:

```
Xp=Q[Q.wave>1070]
Xp=Xp[Xp.wave<1082]
x18=Xp.wave
y18=Xp.intensity
def amp18(x,a18,b18,c18):
    return a18*np.exp(-0.5*((x-b18)/c18)**2)
#    a18=1/(c18*np.sqrt(2*np.pi))
#x=np.random.uniform(120, 140., 100)
x=x18
y=y18

popt, pcov18 = curve_fit(amp18,x18 , y18, maxfev=1500000 ,p0=(12000000,100000,35000))
a18,b18,c18= popt
print(popt)
plt.plot(x18, y18, 'b^-',label='data')
x18_line =arange(min(x), max(x), 1)
y18_line = amp18(x18_line,a18,b18,c18)
#plt.plot(x,amp(x,*popt),'ro:',label='fit')
plt.plot(x18_line, y18_line, 'ro:', color='red',label='fit')
#plt.axis([1000,1200,0.00,1000009])
#plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
plt.grid()
plt.show()
perr18=np.sqrt(np.diag(pcov18))
print(perr18)
```

```
[1.64392953e+05 1.07704084e+03 3.81670250e+00]
```



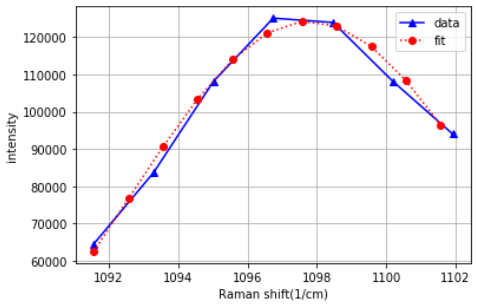

```
[7.07085842e+03 2.04101741e-01 2.52609769e-01]
```

In [26]:

```
Xp=Q[Q.wave>1090]
Xp=Xp[Xp.wave<1102]
x19=Xp.wave
y19=Xp.intensity
def amp19(x,a19,b19,c19):
    return a19*np.exp(-0.5*((x-b19)/c19)**2)
#    a19=1/(c19*np.sqrt(2*np.pi))
#x=np.random.uniform(120, 140., 100)
x=x19
y=y19

popt, pcov19 = curve_fit(amp19,x19 , y19, maxfev=1500000 ,p0=(1200000,100000,35000))
a19,b19,c19= popt
print(popt)
plt.plot(x19, y19, 'b^-',label='data')
x19_line =arange(min(x), max(x), 1)
y19_line = amp19(x19_line,a19,b19,c19)
#plt.plot(x,amp(x,*popt),'ro:',label='fit')
plt.plot(x19_line, y19_line, 'ro:', color='red',label='fit')
#plt.axis([1000,1200,0.00,1000009])
#plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
plt.grid()
plt.show()
perr19=np.sqrt(np.diag(pcov19))
print(perr19)
```

```
[1.24302695e+05 1.09778532e+03 5.30680302e+00]
```



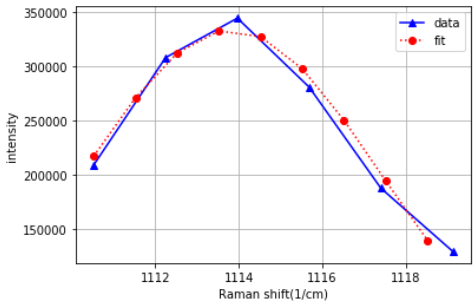

```
[2.07299117e+03 1.32109829e-01 2.07216562e-01]
```

In [27]:

```
Xp=Q[Q.wave>1110]
Xp=Xp[Xp.wave<1120]
x20=Xp.wave
y20=Xp.intensity
def amp20(x,a20,b20,c20):
    return a20*np.exp(-0.5*((x-b20)/c20)**2)
#    a20=1/(c20*np.sqrt(2*np.pi))
#x=np.random.uniform(120, 140., 100)
x=x20
y=y20

popt, pcov20 = curve_fit(amp20,x20 , y20, maxfev=1500000 ,p0=(12000000,100000,35000))
a20,b20,c20= popt
print(popt)
plt.plot(x20, y20, 'b^-',label='data')
x20_line =arange(min(x), max(x), 1)
y20_line = amp20(x20_line,a20,b20,c20)
#plt.plot(x,amp(x,*popt),'ro:',label='fit')
plt.plot(x20_line, y20_line, 'ro:', color='red',label='fit')
#plt.axis([1000,1200,0.00,1000009])
#plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
plt.grid()
plt.show()
perr20=np.sqrt(np.diag(pcov20))
print(perr20)
```

```
[3.33860507e+05 1.11382189e+03 3.55328463e+00]
```



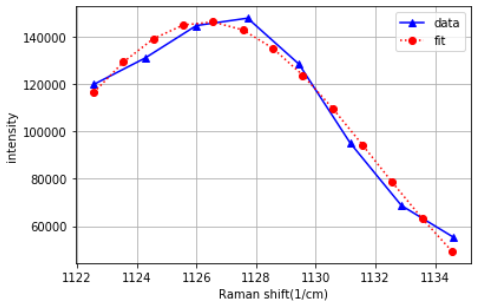

```
[1.19516078e+04 1.67756908e-01 2.17598548e-01]
```

In [28]:

```
Xp=Q[Q.wave>1122]
Xp=Xp[Xp.wave<1135]
x21=Xp.wave
y21=Xp.intensity
def amp21(x,a21,b21,c21):
    return a21*np.exp(-0.5*((x-b21)/c21)**2)
#    a21=1/(c21*np.sqrt(2*np.pi))
#x=np.random.uniform(120, 140., 100)
x=x21
y=y21

popt, pcov21 = curve_fit(amp21,x21 , y21, maxfev=1500000 ,p0=(12000000,100000,35000))
a21,b21,c21= popt
print(popt)
plt.plot(x21, y21, 'b^-',label='data')
x21_line =arange(min(x), max(x), 1)
y21_line = amp21(x21_line,a21,b21,c21)
#plt.plot(x,amp(x,*popt),'ro:',label='fit')
plt.plot(x21_line, y21_line, 'ro:', color='red',label='fit')
#plt.axis([1000,1200,0.00,1000009])
#plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
plt.grid()
plt.show()
perr21=np.sqrt(np.diag(pcov21))
print(perr21)
```

```
[1.46570921e+05 1.12633568e+03 5.57490950e+00]
```



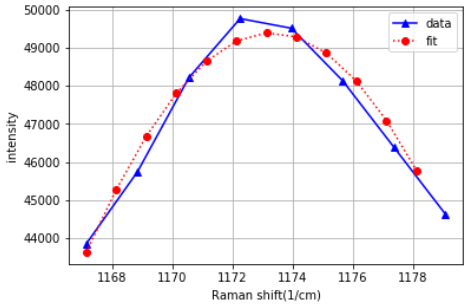

```
[3.52062506e+03 2.39318404e-01 3.03049798e-01]
```

In [29]:

```
Xp=Q[Q.wave>1167]
Xp=Xp[Xp.wave<1180]
x22=Xp.wave
y22=Xp.intensity
def amp22(x,a22,b22,c22):
    return a22*np.exp(-0.5*((x-b22)/c22)**2)
#    a22=1/(c22*np.sqrt(2*np.pi))
#x=np.random.uniform(120, 140., 100)
x=x22
y=y22

popt, pcov22= curve_fit(amp22,x22 , y22, maxfev=1500000 ,p0=(100000,100000,35000))
a22,b22,c22= popt
print(popt)
plt.plot(x22, y22, 'b^-',label='data')
x22_line =arange(min(x), max(x), 1)
y22_line = amp22(x22_line,a22,b22,c22)
#plt.plot(x,amp(x,*popt),'ro:',label='fit')
plt.plot(x22_line, y22_line, 'ro:', color='red',label='fit')
#plt.axis([1000,1200,0.00,1000009])
#plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
plt.grid()
plt.show()
perr22=np.sqrt(np.diag(pcov22))
print(perr22)
```

```
[4.94031075e+04 1.17329831e+03 1.23691588e+01]
```




```
[2.57125978e+02 1.44094642e-01 5.11814930e-01]
```

