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Structural and energetic description of transition metal compounds with advanced density functionals

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Contents

1 Acknowledgement

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2 Abstract

A correct energetic description is a fundamental parameter to reach chemical accuracy with computational methods. The ground state energy, for example, determines the stability of crystal structures for polymorphic compounds, and the formation energy indicates the overall chemical stability. The fundamental methods to computationally obtain such parameters are under continuous development. While main group compounds are generally easier to describe with density functional theory (DFT), the method of choice in this work, the main emphasis here is on transition metal compounds which feature correlated electrons. This poses a much more complicated problem. To try and solve it, two state-of-the-art functionals, PBE and SCAN, are enhanced with the on-site hybrid functional EECE and compared to each other regarding the polymorphic energy ordering and formation energy. The EECE functional features a hybrid approach, where only strongly correlated electrons are treated with the exact Hartree-Fock (HF) exchange energy. In contrast to other functionals, which aim to solve similar problems, such as LDA+U, the EECE is parameter-free. Further, it is computationally much less demanding than an entire HF calculation. The results for the polymorphic energy ordering show a benefit for both pairings with the EECE functional, where SCAN-EECE gives the best predictions. However, the calculation of the formation energy offers mixed results. SCAN, on average, results in larger formation energies compared to literature, and SCAN-EECE in smaller formation energies.

3 Kurzfassung

Eine korrekte energetische Beschreibung ist ein grundlegender Parameter, um mit computergestützten Berechnungsmethoden chemische Genauigkeit zu erreichen. Die Grundzustandsenergie bestimmt zum Beispiel die Stabilität von Kristallstrukturen für polymorphe Verbindungen und die Bildungsenergie gibt die allgemeine chemische Stabilität an. Die grundlegenden Methoden zur rechnerischen Ermittlung solcher Parameter werden ständig weiterentwickelt. Während Verbindungen der Hauptgruppe im Allgemeinen leichter mit der

Dichtefunktionaltheorie (DFT), der Methode der Wahl in dieser Arbeit, zu beschreiben sind, liegt der Schwerpunkt hier auf Übergangsmetallverbindungen, die korrelierte Elektronen aufweisen. Dies stellt ein viel komplizierteres Problem dar. Um es zu lösen, werden zwei moderne Funktionale, PBE und SCAN, mit dem hybriden on-site-Funktional EECE erweitert und hinsichtlich der polymorphen Energieordnung und der Bildungsenergie miteinander verglichen. Das EECE-Funktional zeichnet sich durch einen hybriden Ansatz aus, bei dem nur stark korrelierte Elektronen mit der exakten Hartree-Fock (HF) Austauschenergie behandelt werden. Im Gegensatz zu anderen Funktionalen, die auf die Lösung ähnlicher Probleme abzielen, wie z.B. LDA+U, ist das EECE-Funktional parameterfrei. Außerdem ist es rechnerisch viel weniger anspruchsvoll als eine vollständige HF-Berechnung. Die Ergebnisse für die polymorphe Energieordnung zeigen einen Vorteil für beide Kombinationen mit dem EECE-Funktional, wobei SCAN-EECE die besten Vorhersagen liefert. Die Berechnung der Bildungsenergie liefert jedoch gemischte Ergebnisse. SCAN führt im Durchschnitt zu größeren Bildungsenergien und SCAN-EECE zu kleineren Bildungsenergien im Vergleich zur Literatur.

4 Theory

4.1 Density functional theory

4.1.1 The Kohn-Sham equations

The foundation for the density functional theory (DFT) was laid by P. Hohenberg and W. Kohn in 1964. Their publication describes the ground state of an interacting electron gas in an external potential. The Hohenberg-Kohn-theorem says that the ground state electronic energy E is entirely defined by the electron density $n(\boldsymbol{r})$ [1].

$$E = \int v(\boldsymbol{r})n(\boldsymbol{r})d\boldsymbol{r} + \frac{1}{2}\iint \frac{n(\boldsymbol{r})n(\boldsymbol{r'})}{|\boldsymbol{r}-\boldsymbol{r'}|}d\boldsymbol{r}d\boldsymbol{r'} + G[n] \tag{1}$$

Where $v(\boldsymbol{r})$ is a static potential, and $G[n]$ is a universal functional of the electron density. Therefore, the first term of equation 1 describes the interaction between the nuclear charges and the electrons as a functional of n, also called the external energy $E_{ext}[n]$. It is uniquely defined by the atomic composition and the positions of the atoms. The second term represents the classical electron-electron Coulomb repulsion, also known as the Hartree energy $E_H[n]$. Furthermore, $G[n]$ can be described as

$$G[n] \equiv T_s[n] + E_{xc}[n] \tag{2}$$

where $T_s[n]$ is the kinetic energy of non-interacting electrons and $E_{xc}[n]$ is the exchange and correlation energy as a functional of n [2]. $E_{xc}[n]$ acts as a correction for replacing the many-body problem of the true kinetic energy with $T_s[n]$ and the electron-electron interaction with $E_H[n]$, further $E_{xc}[n]$ is

not known exactly [3]. Combining the above equations leads to a general equation of

$$E = E_{ext}[n] + E_H[n] + T_s[n] + E_{xc}[n] \tag{3}$$

for the electronic energy. Equation 3 still results in the exact electronic energy, it is called the Kohn-Sham energy functional. This functional can be minimised, leading to a set of one-electron Schrodinger equations, known as the Kohn-Sham equations [4, 5].

$$\left(-\frac{1}{2}\nabla^2 + V_{eff}(\boldsymbol{r})\right)\psi_i(\boldsymbol{r}) = \varepsilon_i\psi_i(\boldsymbol{r}) \tag{4}$$

$\psi_i(\boldsymbol{r})$ characterises a single-particle orbital and ε_i the eigenvalue, a quasi-particle energy. The effective potential $V_{eff}(\boldsymbol{r})$ is

$$V_{eff}(\boldsymbol{r}) = V_{ext}(\boldsymbol{r}) + V_H[n] + V_{xc}[n] \tag{5}$$

where $V_{ext}(\boldsymbol{r})$ is the external potential, $V_H[n]$ is the Hartree potential and $V_{xc}[n]$ is the exchange and correlation potential.

$$n(\boldsymbol{r}) = \sum_{i=1}^{N} |\psi_i(\boldsymbol{r})|^2 \tag{6}$$

The electron density is now given as the sum over all occupied wave functions $\psi_i(\boldsymbol{r})$ where N is the total number of electrons in the considered system. To solve these equations E_{xc} and, therefore, V_{xc} must be approximated, and self-consistent field (scf) calculations must be performed as the Kohn-Sham equations depend on their own solutions. In the following chapters, first, the scf method will be explained, followed by an introduction regarding approximations of $E_{xc}[n]$.

4.1.2 Self-consistent field methods

A self-consistent field method must be applied to solve the Kohn-Sham equations, which depend on their own solutions, namely the electron density $n(\boldsymbol{r})$. Figure 1 shows a schematic flow chart to search for a self-consistent solution of the Kohn-Sham equations [6].

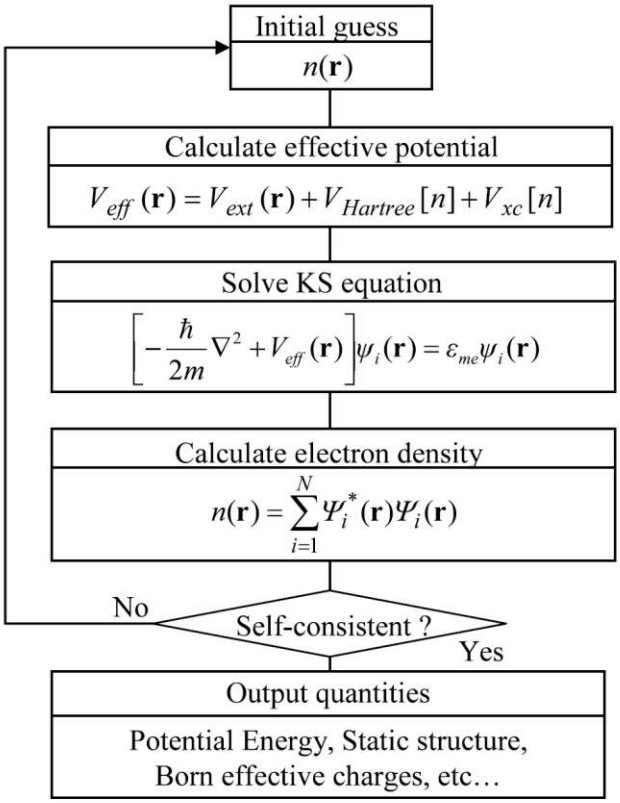


Figure 1: Flow chart describing the self-consistent field method for solving the Kohn-Sham equations from guessing the initial density (top) to the final, self-consistent output (bottom). Picture adapted from E. Nakamachi et al. [6].

The initial electron density is an educated guess, for example, the resulting density of the overlapping atomic densities [3]. It is very beneficial for the number of calculation cycles that need to be performed and thus for the computational effort that this guess is close to the actual electron density. A perfect guess would result in just one iteration to finish the procedure and the calculated electron density would be the same as the initial guess.
In the next step, the effective potential is calculated with regard to the input electron density (equation 5). Then the eigenvalue problem of the Kohn-Sham equations is solved (equation 4), resulting in a set of new eigenfunctions $\psi_i(\boldsymbol{r})$. With this, a new electron density can be obtained (equation 6), and the convergence criteria for self-consistency can be applied to the outcome. If it fits the requirements, the calculation is finished. If it does not fit the requirements, an additional mixing step with the initial electron density is usually performed, which is not displayed in figure 1, and the cycle continues until the stop criteria are met.
Figure 2 further illustrates the process which was described above. The initial input density n_{guess} gets refined with several iterations until it reaches the convergence criteria resulting in the self-consistent or converged electron density $n_{converged}$ [7].

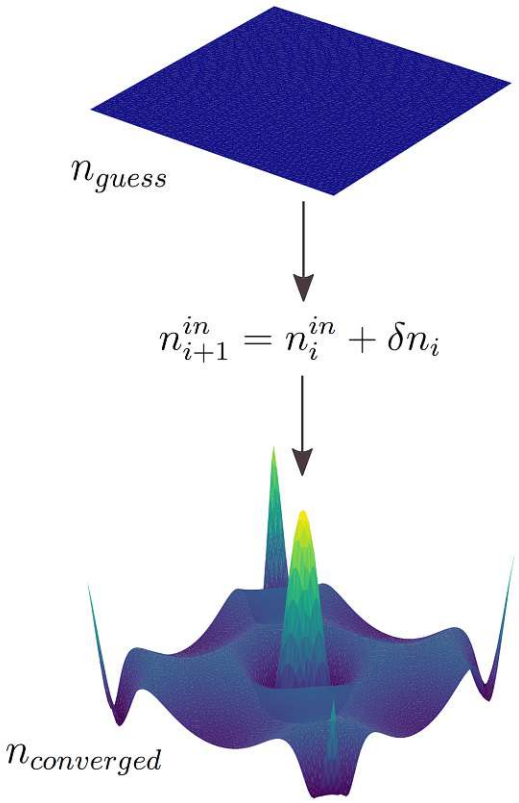


Figure 2: Example illustration (idealised) for finding the converged electron density, beginning from the initial guess (top), then the self-consistent field iterations (middle), to the final converged density (bottom). Picture adapted from N. D. Woods et al. [7].

4.1.3 Exchange-correlation functionals

The exact form of the exchange and correlation energy as a functional of n is unknown and, therefore, it needs to be approximated in a meaningful way. A local approximation shows, that $E_{xc}[n]$ can be expressed as a single-electron energy density $\epsilon_{xc}(n(\boldsymbol{r}))$ at a point $\boldsymbol{r}$, depending only on $n(\boldsymbol{r})$ in an area around $\boldsymbol{r}$ (equation 7) [1, 2, 5].

$$E_{xc}[n] = \int n(\boldsymbol{r})\epsilon_{xc}(n(\boldsymbol{r}))d\boldsymbol{r} \tag{7}$$

This implies that $E_{xc}[n]$ can be approximated as a local functional of the density [5].

4.1.4 Local density approximation (LDA)

W. Kohn and L. J. Sham introduced the local density approximation (LDA) in their publication in 1965 [2]. The LDA approximates $\epsilon_{xc}(n(\boldsymbol{r}))$ with the results from the model of the homogeneous electron gas (HEG) (equation 8 and 9).

$$E_{xc}^{LDA}[n] = \int n(\boldsymbol{r})\epsilon_{xc}^{HEG}(n(\boldsymbol{r}))d\boldsymbol{r} \tag{8}$$

$$\epsilon_x^{HEG}(n) = -\frac{3}{4}\left(\frac{3}{\pi}\right)^{\frac{1}{3}} n^{\frac{4}{3}} \tag{9}$$

The result of the LDA depends only on the value of the electron density at $\boldsymbol{r}$. $\epsilon_x^{HEG}(n)$ is the exchange energy density of the HEG, and the correlation energy density $\epsilon_c^{HEG}(n)$ can be calculated from the results of quantum Monte Carlo methods [8]. E_{xc} is given by the sum of E_x and E_c.

$$E_{xc} = E_x + E_c \tag{10}$$

In their original publication, Kohn and Sham also stated that they did not expect an accurate description of chemical bonding for their theory [2]. Still, with increasing computing power, calculations using the LDA showed promising results, for example, for predicting the ground state structure of Si or the cohesive energy of CO [3]. Although some results fit very well with the experimentally observed parameters, the LDA is by no means perfect.
A well-known problem of the LDA is to overbind [3,9]. This means that lattice parameters are typically predicted to be smaller than the experimental results. This further results in over-predicted cohesive energies, phonon frequencies and elastic moduli [10].

4.1.5 Generalised gradient approximation (GGA)

In 1986 J. P. Perdew and Y. Wang proposed the generalised gradient approximation (GGA) as an improved density functional for the electronic exchange energy [11]. Here, ϵ_x is approximated with the gradient of the electron density $\nabla n(\boldsymbol{r})$ in addition to the LDA, see equation 11 and equation 12.

$$\epsilon_x^{GGA} = \epsilon_x^{LDA}[n]F[s] \tag{11}$$

$$s(\boldsymbol{r}) = \frac{|\nabla n(\boldsymbol{r})|}{n(\boldsymbol{r})^{\frac{4}{3}}} \tag{12}$$

$s(\boldsymbol{r})$ is the dimensionless density gradient, and the exchange enhancement factor $F[s]$ describes the way this gradient is treated; see equation 13 for an example. In addition to the LDA, for the GGA, the electron density gradient is included (equation 12), resulting in much better information about the shape of the electron density, see figure 3.

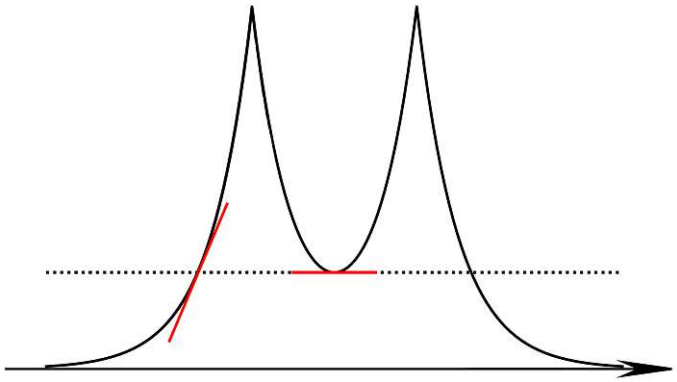


Figure 3: Illustration showing an example shape of an electron density (black line). The LDA would treat the three intersections of the dotted black line with the electron density all in the same way. The GGA provides more information on the shape of the density due to the gradient, illustrated with the red lines. Picture adapted from G. K. H. Madsen [3].

For $F[s]$, there are numerous approaches. One of them, which was also used in this work, is the method developed by J. P. Perdew, K. Burke and M. Ernzerhof in 1996, called PBE [12] (equation 13).

$$F_X^{PBE} = 1 + \kappa - \frac{\kappa}{1 + \mu s^2/\kappa} \tag{13}$$

Where $\kappa = 0.804$ and $\mu = 0.21951$. For small s equation 13 reduces to 1 and for big s it approaches $1 + \kappa$ for the exchange enhancement factor. Figure 4 shows the form of the enhancement factor for PBE-GGA compared to two other well-known GGAs, B88 and PW91, and the LDA [5].