In [30]:

```
print(a,b,c,a2,a2,b2,c3,a2,b3,c3,a4,b4,c4,a5,b5,c5,a6,b6,c6,a7,b7,c7,a8,b8,c8,a9,b9,c9,
a11,b11,c11,a12,a12,b12,c13,a12,b13,c13,a14,b14,c14,a15,b15,c15,a16,b16,c16,a17,b17,c17
,a18,b18,c18,a19,b19,c19,a20,b20,c20,a21,b21,c21,a22,b22,c22)
```

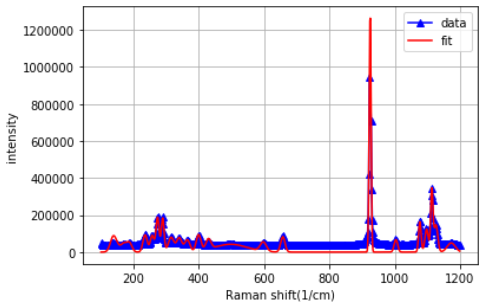
```
50961.79182500722 135.8876327170803 8.6603799688615 45588.07152775322 4558
8.07152775322 144.0113653767824 8.781775849046484 45588.07152775322 170.08
987406095264 8.781775849046484 48193.57066116601 187.45841644964412 7.7851
8979740763 93031.1502362745 235.1587529509383 6.627883819586427 89478.7181
7928331 256.8851872862778 5.9094780845763 59 183025.07450836798 289.1132894
8213753 4.319250988990481 79542.24975702904 314.9044930954107 8.5735308301
07966 76539.94805536408 339.82748138480287 8.007557484239396 88258.0598462
7648 398.8984337344434 7.127526008118037 56266.59294082497 56266.592940824
97 429.0619599965509 50.41512428577877 56266.59294082497 497.1052018521953
50.41512428577877 49554.06312306759 597.4167194840196 9.336120251977745 82
623.75884111467 657.2928800793715 6.672766457778943 1275414.6916343549 92
4.7372842405614 2.83341428863758 67449.71615243719 1003.7231049859892 5.28
1476023459921 164392.95250825808 1077.0408371187789 3.816702495353355 1243
02.69514475921 1097.785322455475 5.306803023453938 333860.5071697533 1113.
821890171552 3.5532846252491392 146570.92104175984 1126.335682909583 5.574
909497878116 49403.107502281666 1173.2983119638436 12.369158843869002
```

In [32]:

```
Xp=Q[Q.wave>100]
Xp=Xp[Xp.wave<1200]
x=Xp.wave
y=Xp.intensity
def ampa(x,a,b,c,a2,b2,c2,a3,b3,c3,a4,b4,c4,a5,b5,c5,a6,b6,c6,a61,b61,c61,a7,b7,c7,a8,b
8,c8,a9,b9,c9,a10,b10,c10,a11,b11,c11,a12,b12,c12,a13,b13,c13,a14,b14,c14,a15,b15,c15,a
16,b16,c16,a17,b17,c17,a18,b18,c18,a19,b19,c19,a20,b20,c20,a21,b21,c21,a22,b22,c22):
    return a*np.exp(-0.5*((x-b)/c)**2)+a2*np.exp(-0.5*((x-b2)/c2)**2)+a3*np.exp(-0.5*((
x-b3)/c3)**2)+a4*np.exp(-0.5*((x-b4)/c4)**2)+a5*np.exp(-0.5*((x-b5)/c5)**2)+a6*np.exp(-
0.5*((x-b6)/c6)**2)+a61*np.exp(-0.5*((x-b61)/c61)**2)+a7*np.exp(-0.5*((x-b7)/c7)**2)+a8
*np.exp(-0.5*((x-b8)/c8)**2)+a9*np.exp(-0.5*((x-b9)/c9)**2)+a10*np.exp(-0.5*((x-b10)/c1
0)**2)+a11*np.exp(-0.5*((x-b11)/c11)**2)+a12*np.exp(-0.5*((x-b12)/c12)**2)+a13*np.exp(-
0.5*((x-b13)/c13)**2)+a14*np.exp(-0.5*((x-b14)/c14)**2)+a15*np.exp(-0.5*((x-b15)/c15)**
2)+a16*np.exp(-0.5*((x-b16)/c16)**2)+a17*np.exp(-0.5*((x-b17)/c17)**2)+a18*np.exp(-0.5*
((x-b18)/c18)**2)+a19*np.exp(-0.5*((x-b19)/c19)**2)+a20*np.exp(-0.5*((x-b20)/c20)**2)+a
21*np.exp(-0.5*((x-b21)/c21)**2)+a22*np.exp(-0.5*((x-b22)/c22)**2)
xa=x
x=np.random.uniform(100, 1200., 10000)
#x=x
y=y

plt.plot(xa, y, 'b^-',label='data')
xa_line =arange(min(x), max(x), 1)
ya_line = ampa(xa_line,a,b,c,a2,b2,c2,a3,b3,c3,a4,b4,c4,a5,b5,c5,a6,b6,c6,a61,b61,c61,a
7,b7,c7,a8,b8,c8,a9,b9,c9,a10,b10,c10,a11,b11,c11,a12,b12,c12,a13,b13,c13,a14,b14,c14,a
15,b15,c15,a16,b16,c16,a17,b17,c17,a18,b18,c18,a19,b19,c19,a20,b20,c20,a21,b21,c21,a22,
b22,c22)

plt.plot(xa_line, ya_line, 'r-', color='red',label='fit')
#plt.axis([130,140,0.00,1000009])
#plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Raman shift(1/cm)')
plt.ylabel('intensity')
plt.legend()
plt.grid()
plt.show()
```



In [33]:

```
def makeTable(headerRow,columnizedData,columnSpacing=2):
    from numpy import array,max,vectorize

    cols = array(columnizedData,dtype=str)
    colSizes = [max(vectorize(len)(col)) for col in cols]

    header = ''
    rows = ['' for i in cols[0]]

    for i in range(0,len(headerRow)):
        if len(headerRow[i]) > colSizes[i]: colSizes[i]=len(headerRow[i])
        headerRow[i]+=' '*(colSizes[i]-len(headerRow[i]))
        header+=headerRow[i]
        if not i == len(headerRow)-1: header+=' '*columnSpacing

        for j in range(0,len(cols[i])):
            if len(cols[i][j]) < colSizes[i]:
                cols[i][j]+=' '*(colSizes[i]-len(cols[i][j])+columnSpacing)
            rows[j]+=cols[i][j]
            if not i == len(headerRow)-1: rows[j]+=' '*columnSpacing

    line = '-'*len(header)
    print(line)
    print(header)
    print(line)
    for row in rows: print(row)
    print(line)
header = ['Name','Age']
names = ['George','Alberta','Frank']
ages = [8,9,11]
makeTable(header,[names,ages])
```

```
------------
Name     Age
------------
George   8
Alberta  9
Frank    11
------------
```

In [34]:

```
header=['Intensity','Remanshift','width']
#header=[a,a2,a3,a4,a5,a6,a61,a7,a8,a9,a12,a11,a11,a12,a13,a14,a15,a16,a17,a18,a19,a20,
a21,a22]
Intensity=[a,a2,a3,a4,a5,a6,a61,a7,a8,a9,a12,a11,a11,a12,a13,a14,a15,a16,a17,a18,a19,a2
0,a21,a22]
Remanshift=[b,b2,b3,b4,b5,b6,b61,b7,b8,b9,b10,b11,b12,b13,b14,b15,b16,b17,b18,b19,b20,b
21,]
width=[c,c2,c3,c4,c5,c6,c61,c7,c8,c9,c10,c11,c12,c13,c14,c15,c16,c17,c18,c19,c20,c21,c2
2]
#makeTable(header,[Intensity,Remanshift,width])
```