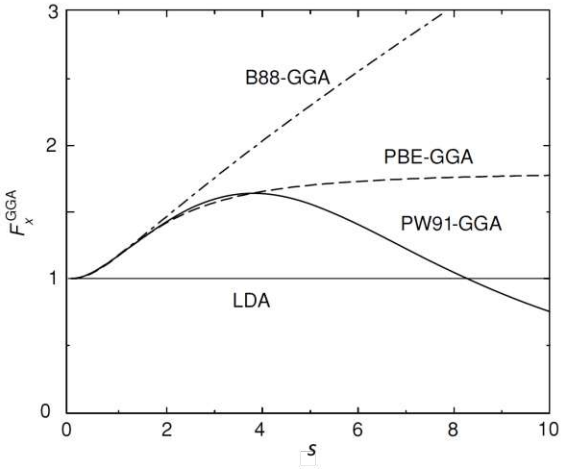


Figure 4: Comparison of the enhancement factor as a function of the dimensionless density gradient for different GGAs (B88, PW91 and PBE) and also the LDA. The LDA provides no enhancement factor, as only the density is observed. The PBE-GGA shows what was already described above: For $s = 0$ no enhancement is given, and for bigger s the enhancement approaches a limit $1 + \kappa = 1.804$. B88-GGA and PW91-GGA show quite different enhancement behaviours illustrating the diversity of GGA approximations. Picture adapted from R. M. Martin [5].

4.1.6 Meta-GGAs

In addition to the gradient of the electron density, meta-GGAs also consider the Laplacian of the electron density $\nabla^2 n(\boldsymbol{r})$ or the kinetic energy density $\tau(\boldsymbol{r})$ (equation 14) [13, 14].

$$\tau(\boldsymbol{r}) = \frac{1}{2}\sum_{i=1}^{N} |\nabla\psi_i(\boldsymbol{r})|^2 \tag{14}$$

A dimensionless variable that is often used for the calculation of meta-GGAs is the iso-orbital indicator $\alpha^{iso}(\boldsymbol{r})$ (equation 15). Where $\tau^W(\boldsymbol{r})$ is the Weizsäcker kinetic energy density (equation 16) and $\tau^{TF}(\boldsymbol{r})$ is the Thomas-Fermi kinetic energy density (equation 17).

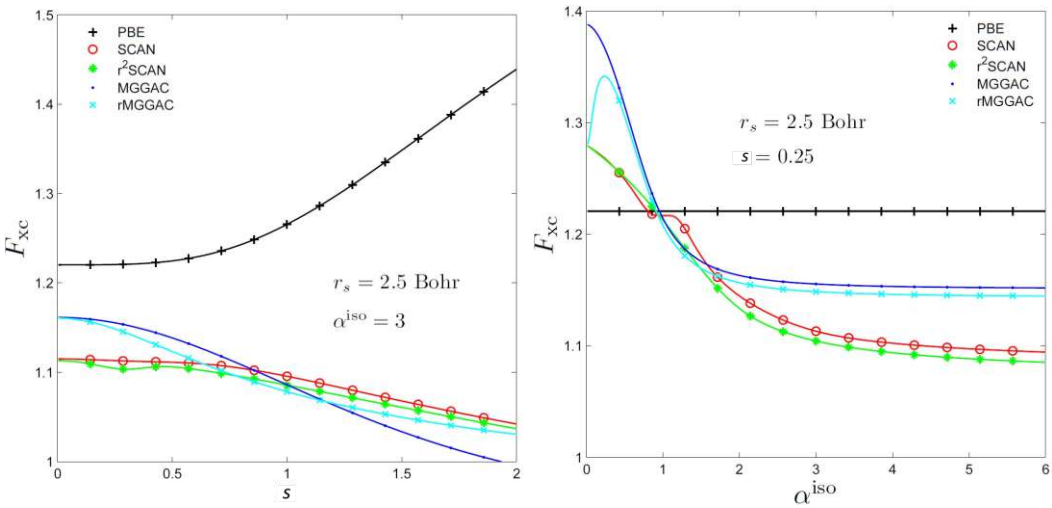
$$\alpha^{iso}(\boldsymbol{r}) = \frac{\tau(\boldsymbol{r}) - \tau^W(\boldsymbol{r})}{\tau^{TF}(\boldsymbol{r})} \tag{15}$$

$$\tau^W(\boldsymbol{r}) = \frac{1}{8}\frac{|\nabla n(\boldsymbol{r})|^2}{n(\boldsymbol{r})} \tag{16}$$

$$\tau^{TF}(\boldsymbol{r}) = \frac{3}{10}\left(3\pi^2\right)^{\frac{2}{3}} n^{\frac{5}{3}}(\boldsymbol{r}) \tag{17}$$

As for the GGA, also for meta-GGAs, a lot of different approximations are developed. Here, two approximations used in this work will be described shortly. One of them is the strongly constrained and appropriately normed meta-GGA (SCAN) [15]. The other is a meta-GGA constructed from the cuspless hydrogen model and Pauli kinetic energy density (MGGAC) [16].
SCAN is a fully constrained meta-GGA obeying all 17 known exact constraints, and it contains no empirical parameters [15]. Since its development in 2015, it has become more and more popular, mainly in the field of solid-state physics.
For MGGAC, the exchange component is a meta-GGA, whereas a GGA describes the correlation, and further, F_X^{MGGAC} is only dependent on α^{iso} but not on s [16, 17].
Figure 5 shows a comparison of the enhancement factor depending on s and α^{iso} for these functionals. Additionally, PBE and two other meta-GGAs are displayed, r^{2}SCAN and rMGGAC, which are revised versions of SCAN and MGGAC.

$$r_s = \left(\frac{3}{4\pi n}\right)^{\frac{1}{3}} \tag{18}$$



(a) (b)

Figure 5: (a) shows F_{XC} as a function of the dimensionless density gradient for the different functionals, and (b) shows the dependence of F_{XC} on the iso-orbital indicator. r_s is the Wigner-Seitz radius (equation 18) and the parameters which are kept constant are displayed in the graphs. Picture adapted from S. Jana et al. [17].

4.1.7 Hybrid functionals

A. D. Becke proposed another step to improve the exchange and correlation energy description in 1993 [18]. The proposed hybrid functionals are linear combinations of the orbital-dependent Hartree-Fock exchange energy E_x^{HF} (equation 20) with the exchange energy of a Kohn-Sham density functional E_x^{DFA} (GGA or meta-GGA), where α is the mixing parameter (equation 19) [3, 5].

$$E_x^{Hybrid} = \alpha E_x^{HF} + (1-\alpha) E_x^{DFA} \tag{19}$$

$$E_x^{HF} = -\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\iint \frac{\psi_i^*(\boldsymbol{r})\psi_j(\boldsymbol{r})\psi_j^*(\boldsymbol{r'})\psi_i(\boldsymbol{r'})}{|\boldsymbol{r}-\boldsymbol{r'}|} d\boldsymbol{r} d\boldsymbol{r'} \tag{20}$$

In contrast to LDA and GGA functionals, the Hartree-Fock exchange energy includes the exchange exactly and is self-interaction free. Therefore hybrid functionals can provide better results, for example, for the electronic structure and thermochemistry, especially for molecules [5, 19, 20]. Today they are the most popular functionals used in molecular chemistry. The main disadvantage is that calculating the Hartree-Fock exchange energy requires far more computational power (10 - 1000 times more than LDA/GGA/MGGA), and the methods are not very accurate for metals, especially regarding the magnetic moments [19].
An example of a hybrid functional, which is also the primary test object for this work, is the exact exchange for correlated electrons (EECE) on-site hybrid functional proposed by Novák et al. [20, 21]. The EECE will be explained in detail in section 4.2.4.

4.1.8 Jacob's ladder

It seems like every functional described in the previous sections is another step towards reaching actual chemical accuracy by use of computational methods. J. Perdew imagined these steps with a biblical metaphor, Jacob's ladder [22]. Figure 6 shows one of the many artistic illustrations of the exhausting climb towards perfection.

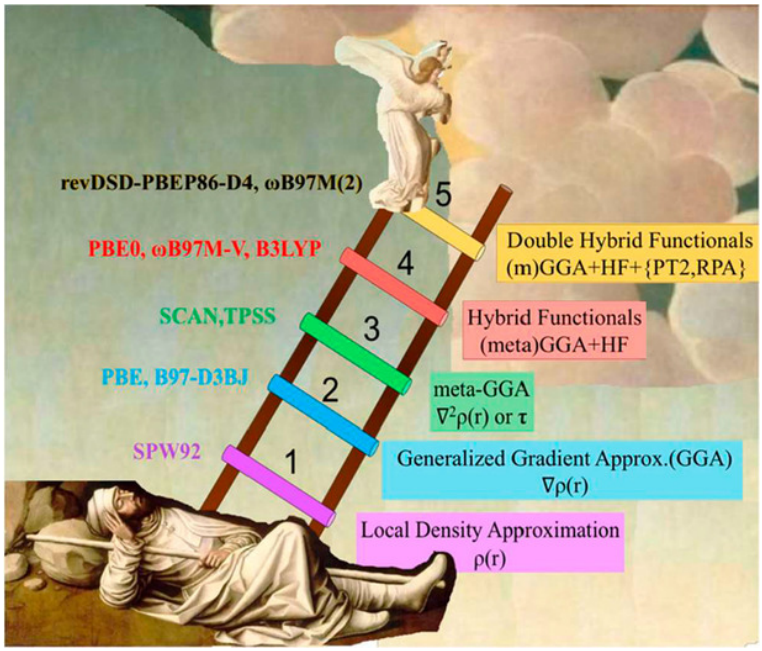


Figure 6: The Jacob's ladder begins at the earthen level where neither exchange nor correlation exists. Each step upwards symbolises a new milestone to describe the exchange and correlation energy better. Heaven is reached when the Schrodinger equation can be solved exactly, resulting in chemical accuracy via computational methods. Picture adapted from J. M. L. Martin et al. [23].

To conclude this section about density functional theory, Jacob's ladder allows a small revisitation of the previous chapters. The LDA, which W. Kohn and L. J. Sham proposed in its general form [2], makes use of just the electron density. This resembles the first step of the ladder. The GGA additionally considers the gradient of the electron density and, to a certain degree, compensates for the well known overbinding problem of the LDA. A prime example of a widely used GGA would be the PBE-GGA [12]. With every further step on the ladder, the overall results improve, but also, the functionals get more intricate and computationally expensive. It is also essential to keep in mind that these functionals are very recent. Some of them may not be thoroughly tested yet or are still under development. Step 3 introduces the Laplacian of the electron density and the kinetic energy density into the exchange and correlation energy description. The SCAN method is one of the recently emerging meta-GGA functionals [15]. Hybrid functionals make use of the exact and self-interaction free Hartree-Fock exchange mixed with the exchange from GGAs or meta-GGAs. The presented EECE method keeps the resources needed for running

low by only using the Hartree-Fock exchange energy for strongly correlated electrons inside the atomic spheres [20, 21]. The fifth step is occupied by double hybrid functionals, followed by most likely many further steps until heaven is reached.

4.2 Computational details

4.2.1 WIEN2k

WIEN2k, version 21.1, released on 30.04.2021, is the program which was used to obtain the results throughout this work. It allows to solve the Kohn-Sham equations based on the augmented plane wave plus local orbitals method (APW+lo) [24, 25]. For this, a variety of approximations for the exchange-correlation functional are implemented. This work features the already introduced PBE-GGA [12], the SCAN [15] and MGGAC [16] meta-GGAs and the on-site hybrid functional EECE [21]. The APW+lo method considers all electrons self-consistently in a full-potential treatment [26]. WIEN2k is developed at TU Wien and more than 3500 licences have been issued up to now. It enables the calculation of a wide variety of material properties and parameters, for example:

- total energy, forces, elastic constants
- structure optimisation, equilibrium geometries
- energy bands, density of states
- electron densities, spin densities, fermi surfaces
- phonons
- electric field gradient, NMR chemical shifts and NMR Knight shifts
- x-ray emission and absorption spectra, electron energy loss spectra

4.2.2 Setup of calculations and flow of programs

To set up a calculation first the structural data of the compound is needed. The information must contain:

- lattice type or space group
- lattice parameters and angles
- atoms and positions

After this, the nearest neighbour distances are calculated via the program *nn* and the optimal RMT values will be determined with *setrmt_lapw* (see the following section for a description of the RMT parameter). The then generated **.struct* master-file includes the required information for all further programs.

After this the initialisation is performed to set up the input files needed for the upcoming calculations. The script for this is *init_lapw*. In batch mode it runs a selection of subprograms such as *lstart* which generates the free atomic densities or *kgen* which generates a **k**-mesh in the Brillouin zone [27]. Various parameters can be set throughout the initialisation. In the following section the parameters *-rkmax* and *-numk*, which correspond to the size of the basis set and the **k**-mesh will be explained with more detail. The generated **.in0* file can then be adjusted to enable the computation with different functionals. By default the PBE functional is used which is signalled by the line *XC_PBE*. This can be modified for example to use the SCAN functional by changing the line to *XC_SCAN*.
However, the focus of this work is to compare the results obtained with the EECE functional, which requires a somewhat different initialisation process. Here the script *init_orb_lapw -eece* is called which results in an interactive dialogue where the user has to input the atoms and the orbitals which are then treated with the EECE. This generates an **.ineece* file where relevant parameters are stored, such as the mixing parameter α or the indices of the chosen atoms and orbitals.
When everything is set up the script *run_lapw* (or *runsp_lapw* for spin-polarised calculations) can be executed and the scf-calculations begin. The calculation with the EECE requires adding the parameter *-eece*. Figure 7 illustrates the program flow in WIEN2k. For further information on the individual subprograms depicted in this figure see the WIEN2k User's Guide [27].

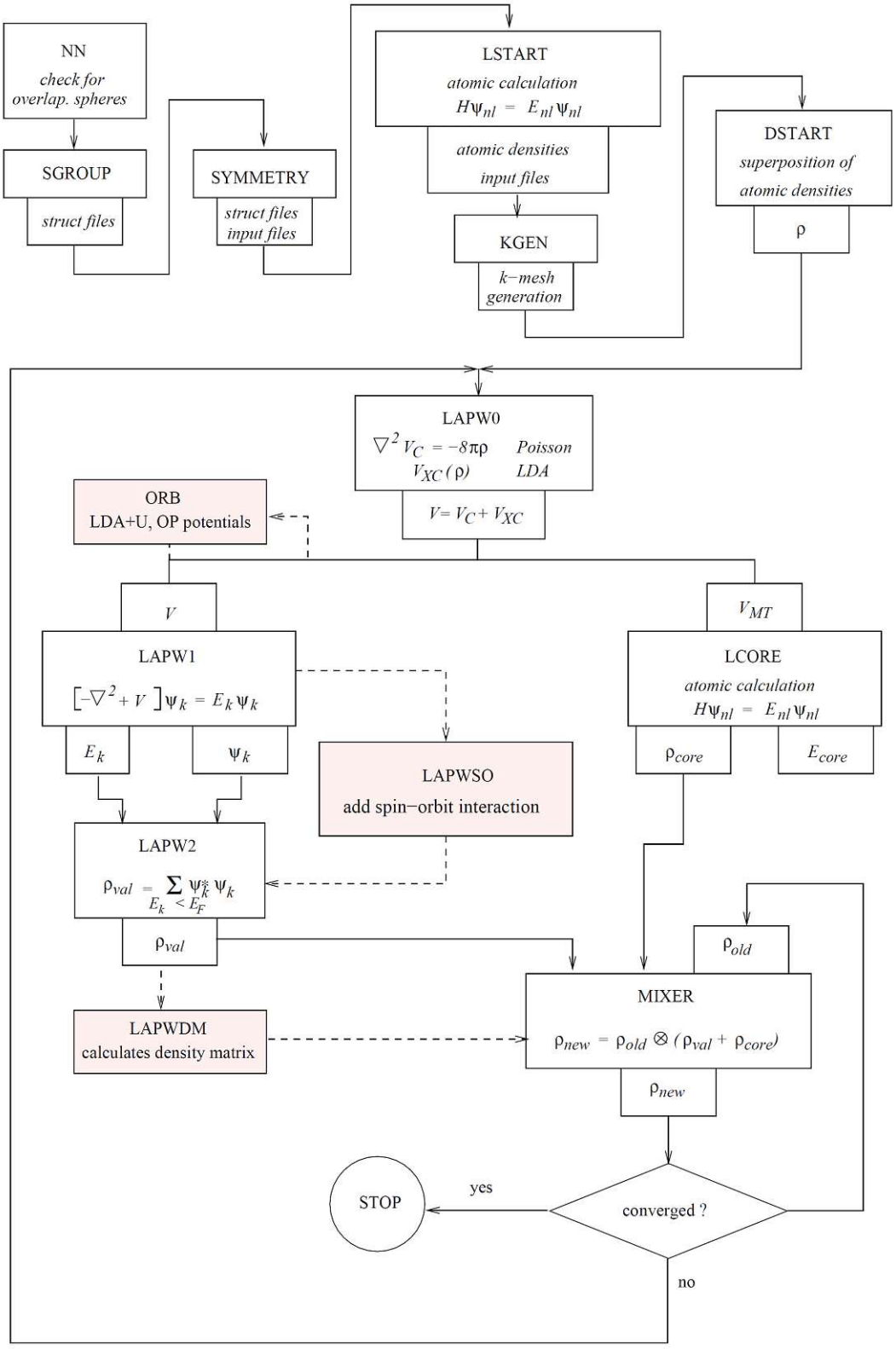
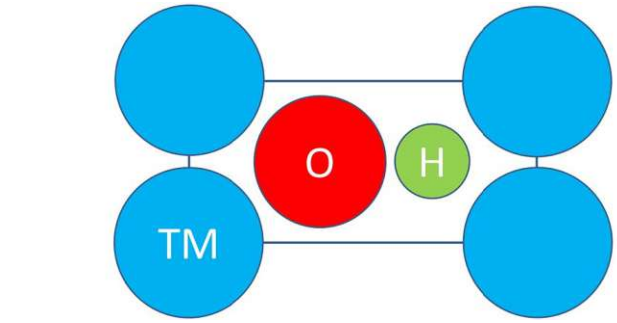


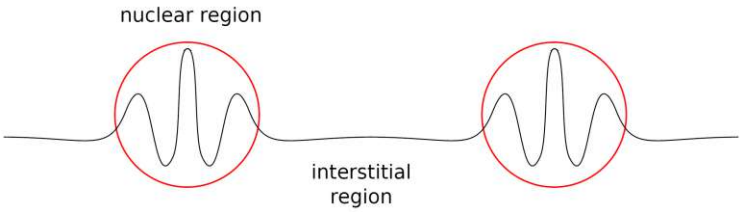
Figure 7: The program flow of WIEN2k. The upper part of the flow chart shows structure generation and initialisation and the subprograms that are executed within this process. The lower part illustrates the scf-cycle with the corresponding subprograms. Picture adapted from P. Blaha et al. [27].

4.2.3 Important initialisation parameters

This section will explain a selection of important parameters that can be set during structure generation and initialisation in WIEN2k.
The muffin-tin radius (RMT) defines the radius of the spheres centred on the atomic cores. These spheres mark the transition from the nuclear region to the interstitial region in the unit cell and their radius depends on the respective atoms and geometry of the unit cell, see figure 8 (a) for an example illustration. This is due to the APW-based aproach of WIEN2k which facilitates a different treatment of the quickly varying potential in the nuclear region and the slowly varying interstitial potential, see figure 8 (b). The spheres shall not overlap, but it is beneficial for the computational efficiency to choose them as large as possible [26].



(a)



(b)

Figure 8: (a) Example of a crystal structure where the radii of the spheres represent different values for the RMT. TM stands for a transition metal, which allows a large RMT, whereas for oxygen in red and hydrogen in green a smaller RMT is required. Picture adapted from P. Blaha et al. [26]. (b) Illustration of the wave function (black line) in the nuclear and interstitial area. The red circles show the muffin-tin areas centred on the atoms. Picture adapted from E. J. G. McDermott [28].

The parameter for the plane wave cut-off is the $R_{MT}^{min}K_{max}$ or short RKmax. This is a crucial parameter for both the quality of the results and also the computing time. It determines the number of basis functions used in the APW+lo method and therefore the size of the matrices that need to be computed [29]. RKmax defines the result of the smallest muffin-tin radius multiplied by the largest wave vector used in the plane wave expansion.
Another important parameter for the quality of the results and also the computing time is the **k**-mesh. The number of **k**-points specifies, how the irreducible part of the Brillouin zone (IBZ) is sampled in the calculations, see

figure 9. A dense **k**-mesh favours the convergence of the final result but also requires more computational power. Both for the **k**-mesh and also RKmax an optimum can be found, where the final results converge sufficiently and the computing time is as low as possible. See figure 10 for an example calculation of the total energy of ScAs with respect to the number of **k**-points and RKmax. It is important to note, that the results for the parameters of this example are just valid for the chosen settings and compound.

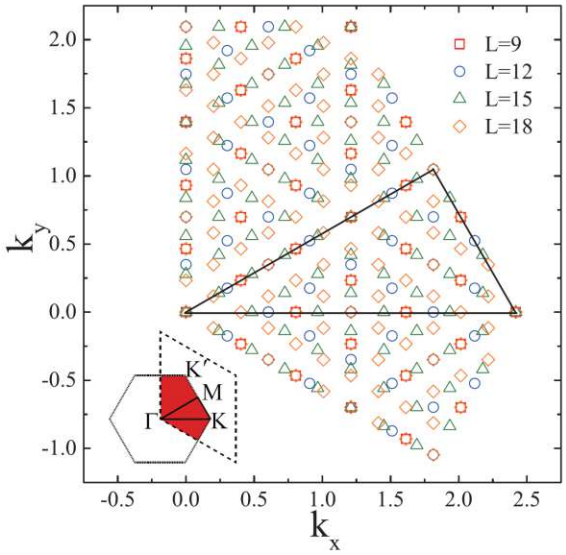
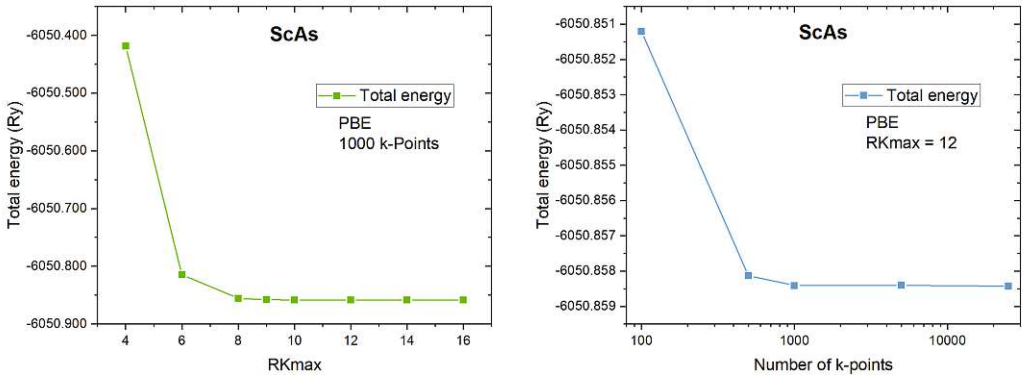


Figure 9: On the bottom left a 2-dimensional Brillouin zone is illustrated. The part coloured in red is shown enlarged in the rest of the graph. The black line corresponds to the high-symmetry path $\Gamma \rightarrow M \rightarrow K \rightarrow \Gamma$. A bigger L means more **k**-points and therefore a denser **k**-mesh, which is depicted with the different symbols. Picture adapted from H. Q. Wu et al. [30].



(a) Results for the calculated total energy as a function of RKmax

(b) Results for the calculated total energy as a function of the number of **k**-points

Figure 10: (a) shows that with the chosen settings the total energy of ScAs converges for RKmax ≥ 8. (b) shows a convergence for the total energy at ≥ 1000 **k**-points. The functional and the fixed parameters are shown in the graphs. Pictures are adapted from own calculations.

4.2.4 Exact exchange for correlated electrons (EECE)

The main objective of this work is to compare the EECE functional to widely used functionals such as PBE or SCAN. The EECE specifically aims to improve the description of systems containing correlated electrons [20], where PBE and SCAN are known to perform poorly [15]. In comparison to another commonly used method which also aims to improve this problem, the LDA+U [31, 32], the EECE is parameter-free [20]. Works by Tran et al. [21] show promising results in the application of the EECE to transition metal monoxides.
For the EECE only strongly correlated electrons are treated with the Hartree-Fock (HF) exchange energy (equation 20), for example d or f electrons. Further, this treatment is applied only inside the atomic spheres using an augmented plane wave scheme [21], whereas the residual space and electrons are treated with GGAs or mGGAs (equation 21). This allows maintaining a low computational demand whilst optimising the description of the correlated electrons with the exact results from the Hartree-Fock equation.

$$E_{xc}^{EECE}[n] = E_{xc}^{(m)GGA}[n] + \alpha \left(E_{x}^{HF}[\psi_{sel}] - E_{x}^{(m)GGA}[n_{sel}] \right) \tag{21}$$

The exchange and correlation energy of the EECE $E_{xc}^{EECE}[n]$ is calculated from the exchange and correlation energy of a GGA or mGGA functional $E_{xc}^{(m)GGA}[n]$ where the exchange energy for the selected electrons $E_{x}^{(m)GGA}[n_{sel}]$ is replaced with the HF exchange energy $E_{x}^{HF}[\psi_{sel}]$ by a factor of α. The default for the mixing parameter α in the implementation in WIEN2k is 0.25 and ψ_{sel} and n_{sel} are the wave function and electron density of the selected (sel) electrons.

4.2.5 Energy minimisation

To find the minimum energy structure with respect to the chosen parameters a variation of the unit cell volume is performed. In this work mainly two different methods were used. The first one is the classic volume optimisation, which takes the unit cell volume and varies it by predefined percentages, for example 0, ±2, ±4 and ±6 %. The result is a energy versus volume function which can be evaluated to find the minimum energy of the structure. For an example of a volume optimisation see figure 11. To obtain the minimum energy E_0 and the volume at this point V_0 as well as various other characteristic values, WIEN2k enables the fitting with different equations of state, for example Birch-Murnaghan [33, 34], Vinet-Rose [35] or Poirier-Tarantola [36]. Throughout this work the results obtained with the Birch-Murnaghan equation of state are used. The second method is more elaborate and computationally expensive as it varies the lattice parameter separately to find the minimum energy structure. In WIEN2k the script for this is *optimize_abc* and it enables a optimisation of lattice parameters for hexagonal and tetragonal (2D) unit cells as well as orthorhombic or even monoclinic (3D) ones [27].

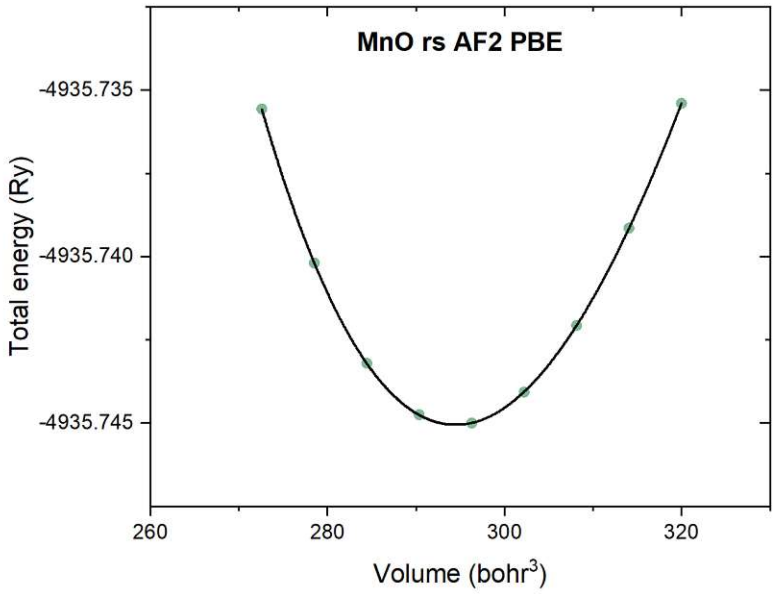
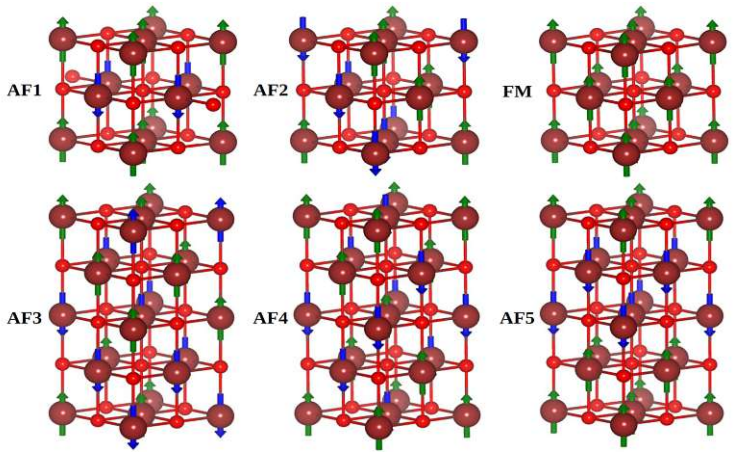


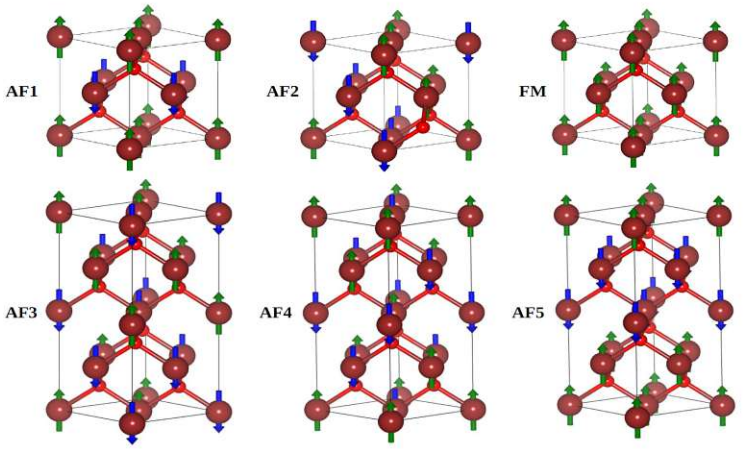
Figure 11: Volume optimisation of MnO in the rocksalt AF2 structure (this structure will be explained in the next section) with the PBE-GGA functional. The black curve is a polynomial fit, whereas the green dots show the calculated energies for different volumes. Picture is adapted from own calculations.

4.2.6 Magnetic structures

For a lot of the inspected transition metal compounds, especially the Mn/Fe/Co /Ni-monoxides (TMOs) with more localised electrons, the magnetic characteristics are an important factor to find the correct energetic minimum. Magnetism mostly comes from exchange splitting and this results in an occupation of states with different numbers of spin-up and spin-down electrons [26]. For this a spin-polarised calculation must be performed in WIEN2k via *runsp_lapw*. By default this method performs a ferromagnetic calculation with all magnetic moments aligned in the same direction. This ordering may be correct for Fe, but TMOs can theoretically exhibit various different ferromagnetic and antiferromagnetic configurations, as well as different crystal structures, see figure 12. Studies by A. Schrön et al. [37, 38] show that the *rs* structures preferably exhibit AF2 ordering and the *zb* structures exhibit AF1 ordering for the above mentioned TMOs. Additionally experimental data shows, that the *rs* structure is energetically more stable than the *zb* structure for all of them [37].



(a) Magnetic configurations of the rocksalt (*rs*) structure.

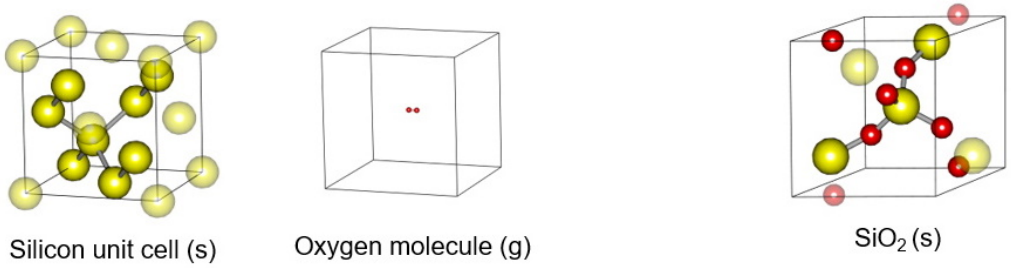


(b) Magnetic configurations of the zinc-blende (*zb*) structure.

Figure 12: (a) shows the magnetic configurations of the rocksalt structure. There are 5 anti-ferromagnetic orderings (AF1-AF5) and one ferromagnetic ordering (FM) displayed. (b) shows the configurations of the zinc-blende structure and there are also 5 anti-ferromagnetic orderings (AF1-AF5) and one ferromagnetic ordering (FM). The different spin directions are illustrated via green (spin-up) and blue (spin-down) arrows. Pictures are adapted from A. Gosh et al. [17].

4.2.7 Formation energy calculation

The calculation of the formation energy is an important benchmark for DFT calculations. This work compares the formation energies calculated with different functionals with the experimentally obtained formation energies. With this comparison the effectiveness of the functionals can be reviewed. Further the correct prediction for the ground state structure can be tested by calculating the formation energies of different structures, for example *zb* versus *rs* in TMOs. Figure 13 illustrates how the formation energy can be calculated for the example of SiO_2. Experimentally it is mostly determined with calorimetry.



$$\mathrm{Si}\,(s) \quad + \quad O_2\,(g) \quad + \Delta E_{form} \rightarrow \quad SiO_2\,(s)$$

$$E_{formation} = E_{products} - E_{reactants}$$

Figure 13: The calculation of the formation energy of SiO_2. On the reactant side the ground state energy of the most stable configuration of Si and O must be known. For this example this would be cubic Si and the O_2 molecule. Same must be known for the product side. A subtraction of these energies gives the formation energy of the compound. A negative energy means the product is energetically more stable than the two separate educts and vice versa. Picture adapted from `https://www.materialssquare.com/blog` (12.04.2022)

5 Practical part

The structural data of the calculated compounds are summarised in the separate appendix in the form of the **.struct* files with excluded symmetry operations.