In [35]:

```
print(header,[Intensity,Remanshift,width])
```

```
['Intensity', 'Remanshift', 'width'] [[50961.79182500722, 45588.0715277532
2, 45254.73573767178, 48193.57066116601, 93031.1502362745, 89478.718179283
31, 186883.22282184276, 183025.07450836798, 79542.24975702904, 76539.94805
536408, 56266.59294082497, 88258.05984627648, 88258.05984627648, 56266.592
94082497, 42316.5003380786, 49554.06312306759, 82623.75884111467, 1275414.
6916343549, 67449.71615243719, 164392.95250825808, 124302.69514475921, 333
860.5071697533, 146570.92104175984, 49403.107502281666], [135.887632717080
3, 144.0113653767824, 170.08987406095264, 187.45841644964412, 235.15875295
09383, 256.8851872862778, 273.47140999626083, 289.11328948213753, 314.9044
930954107, 339.82748138480287, 364.3422508310457, 398.8984337344434, 429.0
619599965509, 497.1052018521953, 597.4167194840196, 657.2928800793715, 92
4.7372842405614, 1003.7231049859892, 1077.0408371187789, 1097.78532245547
5, 1113.821890171552, 1126.335682909583], [8.6603799688615, 10.51776498152
098, 8.781775849046484, 7.78518979740763, 6.627883819586427, 5.90947808457
6359, 4.819309541099333, 4.319250988990481, 8.573530830107966, 8.007557484
239396, 7.991315577543902, 7.127526008118037, 7.838729317645064, 50.415124
28577877, 9.336120251977745, 6.672766457778943, 2.83341428863758, 5.281476
023459921, 3.816702495353355, 5.306803023453938, 3.5532846252491392, 5.574
909497878116, 12.369158843869002]]
```

In [36]:

```
#data = {'First Column Name':  ['First value', 'Second value',...],
#        'Second Column Name': ['First value', 'Second value',...],
#        }
data={'Intensity':[a,a2,a3,a4,a5,a6,a61,a7,a8,a9,a10,a11,a12,a13,a14,a15,a16,a17,a18,a1
9,a20,a21,a22],
        'Remanshift':[b,b2,b3,b4,b5,b6,b61,b7,b8,b9,b10,b11,b12,b13,b14,b15,b16,b17,b18
,b19,b20,b21,b22],
          'width':[c,c2,c3,c4,c5,c6,c61,c7,c8,c9,c10,c11,c12,c13,c14,c15,c16,c17,c18,c1
9,c20,c21,c22]

     }
df = pd.DataFrame (data, columns = ['Intensity','Remanshift','width'])
print(max(Intensity))
df
from IPython.display import display
display(df)
K=df.Intensity
G=df.Remanshift
RK=K/max(K)
```

```
1275414.6916343549
```

	Intensity	Remanshift	width
0	5.096179e+04	135.887633	8.660380
1	4.558807e+04	144.011365	10.517765
2	4.525474e+04	170.089874	8.781776
3	4.819357e+04	187.458416	7.785190
4	9.303115e+04	235.158753	6.627884
5	8.947872e+04	256.885187	5.909478
6	1.868832e+05	273.471410	4.819310
7	1.830251e+05	289.113289	4.319251
8	7.954225e+04	314.904493	8.573531
9	7.653995e+04	339.827481	8.007557
10	6.492138e+04	364.342251	7.991316
11	8.825806e+04	398.898434	7.127526
12	5.626659e+04	429.061960	7.838729
13	4.231650e+04	497.105202	50.415124
14	4.955406e+04	597.416719	9.336120
15	8.262376e+04	657.292880	6.672766
16	1.275415e+06	924.737284	2.833414
17	6.744972e+04	1003.723105	5.281476
18	1.643930e+05	1077.040837	3.816702
19	1.243027e+05	1097.785322	5.306803
20	3.338605e+05	1113.821890	3.553285
21	1.465709e+05	1126.335683	5.574909
22	4.940311e+04	1173.298312	12.369159

In [37]:

```
K

print(RK)
RK*100
```

```
0     0.039957
1     0.035744
2     0.035482
3     0.037787
4     0.072942
5     0.070157
6     0.146527
7     0.143502
8     0.062366
9     0.060012
10    0.050902
11    0.069200
12    0.044116
13    0.033179
14    0.038853
15    0.064782
16    1.000000
17    0.052885
18    0.128894
19    0.097461
20    0.261766
21    0.114920
22    0.038735
Name: Intensity, dtype: float64
```

Out[37]:

```
0       3.995704
1       3.574372
2       3.548237
3       3.778659
4       7.294188
5       7.015657
6      14.652742
7      14.350240
8       6.236579
9       6.001181
10      5.090218
11      6.919950
12      4.411631
13      3.317862
14      3.885329
15      6.478188
16    100.000000
17      5.288454
18     12.889373
19      9.746061
20     26.176624
21     11.492021
22      3.873494
Name: Intensity, dtype: float64
```

In [38]:

```
print('perr[0],'*22)
```

```
perr[0],perr[0],perr[0],perr[0],perr[0],perr[0],perr[0],perr[0],perr[0],perr[0],pe
rr[0],perr[0],perr[0],perr[0],perr[0],perr[0],perr[0],perr[0],perr[0],perr[0],perr
[0],perr[0],perr[0],perr[0],
```

In [42]:

```
#data = {'First Column Name':  ['First value', 'Second value',...],
#        'Second Column Name': ['First value', 'Second value',...],
#        }
data={'Intensity':[a,a2,a3,a4,a5,a6,a61,a7,a8,a9,a10,a11,a12,a13,a14,a15,a16,a17,a18,a1
9,a20,a21,a22],
        'Remanshift':[b,b2,b3,b4,b5,b6,b61,b7,b8,b9,b10,b11,b12,b13,b14,b15,b16,b17,b18
,b19,b20,b21,b22],
         'width':[c,c2,c3,c4,c5,c6,c61,c7,c8,c9,c10,c11,c12,c13,c14,c15,c16,c17,c18,c1
9,c20,c21,c22],
           'err':[perr[0],perr2[0],perr3[0],perr4[0],perr5[0],perr6[0],perr61[0],perr7
[0],perr8[0],perr9[0],perr10[0],perr11[0],perr12[0],perr13[0],perr14[0],perr15[0],perr1
6[0],perr17[0],perr18[0],perr17[0],perr20[0],perr21[0],perr22[0],]
      }
df = pd.DataFrame (data, columns = ['Intensity','Remanshift','width','err'])
print(max(Intensity))
df
from IPython.display import display
display(df)
K=df.Intensity
G=df.Remanshift
RK=K/max(K)
```

```
1275414.6916343549
```