5.1 Polymorphic energy ordering of MnO, FeO, CoO and NiO

The experimental ground state for the transition metal monoxides MnO, FeO, CoO and NiO is the *rs* structure ($Fm\bar{3}m$) with 6-fold, octahedrally coordinated transition metals, as already discussed in section 4.2.6. Studies by A. Schrön et al. [37,38] and Zhang et al. [39] show deviating results for the ground state structures obtained with DFT functionals, for example, PBE and SCAN, which prefer the *zb* structure ($F\bar{4}3m$) with 4-fold, tetrahedrally coordinated transition metals over *rs* for most of the compounds. To improve the description of the correct ground state structure of TMOs, the exact exchange for correlated electrons (EECE) on-site hybrid functional proposed by Novák et al. [20, 21] was tested and compared to the results obtained with PBE and SCAN.

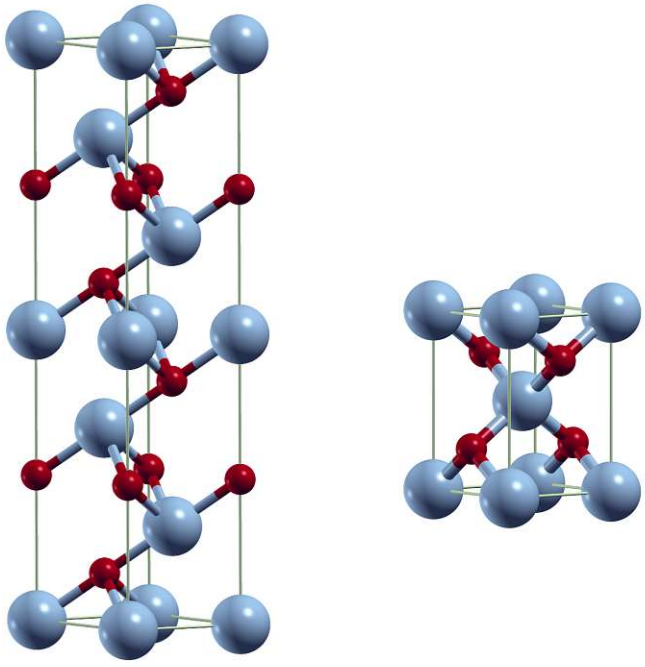
5.1.1 Rocksalt versus zinc-blende structures

First of all the structures of the *rs* AF2 and *zb* AF1 polymorphs of MnO, FeO, CoO and NiO were generated. To take the correct magnetic ordering into

account, a supercell for each structure was set up, see table 1 for the initial supercell parameters and figure 14 for an example illustration of the supercells.

Table 1: Parameters for the initial supercell generation of MnO, FeO, CoO and NiO in the *rs* AF2 and *zb* AF1 structure. The lattice parameters a, b and c are in Å and the angles α, β and γ in degrees.

compound			$a = b$	c	$\alpha = \beta$	γ
MnO	*rs*	AF2	3.14	15.40	90.0	120.0
FeO			3.04	14.91		
CoO			3.01	14.77		
NiO			2.95	14.47		
MnO	*zb*	AF1	3.37	4.77	90.0	90.0
FeO			3.22	4.56		
CoO			3.22	4.55		
NiO			3.11	4.40		



(a) Supercell of the *rs* AF2 structure with hexagonal coordination.

(b) Supercell of the *zb* AF1 structure with tetragonal coordination.

Figure 14: Example illustrations of the supercells generated to take the correct magnetic ordering into account. The gray-blue spheres show the positions of the the transition metal atoms and the red spheres show the positions of the oxygen atoms. Picture adapted from own calculations.

As described in section 4.2.2 the next step was the initialisation via *init_lapw* in WIEN2k. The initialisation parameters were set according to table 2 with

use of the *-prec 1* setting. To obtain comparable results it was important to choose the same parameters for the different polymorphs of the same compound, except for the **k**-mesh which was set according to the values suggested during the initialisation process.

Table 2: Initialisation parameters for the TMOs. The values for the RMTs are shown as: RMT of atom 1 / RMT of atom 2. The value of fftfac defines the enhancement factor of the FFT grid. The lvns value defines the maximum l value for partial waves used in the computation of non-muffin-tin matrix elements and gmax is the value for the Fourier series cutoff for charge densities [27].

Compound			RMT	**k**-mesh	RKmax	fftfac	lvns	gmax
MnO	*rs*	AF2	1.98 / 1.71	12 x 12 x 12	8.00	2	6	16
FeO			1.89 / 1.63					
CoO			1.84 / 1.58	13 x 13 x 13				
NiO			1.83 / 1.57					
MnO	*zb*	AF1	1.98 / 1.71	13 x 13 x 9	8.00	2	6	16
FeO			1.89 / 1.63					
CoO			1.84 / 1.58	14 x 14 x 10				
NiO			1.83 / 1.57					

After the successful initialisation the energy minimisation was performed for the chosen functionals PBE, SCAN and also the on-site hybrid functionals PBE-EECE and SCAN-EECE. Figures 16 - 19 show the obtained energy versus volume curves for all calculated compounds and functionals. The results will be summarised and discussed in section 6.
To validate the results obtained with the initialisation parameters from table 2 the minimum structures were additionally initialised with higher precision parameters with use of the *-prec 2* setting. This setting featured a denser **k**-mesh and increased values for RKmax, fftfac and gmax. Table 3 shows the parameters used for the validation run and figure 15 illustrates the results in form of the energy difference of the zinc-blende and rocksalt structure for each compound with PBE and SCAN in both precision settings. With this results the *-prec 1* setting according to table 2 was decided to be good to go for the upcoming calculations.

Table 3: Initialisation parameters for the validation run of the calculation of the minimum energy structures with higher precision settings compared to the initialisation parameters in table 2.

Compound			RMT	**k**-mesh	RKmax	fftfac	lvns	gmax
MnO	*rs*	AF2	1.98 / 1.71	25 x 25 x 25	9.00	3	6	20
FeO			1.89 / 1.63	28 x 28 x 28				
CoO			1.84 / 1.58	28 x 28 x 28				
NiO			1.83 / 1.57	28 x 28 x 28				
MnO	*zb*	AF1	1.98 / 1.71	21 x 21 x 15	9.00	3	6	20
FeO			1.89 / 1.63	21 x 21 x 15				
CoO			1.84 / 1.58	19 x 19 x 13				
NiO			1.83 / 1.57	22 x 22 x 16				

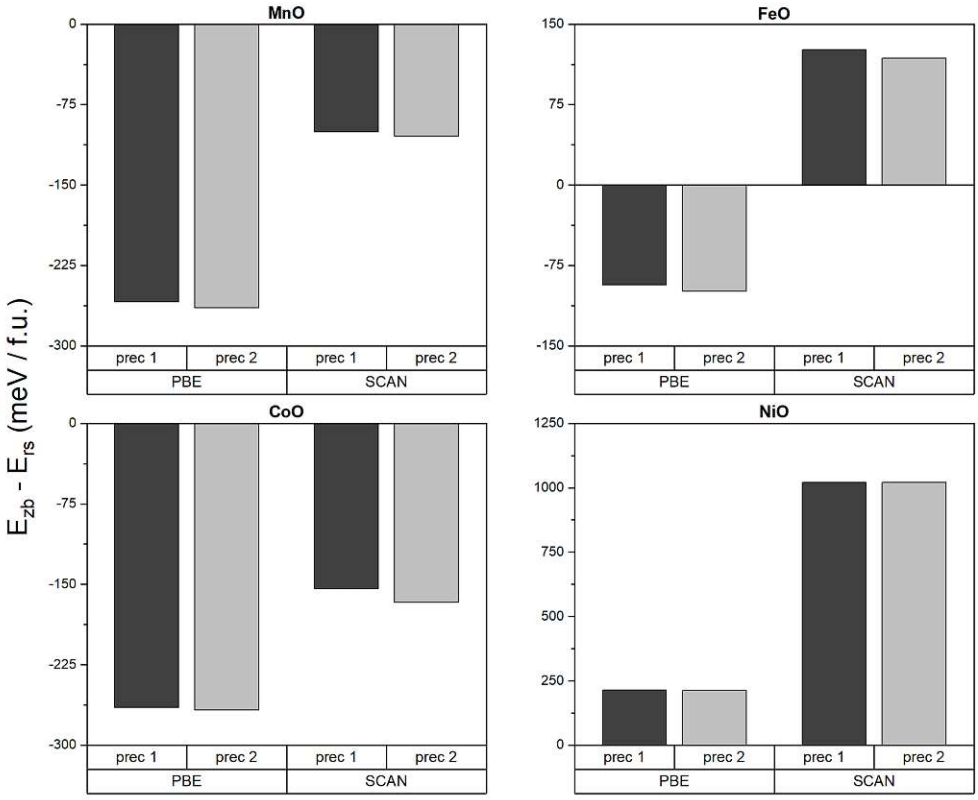


Figure 15: Results of the energy difference between the *zb* and *rs* configuration of MnO, FeO, CoO and NiO calculated with PBE and SCAN and different initialisation parameters, see table 2 and 3.

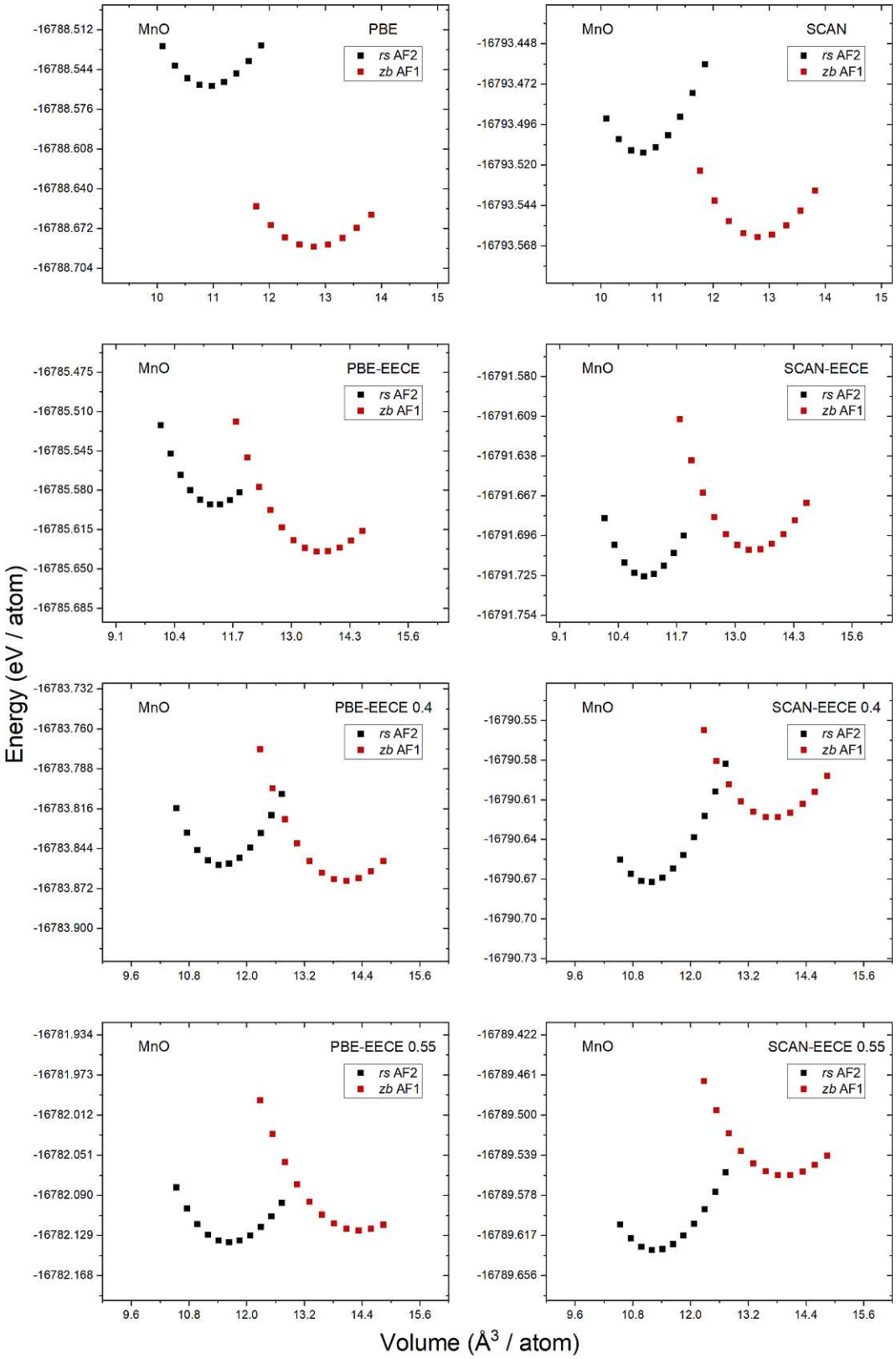


Figure 16: Comparison of the energy minimisation curves of MnO in *rs* AF2 and *zb* AF1 configuration for the PBE and SCAN functional and also for the functionals mixed with the exact exchange for correlated electrons. EECE 0.4 and EECE 0.55 stand for a mixing parameter α of 0.4 and 0.55 (equation 21), whereas the default α is 0.25 (EECE with no number added). Picture adapted from own calculations.

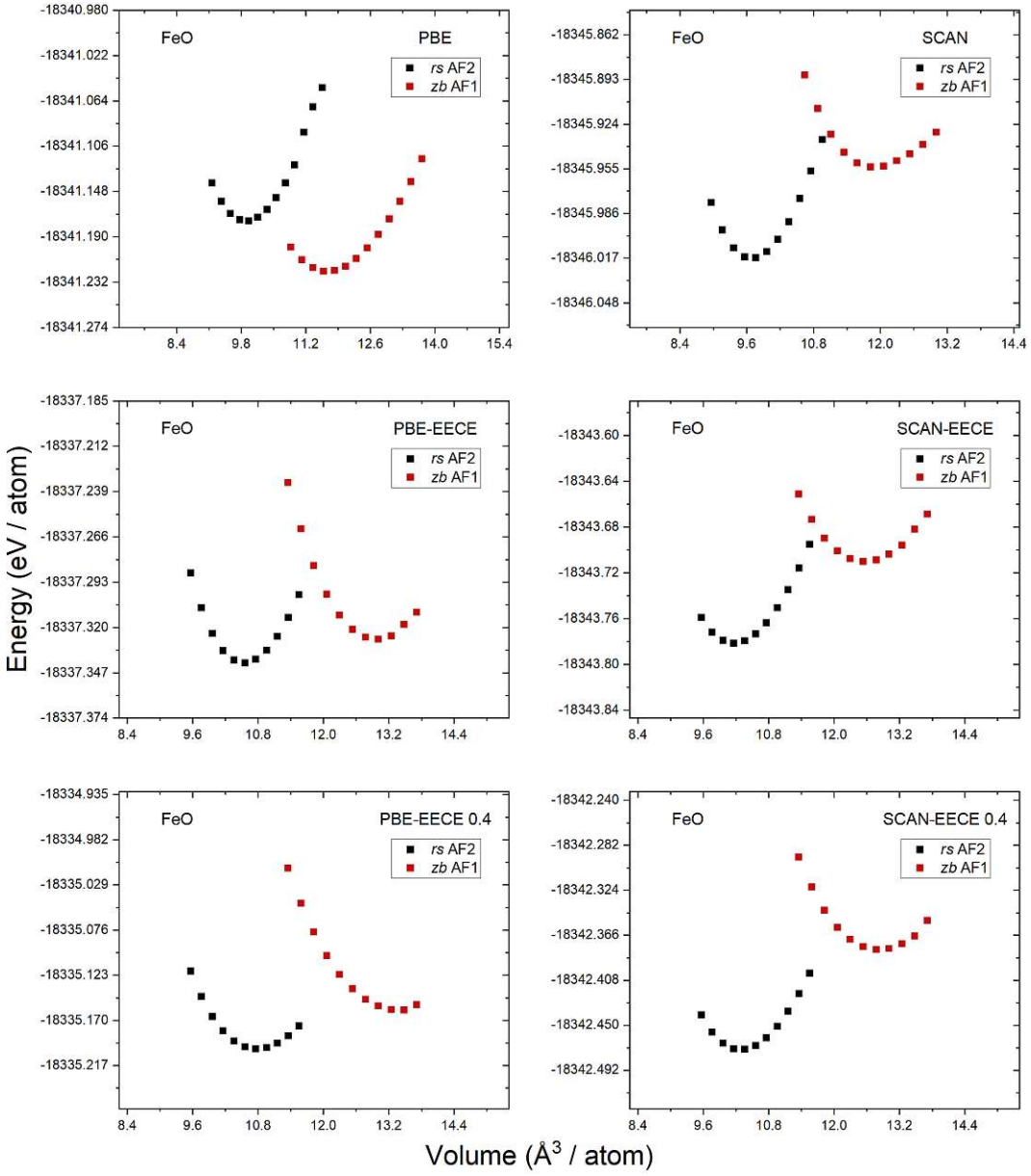


Figure 17: Comparison of the energy minimisation curves of FeO in *rs* AF2 and *zb* AF1 configuration for the PBE and SCAN functional and also for the functionals mixed with the exact exchange for correlated electrons. Picture adapted from own calculations.

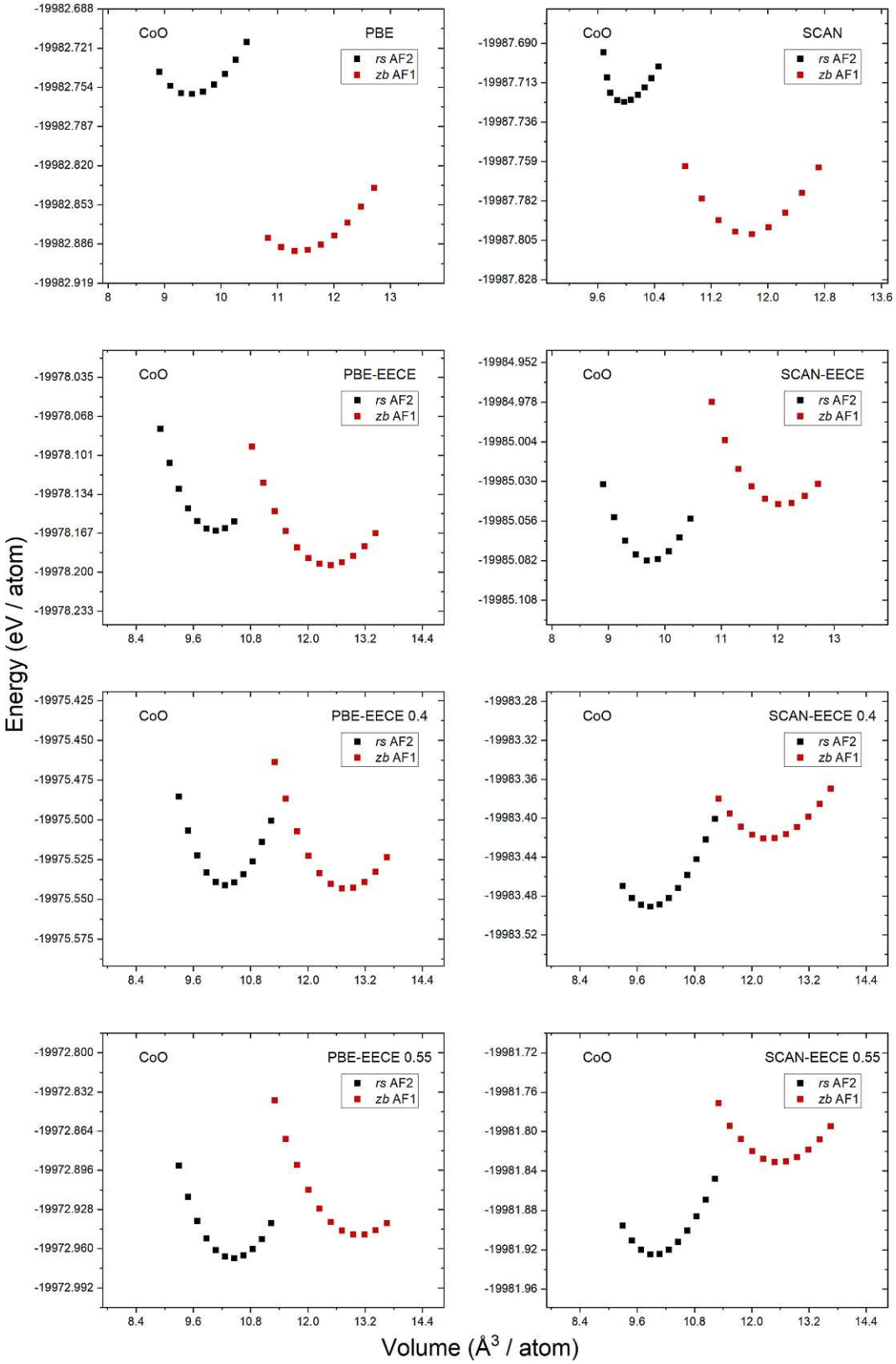


Figure 18: Comparison of the energy minimisation curves of CoO in *rs* AF2 and *zb* AF1 configuration for the PBE and SCAN functional and also for the functionals mixed with the exact exchange for correlated electrons. Picture adapted from own calculations.

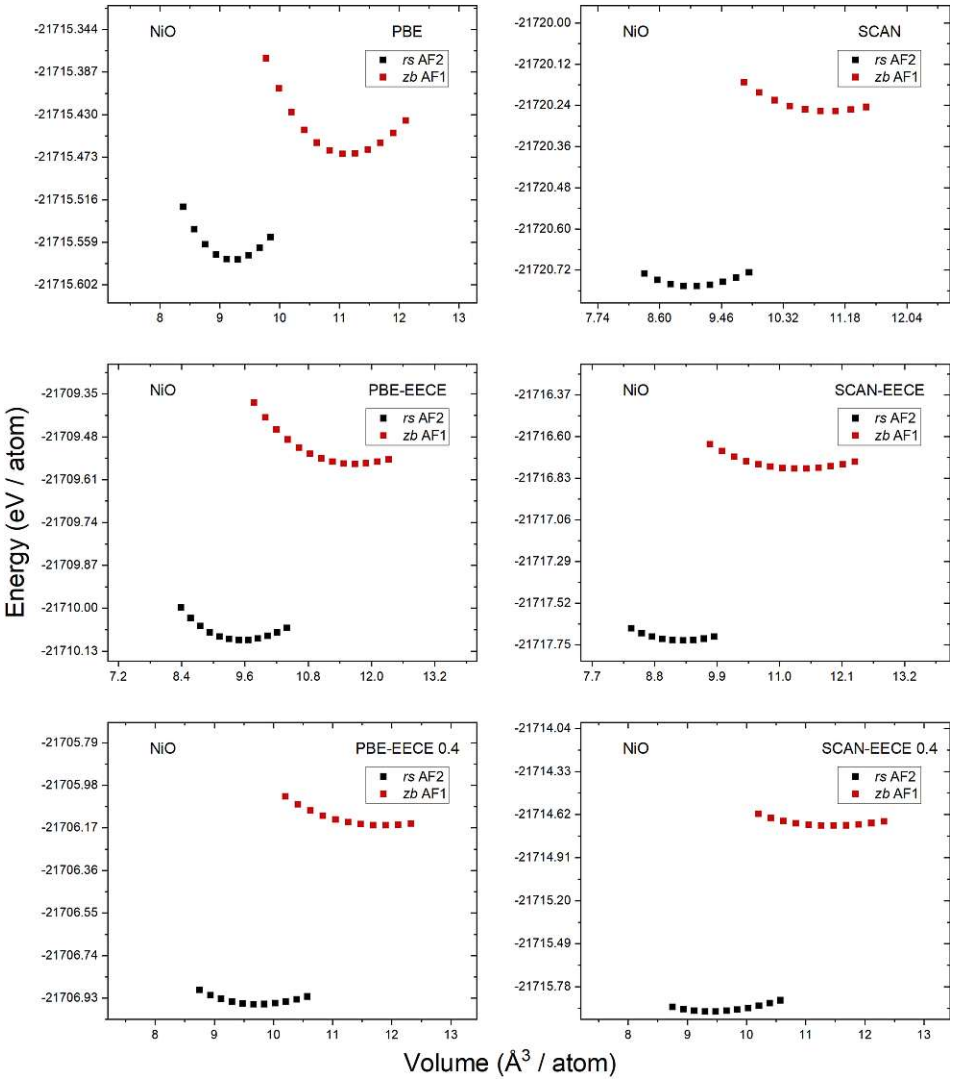


Figure 19: Comparison of the energy minimisation curves of NiO in *rs* AF2 and *zb* AF1 configuration for the PBE and SCAN functional and also for the functionals mixed with the exact exchange for correlated electrons. The seemingly flat curves are a result of the large energy differences between *rs* AF2 and *zb* AF1 for NiO. Picture adapted from own calculations.

5.1.2 Distorted structures

While in section 5.1.1 the polymorphic energy ordering of the ideal *rs* and *zb* structures of MnO, FeO, CoO and NiO was examined this section aims to compare the polymorphic energy ordering of the distorted structures with use of a c/a energy optimisation. For this the lattice parameters c and a were varied for predefined ratios while maintaining a constant volume. Studies from Schrön et al. [38] show, that all of the above mentioned compounds exhibit distortions from the ideal *rs* and *zb* structures both for experimental results and DFT calculations.
To set up the calculations the structures correlating with the energetic minima of the volume optimisations in section 5.1.1 were copied to a new directory and

re-initialised in WIEN2k. After generating the desired c/a - steps with the command *x optimize* and the setting *Vary c/a ratio with constant volume* the energy minimisation could be performed. The results for the minimum energies as well as the c/a distortions and the lattice parameters for each compound and functional can be found in table 4 and will be discussed in section 6.

Table 4: Results of the c/a energy optimisation of the TMOs starting from the ideal *rs* and *zb* minimum structures, calculated with the functionals PBE, PBE-EECE, SCAN and SCAN-EECE. The table displays the c/a distortion in %, the total energy in Rydberg and the unit cell parameters a and c in Angstrom.

compound		functional	c/a distortion in %	total energy in eV / atom	a in Å	c in Å
MnO	*rs*	PBE	−4.3	−16 788.570	3.19	14.95
	zb		−7.0	−16 788.699	3.39	4.46
	rs	PBE-EECE	−2.8	−16 785.602	3.19	15.21
	zb		−6.4	−16 785.645	3.45	4.56
	rs	SCAN	−2.9	−16 793.524	3.15	15.00
	zb		−7.0	−16 793.576	3.39	4.46
	rs	SCAN-EECE	−1.9	−16 791.736	3.16	15.21
	zb		−6.1	−16 791.718	3.42	4.54
FeO	*rs*	PBE	15.9	−18 341.216	2.90	16.45
	zb		−12.2	−18 341.238	3.34	4.15
	rs	PBE-EECE	−4.6	−18 337.355	3.15	14.73
	zb		−16.8	−18 337.358	3.54	4.16
	rs	SCAN	14.4	−18 346.049	2.89	16.20
	zb		−20.7	−18 346.020	3.48	3.91
	rs	SCAN-EECE	−4.6	−18 343.798	3.11	14.54
	zb		−20.2	−18 343.755	3.54	4.00
CoO	*rs*	PBE	14.6	−19 982.803	2.86	16.06
	zb		−2.8	−19 982.899	3.20	4.40
	rs	PBE-EECE	−1.0	−19 978.171	3.06	14.87
	zb		−1.6	−19 978.200	3.30	4.59
	rs	SCAN	−5.0	−19 987.749	3.10	14.42
	zb		1.4	−19 987.810	3.20	4.59
	rs	SCAN-EECE	−0.7	−19 985.090	3.02	14.69
	zb		−2.0	−19 985.054	3.26	4.52
NiO	*rs*	PBE	−0.6	−21 715.582	2.98	14.51
	zb		−15.6	−21 715.482	3.33	3.98
	rs	PBE-EECE	−0.1	−21 710.103	3.00	14.65
	zb		−10.7	−21 709.582	3.33	4.21
	rs	SCAN	−0.1	−21 720.774	2.96	14.46
	zb		−15.3	−21 720.310	3.33	3.99
	rs	SCAN-EECE	−0.3	−21 717.734	2.98	14.54
	zb		−11.8	−21 716.802	3.31	4.12

5.2 Polymorphic energy ordering of other problematic transition metal compounds

In 2018 Zhang et al. [39] demonstrated the efficiency of the SCAN functional in predicting the correct crystal structures of main group compounds, whereas for transition metal compounds this prediction, by their own words, remains a challenge. The EECE functional is suited very well for calculations of transition metal compounds as Tran et al. [21] demonstrated in their work. In this section a selection of transition metal compounds which were already known to perform poorly with SCAN from the works of Zhang et al. [39] were evaluated with the SCAN-EECE functional. Table 5 shows the chosen compounds, their experimentally obtained structures and structures which were wrongfully found to be more stable with use of the SCAN functional.

Table 5: A list of transition metal compounds compiled from the works of Zhang et al. [39] where the experimental structures do not agree with the ground state structures calculated with SCAN. The space groups of the structures are represented with the Hermann-Mauguin notation. For some compounds more than one structure with a total energy lower than the experimental structure was found, therefore they were indexed with whole numbers, beginning with 0 for the most stable of them.

compound	experimental space group	SCAN - more stable space groups		
		0	1	2
AgF	$Fm\bar{3}m$	$Cmcm$	$P\bar{6}m2$	$Pm\bar{3}m$
AgSe	$F\bar{4}3m$	$Fm\bar{3}m$	$P6_3/mmc$	$P\bar{6}m2$
CrO	$Fm\bar{3}m$	Ccm	$P4/mmm$	
Cu_2Se	$Fm\bar{3}m$	$P4_3$		
CuI	$F\bar{4}3m$	$P2_1/m$		
CuSe	$Cmcm$	$F\bar{4}3m$		
LaN	$Fm\bar{3}m$	$Pmmn$		
MnS	$Fm\bar{3}m$	$P2_1$	$I\bar{4}m2$	
MnSe	$Fm\bar{3}m$	$P2_1$	$I\bar{4}m2$	
MoAs	$Pnma$	$P\bar{6}m2$		
NbN	$P6_3/mmc$	$P\bar{6}m2$	$P\bar{6}m2$	
PtO	$P4_2/mmc$	$Pnma$		
TiS	$R\bar{3}m$	$P\bar{6}m2$	$P\bar{6}m2$	$P6_3/mmc$

The structures were imported and initialised in WIEN2k with *init_lapw* with use of the *-prec 2* setting. Again it was very important to use the same parameters for the different structures of each compound to obtain comparable results. In table 6 the initialisation parameters for each structure can be found.

Table 6: Initialisation parameters for the transition metal compounds. The values for the RMTs are shown as: RMT of atom 1 / RMT of atom 2. HDLOs are generally used to remove any larger linearisation errors, they contain the second energy derivative of the radial wave function [27].

compound	RMT	RKmax	fftfac	lvns	gmax	hdlo
AgF	2.27 / 2.05	9.00	3	6	20	yes
AgSe	2.33 / 2.21	9.00	2	6	16	yes
CrO	1.86 / 1.68	8.00	2	6	16	yes
Cu_2Se	2.05 / 1.95	8.50	2	6	16	yes
CuI	2.07 / 2.07	9.00	2	6	16	yes
CuSe	1.92 / 1.83	8.50	2	6	16	yes
LaN	2.26 / 1.85	8.50	2	6	16	yes
MnS	2.17 / 1.86	8.49	3	6	20	yes
MnSe	2.18 / 2.07	9.00	3	6	20	yes
MoAs	2.14 / 2.14	10.00	3	6	20	yes
NbN	2.02 / 1.74	8.05	3	6	20	yes
PtO	1.84 / 1.51	7.20	3	6	20	yes
TiS	2.09 / 1.89	8.60	3	6	20	yes

After this the minimum energies of the cubic structures were calculated via the volume optimisation method, whereas other structures such as hexagonal, orthorhombic or monoclinc were calculated with the *optimize_abc* method. The resulting energies for all structures calculated in WIEN2k with SCAN and SCAN-EECE can be found in table 7 and will be summarised and discussed in section 6.