	Intensity	Remanshift	width	err
0	5.096179e+04	135.887633	8.660380	267.520662
1	4.558807e+04	144.011365	10.517765	236.409066
2	4.525474e+04	170.089874	8.781776	401.587167
3	4.819357e+04	187.458416	7.785190	486.905040
4	9.303115e+04	235.158753	6.627884	1519.845286
5	8.947872e+04	256.885187	5.909478	1183.585713
6	1.868832e+05	273.471410	4.819310	4932.674175
7	1.830251e+05	289.113289	4.319251	9526.503293
8	7.954225e+04	314.904493	8.573531	723.084593
9	7.653995e+04	339.827481	8.007557	1230.584079
10	6.492138e+04	364.342251	7.991316	1279.909973
11	8.825806e+04	398.898434	7.127526	1601.361120
12	5.626659e+04	429.061960	7.838729	776.188316
13	4.231650e+04	497.105202	50.415124	197.597812
14	4.955406e+04	597.416719	9.336120	367.858025
15	8.262376e+04	657.292880	6.672766	2378.624695
16	1.275415e+06	924.737284	2.833414	78433.747867
17	6.744972e+04	1003.723105	5.281476	1142.612205
18	1.643930e+05	1077.040837	3.816702	7070.858416
19	1.243027e+05	1097.785322	5.306803	1142.612205
20	3.338605e+05	1113.821890	3.553285	11951.607798
21	1.465709e+05	1126.335683	5.574909	3520.625062
22	4.940311e+04	1173.298312	12.369159	257.125978

In [ ]:

In [1]:

```
import pandas as pd
import numpy as np
from numpy import arange
from scipy.optimize import curve_fit
from scipy import constants
from scipy.constants import find
from matplotlib import pyplot as plt
import math
from scipy import special
```

In [2]:

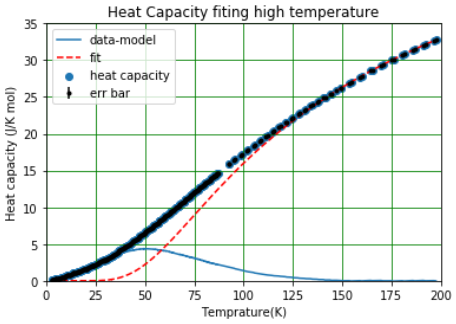
```
#read in data
df=pd.read_csv('fitcp1.csv',',')
#df
```

In [3]:

```
x=df.X
x1=df.X1
y1=df.y1
y2=df.Y3
x3=df.X3
y3=df.Y3
y=df.Y
E=df.E
```

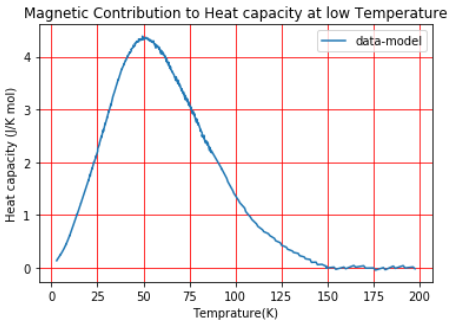
In [4]:

```
plt.plot(x3,y3,label='data-model')
plt.plot(x1,y1,'r--',label='fit')
plt.scatter(x,y,label='heat capacity')
plt.grid(color='g')
plt.xlabel('Temprature(K)')
plt.ylabel('Heat capacity (J/K mol)')
plt.errorbar(x, y, yerr=E, fmt='.k',label= 'err bar')
plt.axis([0,200,0,35])
plt.title('Heat Capacity fiting high temperature')
plt.legend()
plt.show()
```



In [5]:

```
plt.plot(x3,y3,label ='data-model')
plt.grid(color='r')
plt.xlabel('Temprature(K)')
plt.ylabel('Heat capacity (J/K mol)')
plt.title('Magnetic Contribution to Heat capacity at low Temperature')
plt.legend()
plt.show()
max(y3)
```



Out[5]:

4.38912

In [1]:

```
import pandas as pd
import numpy as np
from numpy import arange
from scipy.optimize import curve_fit
from scipy import constants
from scipy.constants import find
from matplotlib import pyplot as plt
import math
from scipy import special
```

In [2]:

```
#read in data
df=pd.read_csv('Cp.txt')
#df=df.tail(403)
#T=df.Sample_Temp_Kelvin
#p=df.Samp_HC_JK
#df
#saturation point reference
qx=[0,350]
qy=[53.17,53.17]
```

In [3]:

```
#create a sub set of data with sample heat capacity and temperature
QS=df[['Samp_HC_JK','Sample_Temp_Kelvin','Samp_HC_Err_mJ_K']]
QC=df[['Total_HC_JK','Samp_HC_JK']]
#removing data with temperature above 200K
QS=QS[QS.Sample_Temp_Kelvin<=200]
#T is temperature in in K and P is heat capacity here in micro J/K
T=QS.Sample_Temp_Kelvin
p=QS.Samp_HC_JK
E=QS.Samp_HC_Err_mJ_K
#QC
#print(T,p)
```

In [4]:

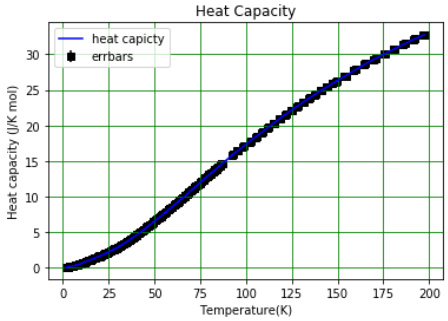
```
#creating the data set for higher temperatures
QS1=QS[QS.Sample_Temp_Kelvin>150]
#QS1
QS2=QS[QS.Sample_Temp_Kelvin<2]
Th=QS1.Sample_Temp_Kelvin
ph=QS1.Samp_HC_JK
#QS2
QSj=pd.concat([QS2,QS1])
#QSj
#the jioned lower and higer temp
Tj=QSj.Sample_Temp_Kelvin
pj=QSj.Samp_HC_JK
```

In [5]:

```
p=QS.Samp_HC_JK
#p is specific heat capacity
p=p
#converting heat capacity to J/K
p= 5981.043*p/1000000
E= 5981.043*E/1000000
p=p
pj=5981.043*pj/1000000
ph=5981.043*ph/1000000
D=df.Debye_Temp_Kelvin
#r=sum(E)/310
#P
#r
```

In [6]:

```
plt.plot(T,p,color='blue' ,label ='heat capicty')
plt.errorbar(T,p,yerr=E,fmt='sk',label = 'errbars',zorder=0)
plt.xlabel('Temperature(K)')
plt.ylabel('Heat capacity (J/K mol)')
plt.title('Heat Capacity')
plt.legend()
plt.grid(color='green')
plt.show()
```



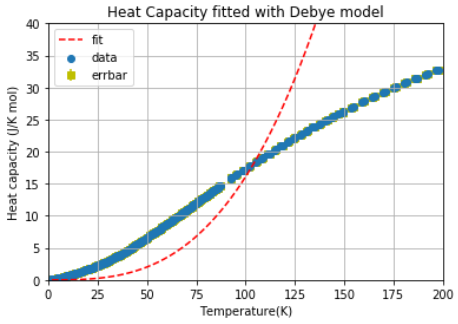
plt.plot(T,p,color='blue' ,label ='heat capicty') plt.errorbar(T,p+E,yerr=100,fmt='none',z color='black',lable = 'err') plt.xlabel('Temprature(K)') plt.ylabel('Heat capacity (J/K mol)') plt.title('Heat Capacity') plt.legend() plt.grid(color='green') plt.show()

In [7]:

```
#fit using debye theory and three Einstein terms
qx=[0,300]
qy=[53.17,53.17]

def objective2(x,K,R):
    return 12*R*(np.pi**4/5)*(x**3)/K**3# + R1*(K1**2/x**2) *(np.e**(K1/x))*(((np.e**(K
1/x))-1)**-2)+R2*(np.pi**4/5)*(x**3)/K2**3
x=T
y=p
#print(x)
#x=temp
#y=U
#method{‘lm’, ‘trf’, ‘dogbox’}, optional
popt, pcov = curve_fit(objective2, x, y, maxfev=150000,bounds =([0,0],[700,0.00005]),si
gma=E)
K,R= popt
print(popt)
plt.scatter(T, p,label='data')
x_line = arange(min(x), max(x), 1)
y_line = objective2(x_line,K,R)
plt.plot(x_line, y_line, '--', color='red',label='fit',zorder=10)
plt.axis([0,200,0.00,40.0075])
plt.errorbar(T,p,yerr=E,fmt='sy',label='errbar',zorder=0)
plt.xlabel('Temperature(K)')
plt.ylabel('Heat capacity (J/K mol)')
plt.legend()
#plt.plot(qx,qy)
plt.title('Heat Capacity fitted with Debye model')
plt.grid()
plt.show()
print(pcov)
# from the graph the material does not follow the dybe theory
```

```
[8.98720375e+00 4.99260269e-05]
```