Table 7: Results of the total energies with SCAN and SCAN-EECE and energy differences to the experimental structures (negative means more stable than exp.).

compound		total energy in eV / atom		difference to exp. in meV / atom	
		SCAN	SCAN-EECE	SCAN	SCAN-EECE
AgF	exp.	−73 712.571	−73 709.184		
	0	−73 712.582	−73 709.186	−10.9	−1.9
	1	−73 712.578	−73 709.181	−6.4	2.9
	2	−73 712.576	−73 709.179	−5.1	5.0
AgSe	exp.	−105 423.425	−105 420.033		
	0	−105 423.553	−105 420.167	−128.0	−133.6
	1	−105 423.505	−105 420.119	−80.1	−86.0
	2	−105 423.460	−105 420.091	−35.0	−57.6
CrO	exp.	−15 326.867	−15 325.260		
	0	−15 327.152	−15 325.435	−284.7	−175.9
	1	−15 326.923	−15 325.300	−56.5	−40.1
Cu_2Se	exp.	−52 076.657	−52 071.858		
	0	−52 076.735	−52 071.896	−78.7	−37.3
CuI	exp.	−119 388.677	−119 385.121		
	0	−119 388.683	−119 385.120	−5.5	0.7
CuSe	exp.	−55 593.065	−55 589.250		
	0	−55 593.074	−55 589.217	−9.5	33.3
LaN	exp.	−116 368.676	−116 368.645		
	0	−116 368.677	−116 368.645	−0.5	0.3
MnS	exp.	−21 202.955	−21 201.331		
	0	−21 203.019	−21 201.330	−63.8	1.8
	1	−21 203.011	−21 201.324	−56.2	7.7
MnSe	exp.	−48 839.708	−48 838.092		
	0	−48 839.782	−48 838.110	−74.4	−18.2
	1	−48 839.778	−48 838.107	−70.8	−15.4
MoAs	exp.	−85 873.992	−85 872.199		
	0	−85 873.996	−85 872.172	−4.5	26.6
NbN	exp.	−52 733.896	−52 732.872		
	0	−52 733.918	−52 732.903	−22.3	−30.1
	1	−52 733.918	−52 732.903	−22.3	−30.1
PtO	exp.	−251 992.879	−251 991.645		
	0	−251 993.046	−251 991.817	−167.2	−172.0
TiS	exp.	−17 055.681	−17 054.641		
	0	−17 055.834	−17 054.848	−153.1	−206.4
	1	−17 055.834	−17 054.848	−153.2	−206.4
	2	−17 055.766	−17 054.749	−84.5	−107.4

5.3 Formation energy calculations

As described in section 4.2.7 the formation energy can be determined when the ground state energy of the compound and the most stable configurations of each atom of the compound are known. In this section the formation energies of the TMOs shown in 5.1 and other problematic transition metal compounds shown in 5.2 were calculated. The ground state structures for the compounds were taken from the already existing calculations in the sections mentioned above. The crystallographic structures of the TMOs were the *rs* structure ($Fm\bar{3}m$) and the *zb* structure ($F\bar{4}3m$). The structures of the problematic transition metal compounds are given in table 5. The most stable crystallographic structures of the atomic components were looked up with help of the Materials Project [40], Aflowlib [41], the Open Quantum Materials Database (OQMD) [42, 43] and the Inorganic Crystal Structure Database (ICSD) [44] and can be found in table 8.

Table 8: Elements and their crystallographic structures in the Hermann-Mauguin notation which were used for the calculation of the formation energy. Gaseous molecules were treated separately, see the following paragraphs.

element	structure	element	structure
Ag	$Fm\bar{3}m$	Mo	$Im\bar{3}m$
As	$R\bar{3}m$	N	N_2 - gaseous
Co	$P6_3/mmc$	Nb	$Im\bar{3}m$
Cr	$Im\bar{3}m$	Ni	$Fm\bar{3}m$
Cu	$Fm\bar{3}m$	O	O_2 - gaseous
F	F_2 - gaseous	Pt	$Fm\bar{3}m$
Fe	$Im\bar{3}m$	S	$Fddd$
I	Cmc	Se	$P3121$
La	$P6_3/mmc$	Ti	$P6_3/mmc$
Mn	$Fm\bar{3}m$		

The structural data of the solids was imported in WIEN2k and ready for the initialisation and energy minimisation. Here I would like to thank Dr. Oleg Rubel for providing me a ready-to-use *.struct* file of the manganese structure, as this structure and its magnetism turned out to be rather complicated to generate. The structures of the gaseous molecules F_2, N_2 and O_2 were generated by hand. For this a primitive unit cell with the lattice parameters (30, 30, 32) Bohr and 90° angles was generated in WIEN2k. Then two atoms were positioned on the edges of the unit cell. For the example of O_2 a bondlenght of 121 pm was estimated, which led to the positions (0, 0, 0.03573) and (0, 0, 0.96427) for the two oxygen atoms. The result was a cell with oxygen molecules separated by vacuum which allowed the calculation of the ground state energy of the molecule, figure 20 illustrates such a structure.

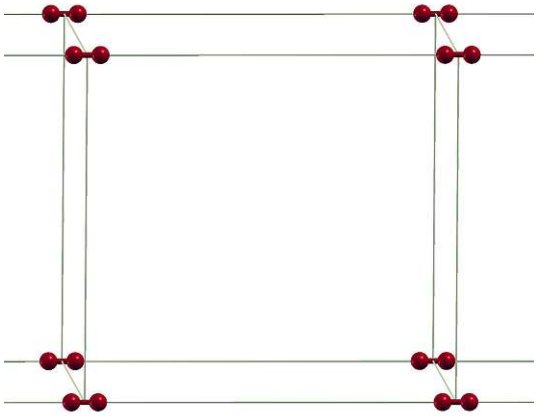


Figure 20: Example illustration of a structure generated for the calculation of the ground state energy of the gaseous molecules in table 8. The red spheres show the positions of the atoms and the bonds are symbolised with a red line connecting two atoms from neighbouring unit cells. The fine grey line illustrates the unit cell.

This structure was then initialised and the energy minimisation was performed with the *-it* setting for an iterative diagonalisation and *-fc 1 -min* to minimise the forces in the scf cycles. The calculations were very resource demanding, especially for memory. Therefore they were performed via MPI parallelisation [27] with a cluster of up to 10 workstations with 32 GB RAM each. For the SCAN functional it was further needed to find the optimal bond length of the molecule by hand as the force minimisation *(-fc 1 -min)* for this functional was not implemented in WIEN2k yet. For this the positions of the atoms were varied by small steps in both directions and the corresponding energies were calculated. The result was an energy versus bond length curve with a distinctive minimum energy. Figure 21 shows the curve calculated for the O_2 molecule with the SCAN functional.

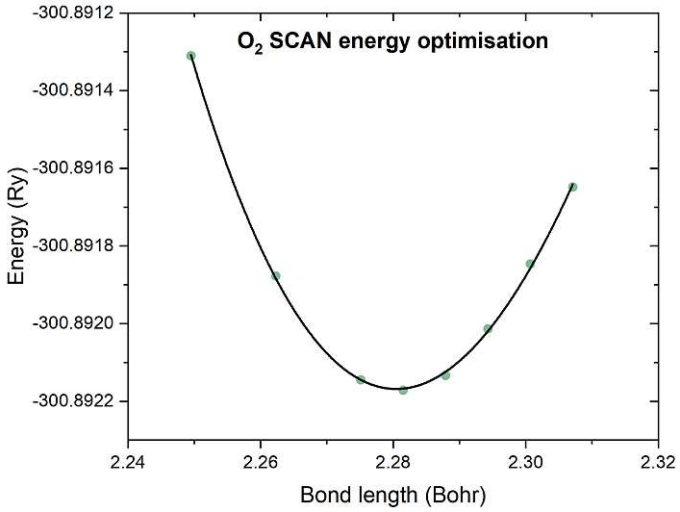


Figure 21: Energy minimisation of the O_2 molecule with the SCAN functional in WIEN2k. The green dots show the calculated energies for different bond lengths and the black line shows a polynomial fit of the results.

With all the structures set up, the initialisation was performed with parameters for RMT and RKmax according to table 9 and the *-prec 2* setting. The initialisation settings were chosen in a uniform way for each compound and the atomic components of this compound to ensure consistent results.

Table 9: Initialisation parameters for the calculation of the formation energies of the transition metal compounds and their atomic components. Each row corresponds to the parameters used for the compound given in the first row.

comp.	RMT	RKmax		RMT	RKmax		RMT	RKmax
AgF	2.07 / 1.27	6.50	Ag	2.07	10.59	F_2	1.27	6.50
AgSe	2.33 / 2.21	9.00	Ag	2.33	9.49	Se	2.21	9.00
CoO	1.84 / 1.10	6.00	Co	1.84	10.04	O_2	1.10	6.00
CrO	1.86 / 1.10	6.00	Cr	1.86	10.15	O_2	1.10	6.00
Cu_2Se	2.05 / 1.95	8.50	Cu	2.05	8.94	Se	1.95	8.50
CuI	2.07 / 2.07	9.00	Cu	2.07	9.00	I	2.07	9.00
CuSe	1.92 / 1.83	8.50	Cu	1.92	8.92	Se	1.83	8.50
FeO	1.89 / 1.10	6.00	Fe	1.89	10.31	O_2	1.10	6.00
LaN	1.91 / 1.00	5.40	La	1.91	10.31	N_2	1.00	5.40
MnO	1.98 / 1.10	6.00	Mn	1.98	10.80	O_2	1.10	6.00
MnS	2.17 / 1.86	8.49	Mn	2.17	9.91	S	1.86	8.49
MnSe	2.18 / 2.07	9.00	Mn	2.18	9.48	Se	2.07	9.00
MoAs	2.14 / 2.14	10.00	Mo	2.14	10.00	As	2.14	10.00
NbN	1.91 / 1.00	5.40	Nb	1.91	10.31	N_2	1.00	5.40
NiO	1.83 / 1.10	6.00	Ni	1.83	9.98	O_2	1.10	6.00
PtO	1.84 / 1.10	6.00	Pt	1.84	10.04	O_2	1.10	6.00
TiS	2.09 / 1.89	8.60	Ti	2.09	9.51	S	1.89	8.60

The results of the ground state energies calculated in WIEN2k for each of the structures can be found in the tables 10, 11, 12 and 13 and will be summarised and discussed in section 6.

Table 10: Results of the ground state energies of the TMOs in the *rs* and *zb* configurations and their atomic components for the PBE and PBE-EECE functional as well as the calculated formation energies in eV / atom.

compound		functional	ground state energy in Ry			form. energy
			compound	atom 1	atom 2	in eV / atom
MnO	*rs*	PBE	−4935.72	−4634.63	−300.72	−1.28
	zb		−4935.76			−1.41
FeO	*rs*		−5392.19	−2545.61		−0.86
	zb		−5392.20			−0.88
CoO	*rs*		−5874.81	−5573.92		−0.61
	zb		−5874.84			−0.70
NiO	*rs*		−6384.24	−3041.67		−0.63
	zb		−6384.21			−0.53
MnO	*rs*	PBE-EECE	−4934.85	−4633.61	−300.72	−1.78
	zb		−4934.86			−1.82
FeO	*rs*		−5391.06	−2544.96		−1.45
	zb		−5391.06			−1.45
CoO	*rs*		−5873.45	−5572.29		−1.51
	zb		−5873.46			−1.54
NiO	*rs*		−6382.63	−3040.73		−1.52
	zb		−6382.47			−1.00

Table 11: Results of the ground state energies of the TMOs for the SCAN and SCAN-EECE functional.

compound		functional	ground state energy in Ry			form. energy
			compound	atom 1	atom 2	in eV / atom
MnO	*rs*	SCAN	−4937.18	−4635.73	−300.89	−1.90
	zb		−4937.20			−1.95
FeO	*rs*		−5393.62	−2546.18		−1.22
	zb		−5393.61			−1.19
CoO	*rs*		−5876.27	−5575.07		−1.04
	zb		−5876.29			−1.10
NiO	*rs*		−6385.77	−3042.26		−1.22
	zb		−6385.63			−0.76
MnO	*rs*	SCAN-EECE	−4936.66	−4635.15	−300.89	−2.08
	zb		−4936.65			−2.06
FeO	*rs*		−5392.95	−2545.76		−1.81
	zb		−5392.94			−1.77
CoO	*rs*		−5875.49	−5574.03		−1.91
	zb		−5875.47			−1.87
NiO	*rs*		−6384.87	−3041.67		−2.18
	zb		−6384.60			−1.25

Table 12: Results of the ground state energies of the problematic transition metal compounds with different crystallographic structures and their atomic components for the SCAN functional as well as the calculated formation energies in eV / atom.

compound		ground state energy in Ry			form. energy
		compound	atom 1	atom 2	in eV / atom
AgF	exp.	−10 835.54	−10635.65	−399.46	−1.10
	0	−21 671.08			−1.11
	1	−10 835.54			−1.10
	2	−10 835.54			−1.11
AgSe	exp.	−15 496.96	−10635.65	−14583.97	0.11
	2	−15 496.98			−0.02
	4	−30 993.94			0.03
	5	−15 496.96			0.07
CrO	exp.	−2253.00	−4204.63	−300.89	−1.60
	0	−4506.08			−1.89
	16	−2253.01			−1.67
Cu_2Se	exp.	−11 482.69	−3310.69	−14583.97	0.02
	1	−45 930.84			−0.05
CuI	exp.	−17 549.81	−3310.69	−56956.43	−0.12
	0	−35 099.63			−0.13
CuSe	exp.	−49 032.18	−3310.69	−14583.97	−0.14
	0	−8172.03			−0.15
LaN	exp.	−17 105.85	−67984.20	−219.15	−1.52
	0	−34 211.70			−1.52
MnS	exp.	−3116.78	−4635.73	−25560.42	−1.00
	0	−3116.79			−1.06
	1	−6233.57			−1.07
MnSe	exp.	−7179.30	−4635.73	−14583.97	−0.78
	0	−7179.32			−0.85
	1	−14 358.63			−0.85
MoAs	exp.	−50 492.98	−8100.20	−9046.01	−0.26
	0	−12 623.25			−0.27
NbN	exp.	−15 503.45	−7641.96	−219.15	−1.30
	0	−7751.73			−1.33
	1	−7751.73			−1.33
PtO	exp.	−74 084.54	−36891.76	−300.89	−0.42
	0	−148 169.18			−0.59
TiS	exp.	−7521.42	−3416.30	−25560.42	−1.54
	0	−2507.16			−1.69
	1	−2507.16			−1.69
	5	−5014.30			−1.62

Table 13: Results of the ground state energies of the problematic transition metal compounds with different cryst. structures and their atomic components for the SCAN-EECE functional as well as the calculated formation energies in eV / atom.

compound		ground state energy in Ry			form. energy
		compound	atom 1	atom 2	in eV / atom
AgF	exp.	−10 835.00	−10635.10	−399.46	−1.18
	0	−21 669.99			−1.18
	1	−10 835.00			−1.16
	2	−10 835.00			−1.17
AgSe	exp.	−15 496.46	−10635.15	−14583.97	0.11
	2	−15 496.48			−0.02
	4	−30 992.95			0.02
	5	−15 496.47			0.05
CrO	exp.	−2252.76	−4204.03	−300.89	−2.04
	0	−4505.57			−2.22
	16	−2252.77			−2.08
Cu2Se	exp.	−11 481.64	−3310.15	−14583.97	−0.11
	1	−45 926.60			−0.14
CuI	exp.	−17 549.29	−3310.15	−56956.43	−0.24
	0	−35 098.59			−0.24
CuSe	exp.	−49 028.81	−3310.12	−14583.97	−0.17
	0	−8171.46			−0.14
LaN	exp.	−17 105.85	−67984.19	−219.15	−1.50
	0	−34 211.69			−1.50
MnS	exp.	−3116.54	−4635.15	−25560.42	−1.35
	0	−3116.54			−1.34
	1	−6233.08			−1.35
MnSe	exp.	−7179.07	−4635.18	−14583.97	−1.03
	0	−7179.07			−1.04
	1	−14 358.14			−1.05
MoAs	exp.	−50 491.92	−8099.95	−9046.01	−0.19
	0	−12 622.98			−0.16
NbN	exp.	−15 503.17	−7641.81	−219.15	−1.35
	0	−7751.59			−1.39
	1	−7751.59			−1.39
PtO	exp.	−74 084.18	−36891.57	−300.89	−0.46
	0	−148 168.46			−0.64
TiS	exp.	−7520.96	−3416.02	−25560.42	−1.43
	0	−2507.02			−1.64
	1	−2507.02			−1.64
	5	−5014.00			−1.54

6 Results and Discussion

6.1 Polymorphic energy ordering of MnO, FeO, CoO and NiO

6.1.1 Rocksalt versus zinc-blende structures

The results for the comparison of the transition metal monoxides MnO, FeO, CoO and NiO in the *rs* AF2 and *zb* AF1 configuration with the functionals PBE, SCAN, PBE-EECE and SCAN-EECE are displayed in table 14 and figure 22.

Table 14: Energy differences of the zinc-blende (E_{zb}) and rocksalt (E_{rs}) structures of the tested TMOs. Positive values mean the rocksalt structure is energetically favoured versus the zinc-blende structure. For FeO and NiO, the EECE functionals with a mixing parameter of 0.55 are not calculated, the 0.4 mixing parameter already prefers the rocksalt configuration for PBE-EECE and SCAN-EECE. Generally, a change of the mixing parameter α from its standard value of 0.25 is not recommended and is used in this work just for scientific interest.

functional	E_{zb} - E_{rs} in meV / f.u.			
	MnO	FeO	CoO	NiO
PBE	-259	-92	-264	213
SCAN	-100	127	-156	1020
PBE-EECE	-84	29	-58	1069
SCAN-EECE	38	143	75	1897
PBE-EECE 0.4	-22	82	-5	1597
SCAN-EECE 0.4	98	186	141	2502
PBE-EECE 0.55	23	-	39	-
SCAN-EECE 0.55	145	-	188	-

The results of the PBE functional, a GGA, show a poor energetic description regarding the experimental ground state structure - the rocksalt configuration [37]. For this functional, a correct result can only be obtained for NiO.
All tested TMOs have partially filled 3d-bands where strong electron correlation effects occur. This means that the electrons can not be appropriately described using a non-interacting model such as the LDA or the GGA provide. The SCAN functional, a meta-GGA, although not taking the strong correlation effects into explicit consideration either, provides a trend in the right direction for this problem. With this, the ground state structures of NiO and FeO are described correctly, and the energy differences between *zb* and *rs* are improved for all four materials.
To improve the description of correlated electron systems, a common method is the GGA+U approach [31, 32]. This is an empirical method where parameters that depend on the system and the property under observation have to be adjusted. Within the GGA+U model, the Hubbard U term defines the Coulomb interaction potential and J the exchange constant. This allows a

customised treatment of the orbitals for satisfactory results.
However, this work aims to test the EECE functional in combination with PBE and SCAN. The general idea of this method is that the uncorrelated states are depicted sufficiently with the GGAs mentioned, whereas the correlated electrons are treated with an exact Hartree-Fock (HF) exchange term, see section 4.2.4 for details. With this, a significant improvement is expected for the tested TMOs. Previous works by Tran et al. [21] already showed promising results in the application of the EECE to the TMOs.
PBE-EECE with the standard mixing parameter α of 0.25 gives the correct ground state structure for NiO and FeO, with the trend again pointing in the right direction for all the compounds. PBE-EECE with increased mixing parameters, although a variation of α is not the intended use of the EECE method, continues this trend, resulting in the correct prediction for all tested TMOs with an α of 0.55.
And finally, the SCAN-EECE functional allows predicting the correct ground state structures for all tested compounds. The results discussed above are visualised as bar plots in figure 22.

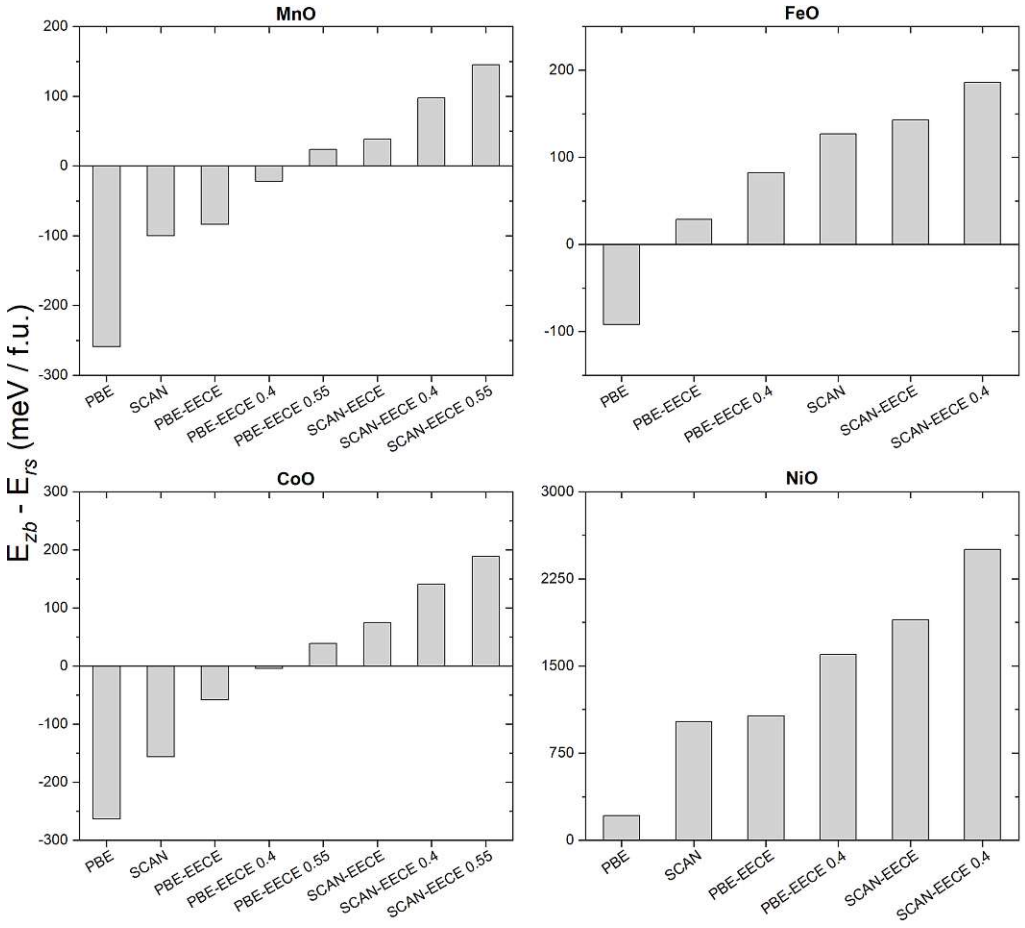


Figure 22: Energy differences of the zinc-blende (E_{zb}) and rocksalt (E_{rs}) structures of the TMOs. A graphical representation of table 14, the energy differences were ordered from lowest to highest.

In table 15 important calculated properties of MnO are listed compared to the experimental results from literature. The lattice constant a_0 is estimated best with PBE, closely followed by SCAN-EECE and SCAN. The bulk modulus B_0 is best assessed with the PBE functional. The band gap E_g is underestimated by more than a factor of 2 for all tested functionals, although combining with the EECE increases the obtained values. Finally, the magnetic moment μ is best represented by the PBE-EECE functional.

Table 15: Results for the lattice constant a_0, the bulk modulus B_0, the band gap E_g and the magnetic moment μ of the Mn atom for the *rs* AF2 configuration of MnO, calculated with different functionals and compared to the experimental data [37]. In WIEN2k, the SCAN functional is not self-consistent. Instead the PBE potential is used for the calculation; therefore E_g and μ for the SCAN functionals were omitted from the results.

functional	a_0 in Å	B_0 in Gpa	E_g in eV	μ in μB
PBE	4.44	149.23	0.86	4.39
SCAN	4.41	166.63	-	-
PBE-EECE	4.49	143.86	1.21	4.65
SCAN-EECE	4.45	160.76	-	-
PBE-EECE 0.4	4.51	141.33	1.34	4.74
SCAN-EECE 0.4	4.47	158.08	-	-
PBE-EECE 0.55	4.53	138.93	1.45	4.80
SCAN-EECE 0.55	4.48	156.12	-	-
Experiment	4.4365, 4.4315	149.6, 146.7	3.6-3.9	4.58

6.1.2 Distorted structures

In table 16 the distorted TMO structures calculated with the *c/a* energy optimisation (see section 5.1.2) are compared to the ideal *rs* and *zb* structures. Table 4 shows that depending on the functional and compound significant *c/a* distortions of the ideal lattice structures from up to 20 % can be observed with this method. The results for the energy comparison show that, as expected [38], the distorted structures are energetically favoured for most of the compounds. For MnO and FeO, all structures calculated with the tested functionals show results that indicate a more stable distorted structure. CoO *rs* exhibits stable distorted structures with PBE and SCAN, whereas the results obtained with the rest of the functionals show minimal energy differences between the ideal and distorted structures. The same applies for NiO, but this time NiO *zb* shows stable distorted structures with SCAN, PBE-EECE and SCAN-EECE. The remaining results only show a slight deviation in energy.

Table 16: Comparison of the minimum energies of the ideal rocksalt and zinc-blende structures versus the distorted structures E_{dis} with the functionals PBE, SCAN, PBE-EECE and SCAN-EECE for MnO, FeO, CoO and NiO.

Functional	Structure	E_{id} - E_{dis} in meV / f.u.			
		MnO	FeO	CoO	NiO
PBE	*rs*	11.2	65.9	69.3	−6.4
	zb	11.5	16.1	−2.6	6.7
SCAN	*rs*	8.2	49.8	34.6	−4.2
	zb	12.2	116.9	0.7	87.5
PBE-EECE	*rs*	4.7	13.0	−3.5	−5.9
	zb	6.1	48.3	−3.9	21.7
SCAN-EECE	*rs*	5.9	17.5	−1.0	−1.5
	zb	8.2	74.2	2.3	30.8

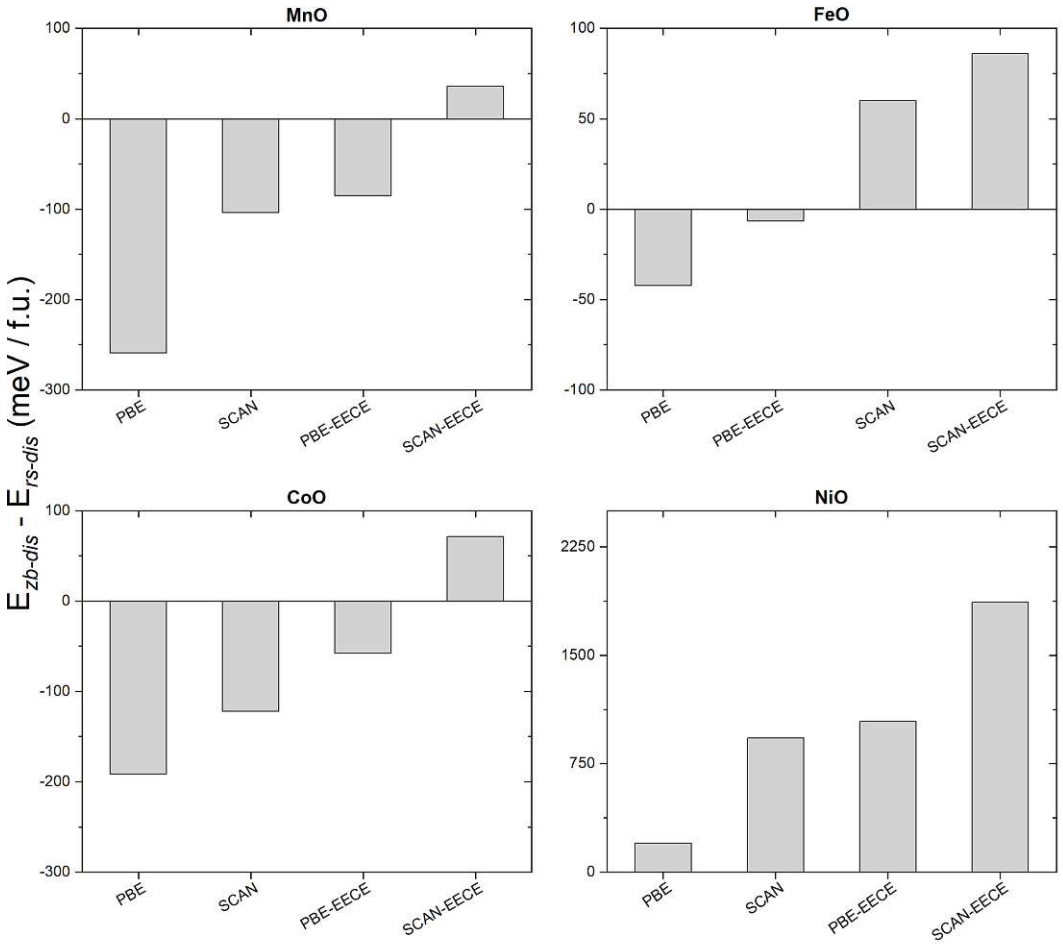


Figure 23: Graphical representation of the energy differences between the distorted zinc-blende and distorted rocksalt structures for MnO, FeO, CoO and NiO calculated with PBE, SCAN, PBE-EECE and SCAN-EECE.

Despite the distorted structures being energetically more stable overall, the comparison between the minimum energies of the distorted zinc-blende (E_{zb-dis}) and distorted rocksalt (E_{rs-dis}) structures remains mostly the same as for the ideal structures. Figure 23 shows the comparison of the distorted structures for the PBE, SCAN, PBE-EECE and SCAN-EECE functional. The verdict from the ideal structures fundamentally remains the same, with just minor energy deviations compared to the distorted structures. SCAN-EECE again is the only tested functional to predict the correct ground state structure for all four TMOs. The only change in prediction is for FeO with the PBE-EECE functional. Here the ideal structure shows a slightly positive value, whereas the distorted structure shows a slightly negative value.

6.2 Polymorphic energy ordering of other problematic transition metal compounds

In addition to the materials discussed in the sections above, further compounds that contain transition metals were tested. This section treats materials which are known to perform poorly with regards to their energetic ground state structure calculated with the SCAN functional, see section 5.2. Figure 24 shows a diagram comparing the energies of the minimum structures (E_{min}) and the experimental structure (E_{exp}) calculated with SCAN and SCAN-EECE. The results confirm that the SCAN functional performs poorly for each selected compound and structure. A negative value of E_{min} - E_{exp} means that the compared minimum structure wrongfully is more stable than the experimentally determined structure. For AgF two of the three tested structures show the correct result with SCAN-EECE and overall, the result is improved for all three tested structures. For AgSe, NbN, PtO and TiS, applying the SCAN-EECE functional worsens the outcome for all structures, whereas the results for CrO, Cu_2Se and MnSe are improved but still not correct. CuI, CuSe, LaN, MnS and MoAs show the proper ground state structure with SCAN-EECE where SCAN failed for each of them. The box-whisker-plot inserted as a small diagram in figure 24 shows an improvement for the mean value of E_{min} - E_{exp} over all tested structures of about 14 meV / atom for the SCAN-EECE functional compared with SCAN.

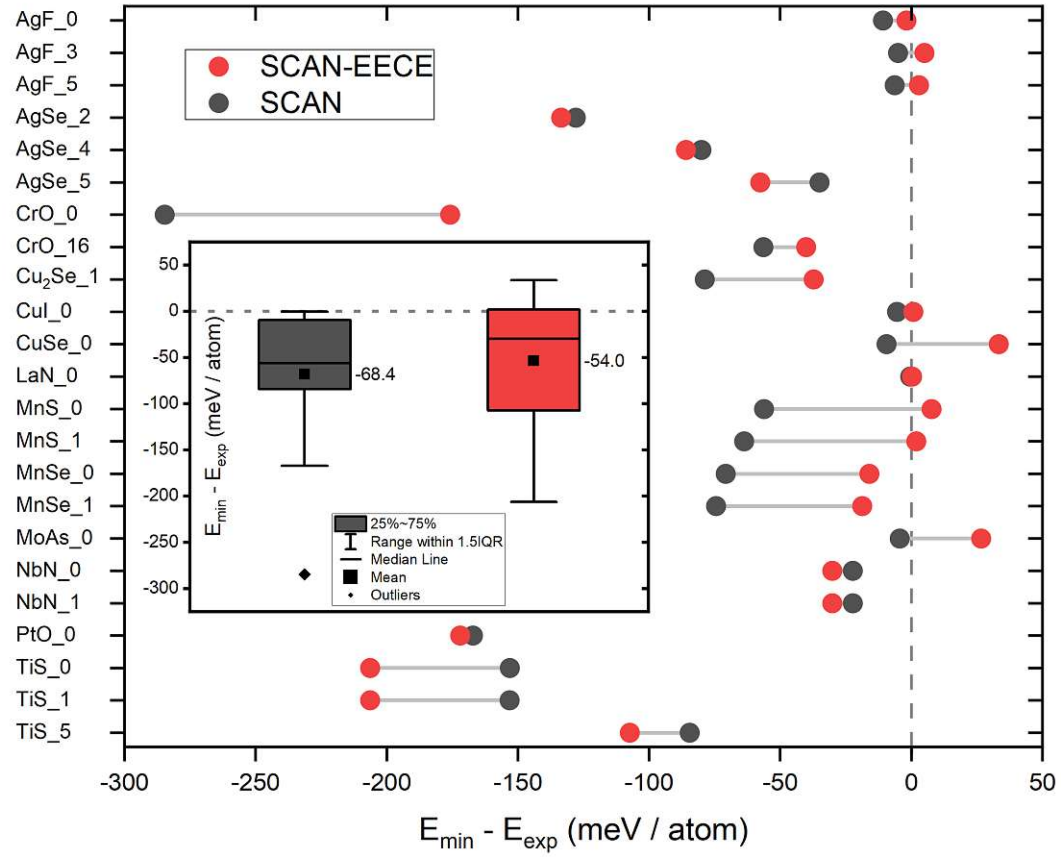


Figure 24: Comparison of the energy differences between the minimum energy structures and the experimental structure. The black dots in the diagram show the results obtained with the SCAN functional and the red dots show the results with the SCAN-EECE functional. Details about the naming scheme of the different minimum structures on the left side of the diagram can be found in table 5. The small inserted diagram shows a box-whisker-plot for all structures calculated with SCAN (black) and SCAN-EECE (red). The boxes show the range from the 25th percentile to the 75th percentile. In these boxes the median (line) and the mean (square) are pictured and the value for the mean is quoted. The whiskers show the range of the obtained values without the outliers. The outliers are pictured diamond shaped. Every value that ranges higher or lower than 1,5 times the interquartile range (IQR) is depicted as an outlier.