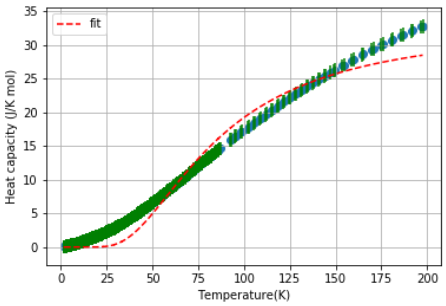



```
[[ 3.63200539e-21 -2.17932913e-16]
 [-2.17932913e-16  1.30767303e-11]]
```

In [8]:

```
def objective2(x,K,R):
    return 3*R*(K**2/x**2) *(np.e**(K/x))*(((np.e**(K/x))-1)**-2)
#work on the u nt and make sure the are in the right unit that crospond
#J=43.50
x=T
y=p
#K=300.4
#print(x)
#x=temp
#y=U
#method{‘lm’, ‘trf’, ‘dogbox’}, optional
popt, _ = curve_fit(objective2, T, p, maxfev=150000,)
K,R= popt
print(popt)
plt.scatter(T, p)
x_line = x #arange(min(x), max(x), 1)
y_line = objective2(x_line,K,R)
plt.plot(x_line, y_line, '--', color='red',label='fit')
#plt.axis([0.0,300,0.00,0.0085])
plt.errorbar(T,p,yerr=1,fmt='none', color='green')
plt.xlabel('Temperature(K)')
plt.ylabel('Heat capacity (J/K mol)')
plt.legend()
plt.grid()
plt.show()
```

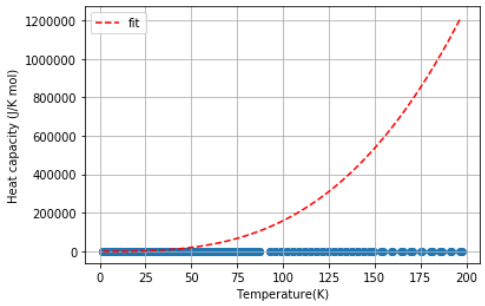
```
[260.20652956  10.94260161]
```



In [9]:

```
#fit using debye theory and three Einstein terms
def objective2(x,K,R,R1,K1,R2,K2):
    return 12*R*(np.pi**4/5)*(x**3)/K**3 + R1*(K1**2/x**2) *(np.e**(K1/x))*(((np.e**(K1
/x))-1)**-2)+R2*(np.pi**4/5)*(x**3)/K2**3
x=T
y=p
#print(x)
#x=temp
#y=U
#method{‘lm’, ‘trf’, ‘dogbox’}, optional
popt, _ = curve_fit(objective2, x, y, maxfev=150000)
K,R,K1,R1,R2,K2= popt
print(popt)
plt.scatter(T, p)
x_line = arange(min(x), max(x), 1)
y_line = objective2(x_line,K,R,K1,R1,K2,R2)
plt.plot(x_line, y_line, '--', color='red',label='fit')
#plt.axis([0,200,0.00,40.0075])
plt.errorbar(T,p,yerr=2,fmt='none', color='green')
plt.xlabel('Temperature(K)')
plt.ylabel('Heat capacity (J/K mol)')
plt.legend()
plt.grid()
plt.show()
# from the graph the material does not follow the dybe theory
```

```
[ 4.00352419e+00  4.37574549e-02  2.01982695e+01  1.96441676e+02
 -8.92920642e+01  2.21804820e+01]
```



In [10]:

```
T=QS.Sample_Temp_Kelvin.head(261)
p=QS.Samp_HC_JK.head(261)
#p is specific heat capacity
p= 5981.043*p/1000000
p1=p.head(261)
T1=df.Sample_Temp_Kelvin.head(261)
#print(p,T1)
```

In [11]:

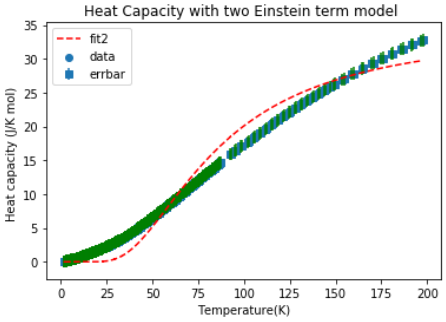
```
#fit with 2term Einstine theory, fiting R(1), scaling factor, and K(1), for eintin Temp
erature mode
p=QS.Samp_HC_JK
#p is specific heat capacity
p= 5981.043*p/1000000
E=5981.043*E/1000000
p1=p
T1=QS.Sample_Temp_Kelvin

def objective2(x,K,R,R1,K1):
    return 3*7*8.314*R*(K**2/x**2) *(np.e**(K/x))*(((np.e**(K/x))-1)**-2) + R1*(K1**2/x
**2) *(np.e**(K1/x))*(((np.e**(K1/x))-1)**-2)#+R2*(K2**2/x**2) *(np.e**(K2/x))*(((np.e*
*(K2/x))-1)**-2)
x=T1
y=p1
#method{‘lm’, ‘trf’, ‘dogbox’}, optional
popt, pcov = curve_fit(objective2, T1, p1,sigma=E, maxfev=150000, bounds =([260,0,0,400
],[1200,100,0.006,1110.1175572375146]))
K,R,R1,K1= popt
print(popt)
plt.scatter(T1, p1, label='data')
x_line = x #arange(min(x), max(x), 1)
y_line = objective2(x_line,K,R,R1,K1)

perr=np.sqrt(np.diag(pcov))
plt.grid()
plt.errorbar(T1,p1,yerr=E,fmt='s',zorder=0,label='errbar')

plt.plot(x_line, y_line, '--', color='red',label='fit2')
#plt.axis([00.0,220,0.00,0.008])
print('K =',K,'K1=',K1,'R =', R, 'R1 =',R1)
plt.xlabel('Temperature(K)')
plt.ylabel('Heat capacity (J/K mol) ')
plt.errorbar(T1,p1,yerr=0.9,fmt='none', color='green')
#plt.plot(qx,qy)
plt.title('Heat Capacity')
plt.title('Heat Capacity with two Einstein term model ')
plt.legend()
plt.grid()
plt.show()
#this shows a better match in the data set after focusing the fit at the 0.0008 point t
his result in the abnormal shapping of mthe fit curve at this point
```

```
[2.60000000e+02 1.96383142e-01 5.99999991e-03 1.11011756e+03]
K = 260.0000000031246 K1= 1110.117555793179 R = 0.19638314211378435 R1 =
0.00599999990906865
```



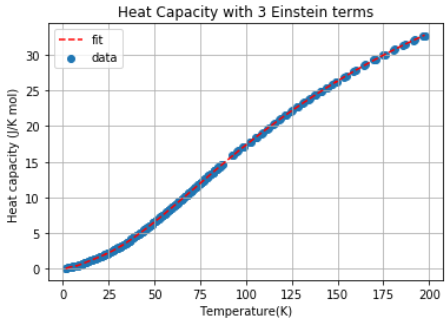
In [12]:

```
#fit with 2term Einstine theory, fiting R(1), scaling factor, and K(1), for eintin Temp
erature mode
p=QS.Samp_HC_JK
#p is specific heat capacity
p= 5981.043*p/1000000
p1=p
T1=QS.Sample_Temp_Kelvin

def objective2(x,R,K,R1,K1,R2,K2,R3,K3,R4,K4,R5,K5,R6,K6,R7,K7):
    return R*(K**2/x**2) *(np.e**(K/x))*(((np.e**(K/x))-1)**-2) + R1*(K1**2/x**2) *(np.
e**(K1/x))*(((np.e**(K1/x))-1)**-2)+R2*(K2**2/x**2) *(np.e**(K2/x))*(((np.e**(K2/x))-1)
**-2)+R3*(K3**2/x**2) *(np.e**(K3/x))*(((np.e**(K3/x))-1)**-2) + R4*(K4**2/x**2) *(np.e
**(K4/x))*(((np.e**(K4/x))-1)**-2)+R5*(K5**2/x**2) *(np.e**(K5/x))*(((np.e**(K5/x))-1)*
*-2)+ R6*(K6**2/x**2) *(np.e**(K6/x))*(((np.e**(K6/x))-1)**-2) + R7*(K7**2/x**2) *(np.e
**(K7/x))*(((np.e**(K7/x))-1)**-2)
x=T1
y=p1
#method{'lm', 'trf', 'dogbox'}, optional
popt, _ = curve_fit(objective2, T1, p1, maxfev=150000,bounds =(0,1000))
K,R,R1,K1,R2,K2,R3,K3,R4,K4,R5,K5,R6,K6,R7,K7= popt
print(popt)
plt.scatter(T1, p1,label='data')
x_line = x #arange(min(x), max(x), 1)
y_line = objective2(x_line,K,R,R1,K1,R2,K2,R3,K3,R4,K4,R5,K5,R6,K6,R7,K7)
plt.plot(x_line, y_line, '--', color='red',label='fit')
#plt.axis([00.0,220,0.00,0.008])
print('K =',K,'K1=',K1,'K2 =',K2,'R =', R, 'R1 =',R1,'R2 =',R2,'R3=',R3 ,'K3=',K3 ,'R4
=', R4, 'K4=',K4, 'R5=',R5 ,'K5=',K5 ,'R6=',R6,'K6=', K6,'R7=', R7,'K7=', K7 )
Dy=(y-y_line)
plt.xlabel('Temperature(K)')
plt.ylabel('Heat capacity (J/K mol) ')
plt.errorbar(T1,p1,yerr=0.0002,fmt='none', color='green')
#plt.plot(x_line,Dy)
#saturation ref
#plt.plot(qx,qy)
plt.title('Heat Capacity with 3 Einstein terms')
plt.legend()
plt.grid()
plt.show()

print(Dy)
#this shows a better match in the data set after focusing the fit at the 0.0008 point t
his result in the abnormal shapping of mthe fit curve at this point
```

```
[1.30767086e-05 4.13866618e+02 8.01528650e+00 4.27468505e+02
 8.54729295e+00 2.55417986e+02 5.80378644e+00 1.56504598e+02
 3.65128011e-01 9.92849812e+00 2.00828266e+00 5.35308900e+01
 1.75543464e+01 8.50790155e+02 1.08737619e+01 4.27570855e+02]
K = 1.3076708636666094e-05 K1= 427.4685050205239 K2 = 255.41798613799375 R
= 413.86661776011545 R1 = 8.01528649581199 R2 = 8.547292946427813 R3= 5.80
37864353414275 K3= 156.50459814131426 R4= 0.3651280109415611 K4= 9.9284981
16531703 R5= 2.0082826634412267 K5= 53.5308900338941 R6= 17.55434642755447
8 K6= 850.790154645761 R7= 10.873761880592037 K7= 427.5708545586373
```




```
0      0.041144
1      0.042513
2      0.041476
3     -0.003415
4     -0.003401
         ...
305   -0.007721
306    0.032250
307   -0.014208
308   -0.006514
309   -0.043909
Length: 310, dtype: float64
```

In [13]:

```
#plt.plot(x_line,Dy)
#plt.axis([0.00,30,-0.01,0.01])
#plt.plot(x,y)
#plt.show()
```

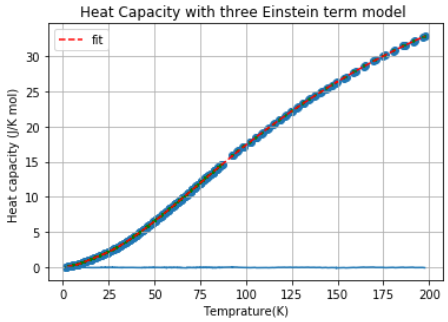
In [14]:

```
#fit with 2term Einstine theory, fiting R(1), scaling factor, and K(1), for eintin Temp
erature mode
p=QS.Samp_HC_JK
#p is specific heat capacity
p= 5981.043*p/1000000 #converted to j/kmol
p1=p
T1=QS.Sample_Temp_Kelvin

def objective2(x,R,K,R1,K1,R2,K2,R3,K3,R4,K4,):
    return R*(K**2/x**2) *(np.e**(K/x))*(((np.e**(K/x))-1)**-2) + R1*(K1**2/x**2) *(np.
e**(K1/x))*(((np.e**(K1/x))-1)**-2)+R2*(K2**2/x**2) *(np.e**(K2/x))*(((np.e**(K2/x))-1)
**-2)+R3*(K3**2/x**2) *(np.e**(K3/x))*(((np.e**(K3/x))-1)**-2) + R4*(K4**2/x**2) *(np.e
**(K4/x))*(((np.e**(K4/x))-1)**-2)#+R5*(K5**2/x**2) *(np.e**(K5/x))*(((np.e**(K5/x))-1)
**-2)+ R6*(K6**2/x**2) *(np.e**(K6/x))*(((np.e**(K6/x))-1)**-2) + R7*(K7**2/x**2) *(np.
e**(K7/x))*(((np.e**(K7/x))-1)**-2)

x=T1
y=p1
#method{‘lm’, ‘trf’, ‘dogbox’}, optional
popt, _ = curve_fit(objective2, x, y, maxfev=150000)
K,R,R1,K1,R2,K2,R3,K3,R4,K4,= popt
print(popt)
plt.scatter(x, y)
x_line = x #arange(min(x), max(x), 1)
y_line = objective2(x_line,K,R,R1,K1,R2,K2,R3,K3,R4,K4,)
plt.plot(x_line, y_line, '--', color='red',label='fit')
#plt.axis([00.0,220,0.00,2.2])
print('K =',K,'K1=',K1,'K2 =',K2,'R =', R, 'R1 =',R1,'R2 =',R2,'R3=',R3 ,'K3=',K3 ,'R4
=', R4, 'K4=',K4, )#'R5=',R5 ,'K5=',K5 ,'R6=',R6,'K6=', K6,'R7=', R7,'K7=', K7 )
Dy=(y-y_line)
plt.xlabel('Temprature(K)')
plt.ylabel('Heat capacity (J/K mol) ')
plt.errorbar(T1,p1,yerr=0.2,fmt='none', color='green')
plt.plot(x_line,Dy)
#saturation ref
#plt.plot(qx,qy)
plt.legend()
plt.title('Heat Capacity with three Einstein term model ')
plt.grid()
plt.show()
G=(R+K+R1+K1+R2+K2+R3+K3+R4+K4)
print(R,R1,R2,R3,R4)
print(K,K1,K2,K3,K4)
print('G=', G)
print(Dy)
#this shows a better match in the data set after focusing the fit at the 0.0008 point t
his result in the abnormal shapping of mthe fit curve at this point
```

```
[ 2.11413887e+01  3.85547863e+02  1.88875896e+01  8.04031246e+02
  9.76797364e+00 -1.82206561e+02  2.22955152e+00 -5.74870701e+01
  4.04707829e-01  1.09117678e+01]
K = 21.141388732291077 K1= 804.0312462603379 K2 = -182.20656113005677 R =
385.54786346607676 R1 = 18.88758962448124 R2 = 9.767973643528759 R3= 2.229
5515174157967 K3= -57.48707011812936 R4= 0.404707829257846 65 K4= 10.911767
79775991
```




```
385.54786346607676 18.88758962448124 9.767973643528759 2.2295515174157967
0.40470782925784665
21.141388732291077 804.0312462603379 -182.20656113005677 -57.4870701181293
6 10.91176779775991
G= 1013.2284576229629
0      0.051813
1      0.053180
2      0.052123
3      0.006990
4      0.007000
         ...
305   -0.007553
306    0.034472
307   -0.011411
308   -0.001128
309   -0.037812
Length: 310, dtype: float64
```

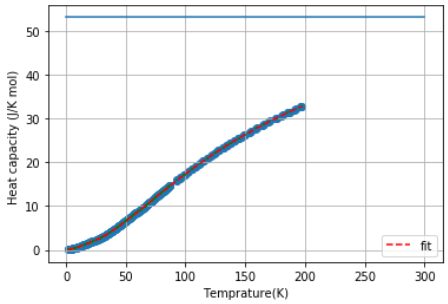
In [15]:

```
#fit with 2term Einstine theory, fiting R(1), scaling factor, and K(1), for eintin Temp
erature mode
p=QS.Samp_HC_JK
#p is specific heat capacity
p= 5981.043*p/1000000 #converted to j/kmol
p1=p
T1=QS.Sample_Temp_Kelvin

def objective2(x,R,K,R1,K1,R2,K2,R3,K3):
    return 3*R*(K**2/x**2) *(np.e**(K/x))*(((np.e**(K/x))-1)**-2) + R1*(2**2/x**2) *(np
.e**(2/x))*(((np.e**(K1/x))-1)**-2)+R2*(K2**2/x**2) *(np.e**(K2/x))*(((np.e**(K2/x))-1)
**-2)+R3*(K3**2/x**2) *(np.e**(K3/x))*(((np.e**(K3/x))-1)**-2) + R4*(K4**2/x**2) *(np.e
**(K4/x))*(((np.e**(K4/x))-1)**-2)#+R5*(K5**2/x**2) *(np.e**(K5/x))*(((np.e**(K5/x))-1)
**-2)+ R6*(K6**2/x**2) *(np.e**(K6/x))*(((np.e**(K6/x))-1)**-2) + R7*(K7**2/x**2) *(np.
e**(K7/x))*(((np.e**(K7/x))-1)**-2)

x=T1
y=p1
#method{‘lm’, ‘trf’, ‘dogbox’}, optional
popt, _ = curve_fit(objective2, x, y, maxfev=150000)
K,R,R1,K1,R2,K2,R3,K3= popt
print(popt)
plt.scatter(x, y)
x_line = x #arange(min(x), max(x), 1)
y_line = objective2(x_line,K,R,R1,K1,R2,K2,R3,K3)
plt.plot(x_line, y_line, '--', color='red',label='fit')
#plt.axis([00.0,220,0.00,2.2])
print('K =',K,'K1=',K1,'K2 =',K2,'R =', R, 'R1 =',R1,'R2 =',R2,'R3=',R3 ,'K3=',K3 )#'R5
=',R5 ,'K5=',K5 ,'R6=',R6,'K6=', K6,'R7=', R7,'K7=', K7 )
Dy=(y-y_line)
plt.xlabel('Temprature(K)')
plt.ylabel('Heat capacity (J/K mol) ')
plt.errorbar(T1,p1,yerr=0.2,fmt='none', color='green')
#plt.plot(x_line,Dy)
#saturation ref
plt.plot(qx,qy)
plt.legend()
plt.grid()
plt.show()
print(R,R1,R2,R3,R4)
print(K,K1,K2,K3,K4)
#print(Dy)
#this shows a better match in the data set after focusing the fit at the 0.0008 point t
his result in the abnormal shapping of mthe fit curve at this point
```

```
[  3.21264555 199.12533958 756.50678744  25.77443082  20.58339379
 404.68277784  18.0019954  836.03478362]
K = 3.2126455530957068 K1= 25.774430823478223 K2 = 404.68277784289734 R =
199.1253395778161 R1 = 756.506787443811 R2 = 20.583393787677192 R3= 18.001
995403399782 K3= 836.0347836226126
```




```
199.1253395778161 756.506787443811 20.583393787677192 18.001995403399782
0.40470782925784665
3.2126455530957068 25.774430823478223 404.68277784289734 836.0347836226126
10.91176779775991
```

In [16]:

```
#fit with 2term Einstine theory, fiting R(1), scaling factor, and K(1), for eintin Temp
erature mode
p=QS.Samp_HC_JK
#p is specific heat capacity
p= 5981.043*p/1000000 #converted to j/kmol
p1=p
T1=QS.Sample_Temp_Kelvin

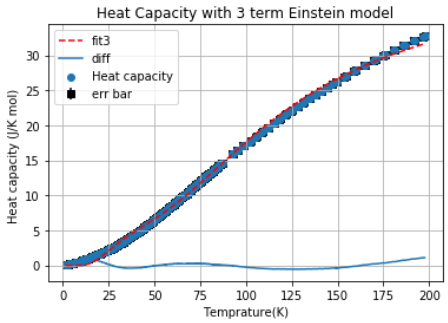
def objective2(x,R,K,R1,K1,R2,K2):
    return 3*7*8.314*R*(3**2/x**2) *(np.e**(K/x))*(((np.e**(K/x))-1)**-2) + R2*(K1**2/x
**2) *(np.e**(K2/x))*(((np.e**(K2/x))-1)**-2)+R1*(K1**2/x**2) *(np.e**(K1/x))*(((np.e**
(K1/x))-1)**-2)
x=T1
y=p1
gess = [0.0734,999.937,0.030251,622.493,0.201873,362]
#method{‘lm’, ‘trf’, ‘dogbox’}, optional
popt, pcov= curve_fit(objective2, x, y, maxfev=150000)#,bounds=([200,0.02,0.01,200,0.0
1,200],[700,10,10,900,10,1200]))
K,R,R1,K1,R2,K2= popt
print(popt)
plt.scatter(x, y,label='Heat capacity')
x_line = x #arange(min(x), max(x), 1)

perr3=np.sqrt(np.diag(pcov))

y_line = objective2(x_line,K,R,R1,K1,R2,K2)
plt.plot(x_line, y_line, '--', color='red',label='fit3',zorder=10)
#plt.axis([00.0,55,0.00,10])
print('K =',K,'K1=',K1,'K2 =',K2,'R =', R, 'R1 =',R1,'R2=',R2,'K2 =',K2)
Dy=(y-y_line)
plt.xlabel('Temprature(K)')
plt.ylabel('Heat capacity (J/K mol) ')
plt.errorbar(T1,p1,yerr=E,fmt='sk', label='err bar',zorder=0)
plt.plot(x_line,Dy,label ='diff')
#saturation ref
plt.title("Heat Capacity with 3 term Einstein model")
#plt.plot(qx,qy)
plt.legend()
plt.grid()
#plt.plot(qx,qy)
G=((R*4/8.31)+(R1*4/24.94)+(R2*4/24.94))
plt.show()
print(R,R1,R2,)
print(K,K1,K2,)
print(G)
print('err=',perr)
#print(Dy)
#this shows a better match in the data set after focusing the fit at the 0.0008 point t
his result in the abnormal shapping of mthe fit curve at this point
```

```
[  70.48942342  111.62642054 -675.76985642  403.63141235  707.97973168
  403.63141874]
K = 70.48942341972356 K1= 403.6314123548167 K2 = 403.63141873981937 R = 11
1.62642053880622 R1 = -675.7698564203533 R2= 707.9797316806927 K2 = 403.63
141873981937

C:\ProgramData\Anaconda3\lib\site-packages\ipykernel_launcher.py:20: Runti
meWarning: invalid value encountered in sqrt
```



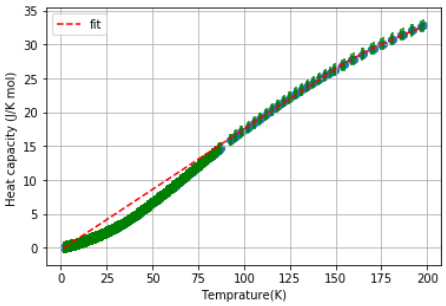

```
111.62642053880622 -675.7698564203533 707.9797316806927
70.48942341972356 403.6314123548167 403.63141873981937
58.89710740967245
err= [1.63291222e+01 2.80901127e-02 6.28738266e+02 2.79745686e+07]
```

In [17]:

```
#fit with 2term Einstine theory, fiting R(1), scaling factor, and K(1), for eintin Temp
erature mode
p=QS.Samp_HC_JK
#p is specific heat capacity
p= 5981.043*p/1000000 #converted to j/kmol
p1=p
T1=QS.Sample_Temp_Kelvin

def objective2(x,R,K,R1,K1,R2,K2):
    return 3*R*(K**2/x**2) *(np.e**(K/x))*(((np.e**(K/x))-1)**-2) + R2*(K1**2/x**2) *(n
p.e**(K2/x))*(((np.e**(K2/x))-1)**-2)+R1*(K1**2/x**2) *(np.e**(K1/x))*(((np.e**(K1/x))-
1)**-2)
x=Tj
y=pj
#method{‘lm’, ‘trf’, ‘dogbox’}, optional
popt, _ = curve_fit(objective2, T1, p1, maxfev=150000)
K,R,R1,K1,R2,K2= popt
print(popt)
plt.scatter(T1, p1)
x_line = x #arange(min(x), max(x), 1)
y_line = objective2(x_line,K,R,R1,K1,R2,K2)
plt.plot(x_line, y_line, '--', color='red',label='fit')
#plt.axis([0.0,220,0.00,40.2])
print('K =',K,'K1=',K1,'K2 =',K2,'R =', R, 'R1 =',R1,'R2=',R2,'K2 =',K2)
Dy=(y-y_line)
plt.xlabel('Temprature(K)')
plt.ylabel('Heat capacity (J/K mol) ')
plt.errorbar(T1,p1,yerr=0.9,fmt='none', color='green')
#plt.plot(x_line,Dy)
#saturation ref
#plt.plot(qx,qy)
plt.legend()
plt.grid()
#plt.plot(qx,qy)
plt.show()
#G is the number of active modes between 92K to 200K and the result is 30 modes, i thin
k the remaining 12 modes will be in the lower temperature region
G=((R*4/8.31)+(R1*4/24.94)+(R2*4/24.94))
print(R,R1,R2)
print(K,K1,K2)
print('G=', G)
#print(Dy)
#this shows a better match in the data set after focusing the fit at the 0.0008 point t
his result in the abnormal shapping of mthe fit curve at this point
```

```
[  9.16157796 543.87037599   2.89406709  50.75395238 306.33510984
 221.37149844]
K = 9.16157796243613 K1= 50.75395237685186 K2 = 221.37149843948322 R = 54
3.8703759931121 R1 = 2.894067093584578 R2= 306.335109838126 K2 = 221.37149
843948322
```



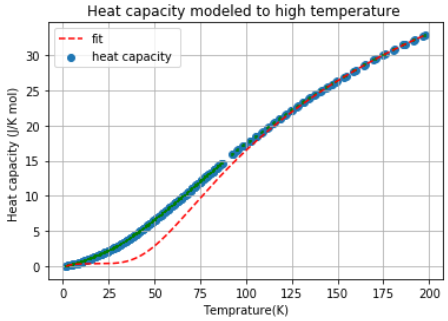

```
543.8703759931121 2.894067093584578 306.335109838126
9.16157796243613 50.75395237685186 221.37149843948322
G= 311.38649268609487
```

In [18]:

```
#fit with 2term Einstine theory, fiting R(1), scaling factor, and K(1), for eintin Temp
erature mode
p=QS.Samp_HC_JK
#p is specific heat capacity
p= 5981.043*p/1000000 #converted to j/kmol
p1=p
T1=QS.Sample_Temp_Kelvin

def objective2(x,R,K,R1,K1,R2,K2):
    return 7*3*R*(K**2/x**2) *(np.e**(K/x))*(((np.e**(K/x))-1)**-2) + R1*(2**2/x**2) *(
np.e**(2/x))*(((np.e**(K1/x))-1)**-2)+R2*(K2**2/x**2) *(np.e**(K2/x))*(((np.e**(K2/x))-
1)**-2)+R3*(K3**2/x**2) *(np.e**(K3/x))*(((np.e**(K3/x))-1)**-2) + R4*(K4**2/x**2) *(np
.e**(K4/x))*(((np.e**(K4/x))-1)**-2)#+R5*(K5**2/x**2) *(np.e**(K5/x))*(((np.e**(K5/x))-
1)**-2)+ R6*(K6**2/x**2) *(np.e**(K6/x))*(((np.e**(K6/x))-1)**-2) + R7*(K7**2/x**2) *(n
p.e**(K7/x))*(((np.e**(K7/x))-1)**-2)
#x=np.random.uniform(1.8, 200., 1000)
x=T1
y=p1
geuss = [0.0734,999.937,0.030251,622.493,0.201873,362]
#method{‘lm’, ‘trf’, ‘dogbox’}, optional
popt, _ = curve_fit(objective2, Th, ph, maxfev=150000,bounds=(0,1000),p0=geuss)
R,R1,R2,K,K1,K2= popt
print(popt)
plt.scatter(T1, p1,label='heat capacity ')
x_line = arange(min(x), max(x), 1)
y_line = objective2(x_line,R,R1,R2,K,K1,K2)
plt.plot(x_line, y_line, '--', color='red',label='fit')
#plt.axis([00.0,220,0.00,2.2])
print('K =',K,'K1=',K1,'K2 =',K2,'R =', R, 'R1 =',R1,'R2 =',R2,)#'R5=',R5 ,'K5=',K5 ,'R
6=',R6,'K6=', K6,'R7=', R7,'K7=', K7 )
#Dy=(y-y_line)
plt.xlabel('Temprature(K)')
plt.ylabel('Heat capacity (J/K mol) ')
plt.errorbar(T1,p1,yerr=0.2,fmt='none', color='green')
#plt.plot(x_line,Dy)
#saturation ref
#plt.plot(qx,qy)
plt.title('Heat capacity modeled to high temperature ')
plt.legend()
plt.grid()
plt.show()
print(R,R1,R2)
print(K,K1,K2)
#print(Dy)
#this shows a better match in the data set after focusing the fit at the 0.0008 point t
his result in the abnormal shapping of mthe fit curve at this point
```

```
[1.73998465e-14 7.25800406e+02 1.28357293e+02 9.87940396e+02
 3.39020660e+01 3.14737227e+02]
K = 987.9403963310415 K1= 33.902066016449716 K2 = 314.737226786176 R = 1.7
399846546301446e-14 R1 = 725.8004056465209 R2 = 128.35729349929306
```




```
1.7399846546301446e-14 725.8004056465209 128.35729349929306
987.9403963310415 33.902066016449716 314.737226786176
```

In [19]:

```
#plt.plot(x_line,Dy)
```

In [20]:

```
3**3
```

Out[20]:

```
27
```