6.3 Formation energies

In figure 25 the formation energies of MnO, FeO, CoO and NiO in the *rs* and *zb* configuration calculated with the PBE, SCAN, PBE-EECE and SCAN-EECE functionals are compared to the values from literature. The formation energy for the experimental ground state structure (*rs*) is best approximated for MnO with SCAN-EECE and SCAN, for FeO with PBE-EECE and for CoO and NiO with SCAN. Figure 25 shows that for the calculation of the formation energies of the TMOs finding the correct ground state structure is not as important compared to the choice of the functional used for the calculations. In this case the SCAN functional is the best overall choice to calculate the formation

energy. In the next paragraph a wider variety of compounds will be compared to their formation energy values from literature and an overview of SCAN versus SCAN-EECE will be discussed.

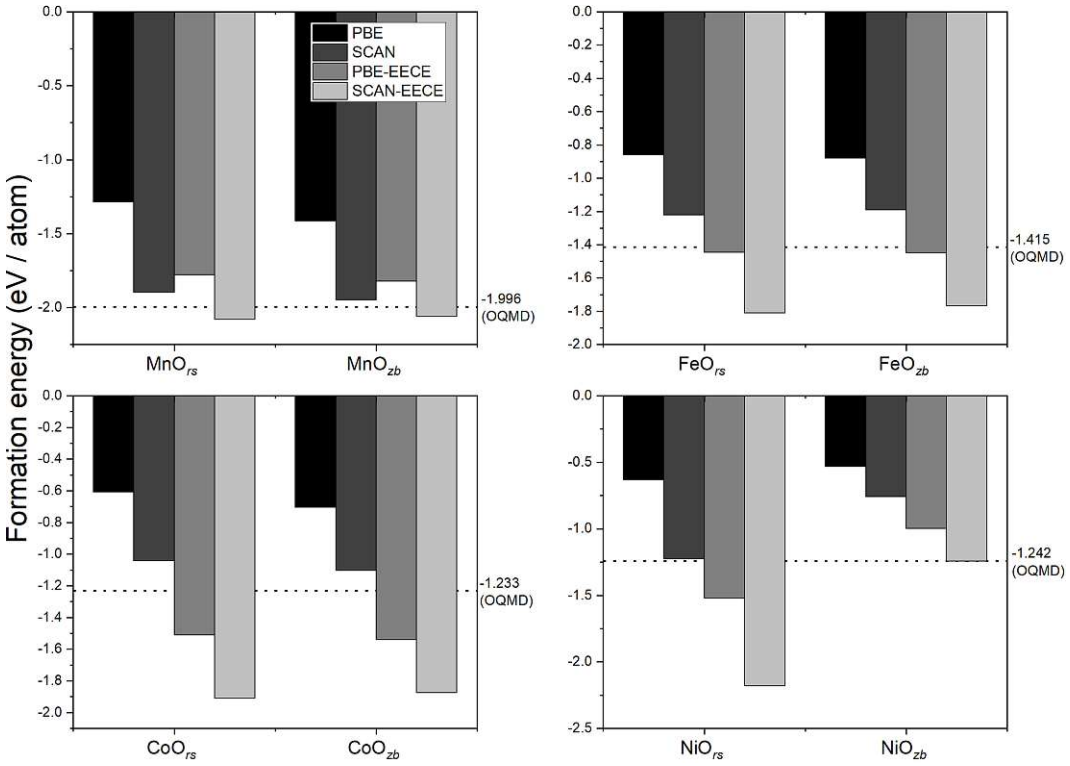


Figure 25: Illustration of the formation energies of MnO, FeO, CoO and NiO in the *rs* and *zb* configuration calculated with the PBE, SCAN, PBE-EECE and SCAN-EECE functionals and compared to the values from literature (dotted line, Source: The Open Quantum Materials Database [42, 43]). See table 17 (appendix) for the literature values.

Figure 26 compares the formation energies of all compounds in their experimental ground state structure which were calculated throughout this work. A result close to 0 means, that the ground state energy obtained with DFT is similar to the experimental ground state energy obtained from literature. For this selection of compounds, of which all are known to be problematic to calculate with DFT, SCAN tends to underestimate the formation energy (more positive values), whereas SCAN-EECE overestimates it. Especially for the transition metal oxides CoO, CrO, FeO and NiO the spread of the calculated formation energy between SCAN and SCAN-EECE is considerable. Although SCAN-EECE predicts the correct ground state structure for CoO, FeO and NiO in contrast to SCAN, the formation energies for these compounds are better predicted with SCAN. The box-whisker-plot in figure 26 further illustrates this conclusion. The mean energy difference of all calculated structures to the literature in figure 26 is 0.072 eV / atom for SCAN and -0.157 eV / atom for SCAN-EECE.

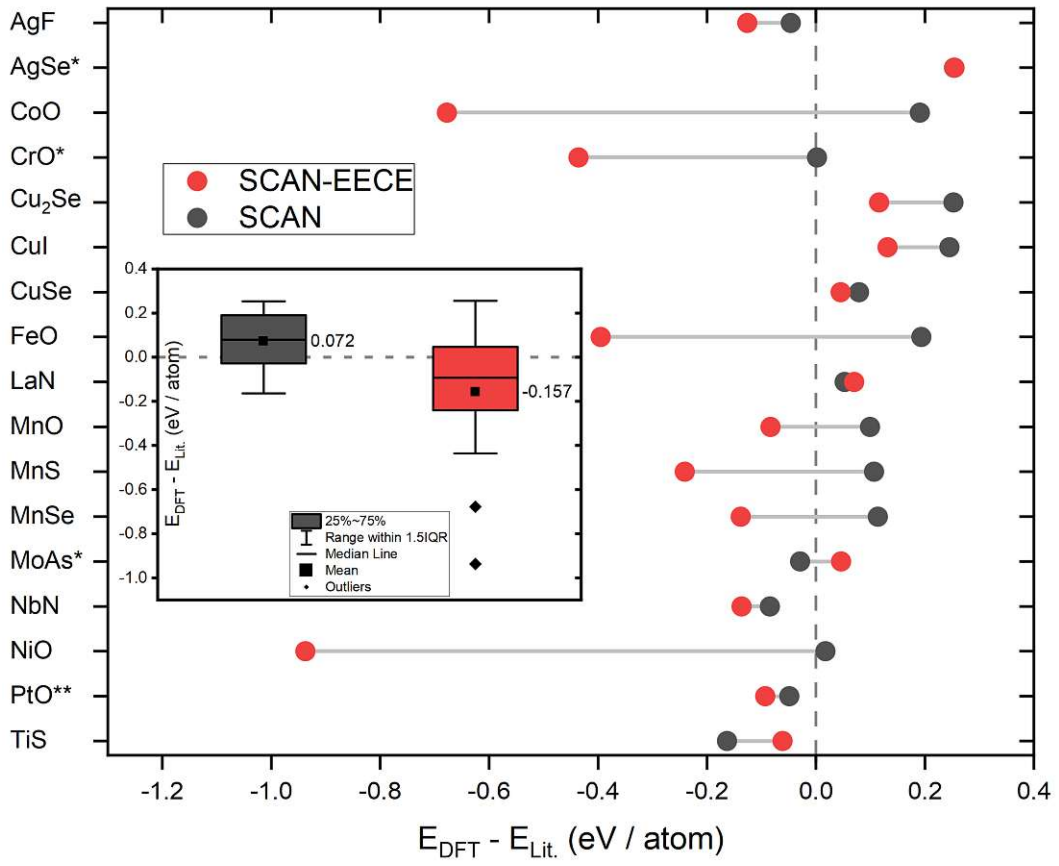


Figure 26: Comparison of the calculated formation energies for the experimental structures with SCAN and SCAN-EECE versus the ground state energies obtained from literature. Sources for the literature energies: The Open Quantum Materials Database [42,43], The Materials Project [40] (*) and the works from Zhang et al. [39] (**). See table 17 (appendix) for the literature values. The small inserted diagram shows a box-whisker-plot for all structures calculated with SCAN (black) and SCAN-EECE (red).

7 Summary

To compare the EECE with the PBE and SCAN functionals, this work focuses mainly on the energetic description of compounds with correlated electrons. A part of the calculation is concentrated in the polymorphic energy ordering, where the compounds MnO, FeO, CoO and NiO are observed in detail regarding the rocksalt and zinc-blende crystal structure. The results of this part are also published in the works of A. Gosh et al. [17]. Further, a wider variety of compounds selected from the works of J. Sun et al. [15] are evaluated for the polymorphic energy ordering.

The results, first of all for MnO, FeO, CoO and NiO, show that PBE predicts the wrong ground state structure for three of four compounds and SCAN for two of four. In contrast, PBE-EECE improves the prediction for all compounds (two of four correct), and SCAN-EECE achieves an accurate prediction of the ground state structure for all four compounds with little to no increase

in computing time (see table 14 and figure 22). The tests with a wider variety of polymorphic compounds confirm the improvement of SCAN-EECE over SCAN. This variety features 13 compounds and 23 structures, excluding the experimentally confirmed ground state structures (see table 5). The mean value of the calculated total energies of the structures subtracted by the total energy of the experimentally confirmed ground state structures is improved by 14 meV / atom (figure 24).
The second part of the work examines the formation energies of the compounds with PBE, SCAN, PBE-EECE and SCAN-EECE. For the formation energies of MnO, FeO, CoO and NiO, none of the functionals perform equally well with all four compounds, and only the PBE functional performs poorly for all of them (see figure 25). Interestingly the formation energies for the rocksalt and zinc-blende structures show very similar results, except for NiO, which concludes that finding the correct ground state structure is not as important compared to the choice of the functional used for the calculations, at least for the tested compounds.
Finally, the formation energies of 17 different compounds obtained with SCAN and SCAN-EECE are compared to the energies from the literature. Overall the calculated formation energies for SCAN differ 0.072 eV / atom to the literature values and for SCAN-EECE -0.157 eV / atom (see figure 26).
The SCAN-EECE functional improves the evaluation of the correct ground state structures of transition metal compounds, especially for the tested transition metal monoxides. All four structures are predicted correctly. Whereas for calculating the formation energies, a combination of SCAN with EECE overall leads to worse results.

8 References

[1] P. Hohenberg and W. Kohn. Inhomogeneous electron gas. Physical Review, 136(3B), 1964.

[2] W. Kohn and L. J. Sham. Self-consistent equations including exchange and correlation effects. Physical Review, 140(4A), 1965.

[3] Georg K. H. Madsen. Introduction to Electronic Structure. TU Wien, 2021.

[4] Richard M. Martin, Lucia Reining, and David M. Ceperley. Interacting electrons theory and computational approaches. Cambridge University Press, 2016.

[5] Richard M. Martin. Electronic structure basic theory and practical methods. Cambridge University Press, 2020.

[6] Eiji Nakamachi, Hwisim Hwang, Yasutomo Uetsuji, and Hiroyuki Kuramae. Three-scale process-crystallographic analysis of a new biocompatible piezoelectric material mgsio3 generation. 2010 2nd International Conference on Computer Technology and Development, 2010.

[7] N D Woods, M C Payne, and P J Hasnip. Computing the self-consistent field in kohn–sham density functional theory. Journal of Physics: Condensed Matter, Aug 2019.

[8] D. M. Ceperley and B. J. Alder. Ground state of the electron gas by a stochastic method. Physical Review Letters, 45(7):566–569, 1980.

[9] C. Fiolhais, F. Nogueira, and Marques Miguel A L. A primer in density functional theory. Springer, 2011.

[10] A. van de Walle and G. Ceder. Correcting overbinding in local-density-approximation calculations. Physical Review B, 59(23):14992–15001, 1999.

[11] John P. Perdew and Wang Yue. Accurate and simple density functional for the electronic exchange energy: Generalized gradient approximation. Physical Review B, 33(12):8800–8802, 1986.

[12] John P. Perdew, Kieron Burke, and Matthias Ernzerhof. Generalized gradient approximation made simple. Physical Review Letters, 77(18):3865–3868, 1996.

[13] Stefan Kurth, John P. Perdew, and Peter Blaha. Molecular and solid-state tests of density functional approximations: Lsd, ggas, and meta-ggas. International Journal of Quantum Chemistry, 75(4-5):889–909, 1999.

[14] Troy Van Voorhis and Gustavo E. Scuseria. A novel form for the exchange-correlation energy functional. The Journal of Chemical Physics, 109(2):400–410, 1998.

[15] Jianwei Sun, Adrienn Ruzsinszky, and John P. Perdew. Strongly constrained and appropriately normed semilocal density functional. Physical Review Letters, 115(3), 2015.

[16] Bikash Patra, Subrata Jana, Lucian A. Constantin, and Prasanjit Samal. Relevance of the pauli kinetic energy density for semilocal functionals. Physical Review B, 100(15), 2019.

[17] Arghya Ghosh, Subrata Jana, Manish K. Niranjan, Fabien Tran, David Wimberger, Peter Blaha, Lucian A. Constantin, and Prasanjit Samal. Correct and accurate polymorphic energy ordering of transition-metal monoxides obtained from semilocal and onsite-hybrid exchange-correlation approximations. arXiv:2112.09022 [cond-mat.mtrl-sci], Dec 2021.

[18] Axel D. Becke. A new mixing of hartree-fock and local density-functional theories. The Journal of Chemical Physics, 98(2):1372–1377, 1993.

[19] Peter Blaha. Density functional theory and beyond, 2020.

[20] P. Novák, J. Kuneš, L. Chaput, and W. E. Pickett. Exact exchange for correlated electrons. physica status solidi (b), 243(3):563–572, 2006.

[21] Fabien Tran, Peter Blaha, Karlheinz Schwarz, and Pavel Novák. Hybrid exchange-correlation energy functionals for strongly correlated electrons: Applications to transition-metal monoxides. Physical Review B, 74(15), 2006.

[22] John P. Perdew. Jacob's ladder of density functional approximations for the exchange-correlation energy. AIP Conference Proceedings, 2001.

[23] Jan M. Martin and Golokesh Santra. Empirical double-hybrid density functional theory: A third way in between wft and dft. Israel Journal of Chemistry, 60(8-9):787–804, 2019.

[24] E Sjöstedt, L Nordström, and D.J Singh. An alternative way of linearizing the augmented plane-wave method. Solid State Communications, 114(1):15–20, 2000.

[25] Georg K. Madsen, Peter Blaha, Karlheinz Schwarz, Elisabeth Sjöstedt, and Lars Nordström. Efficient linearization of the augmented plane-wave method. Physical Review B, 64(19), 2001.

[26] Peter Blaha, Karlheinz Schwarz, Fabien Tran, Robert Laskowski, Georg K. Madsen, and Laurence D. Marks. Wien2k: An apw+lo program for calculating the properties of solids. The Journal of Chemical Physics, 152(7):074101, 2020.

[27] Peter Blaha, Karlheinz Schwarz, Georg KH Madsen, Dieter Kvasnicka, Joachim Luitz, et al. wien2k. An augmented plane wave+ local orbitals program for calculating crystal properties, 60, 2001.

[28] Eamon John Gordon McDermott. Density functional theory study of complex metal oxide surface reconstructions. PhD thesis, Wien, 2016.

[29] Georg KH Madsen, Peter Blaha, Karlheinz Schwarz, Elisabeth Sjöstedt, and Lars Nordström. Efficient linearization of the augmented plane-wave method. Physical Review B, 64(19):195134, 2001.

[30] Han-Qing Wu, Yuan-Yao He, Yi-Zhuang You, Cenke Xu, Zi Yang Meng, and Zhong-Yi Lu. Quantum monte carlo study of strange correlator in interacting topological insulators. Physical Review B, 92(16):165123, 2015.

[31] Sergei L Dudarev, Gianluigi A Botton, Sergey Y Savrasov, CJ Humphreys, and Adrian P Sutton. Electron-energy-loss spectra and the structural stability of nickel oxide: An lsda+ u study. Physical Review B, 57(3):1505, 1998.

[32] AI Liechtenstein, Vladimir I Anisimov, and Jan Zaanen. Density-functional theory and strong interactions: Orbital ordering in mott-hubbard insulators. Physical Review B, 52(8):R5467, 1995.

[33] Francis Birch. Elasticity and constitution of the earth's interior. Journal of Geophysical Research, 57(2):227–286, 1952.

[34] FD Murnaghan. Finite deformation of an elastic solid. new york: Willey, 1951.

[35] PJJR Vinet, J Ferrante, JR Smith, and JH Rose. A universal equation of state for solids. Journal of Physics C: Solid State Physics, 19(20):L467, 1986.

[36] J-P Poirier and A Tarantola. A logarithmic equation of state. Physics of the Earth and Planetary Interiors, 109(1-2):1–8, 1998.

[37] A Schrön, C Rödl, and F Bechstedt. Energetic stability and magnetic properties of mno in the rocksalt, wurtzite, and zinc-blende structures: Influence of exchange and correlation. Physical Review B, 82(16):165109, 2010.

[38] A Schrön, Claudia Rödl, and Friedhelm Bechstedt. Crystalline and magnetic anisotropy of the 3 d-transition metal monoxides mno, feo, coo, and nio. Physical Review B, 86(11):115134, 2012.

[39] Yubo Zhang, Daniil A Kitchaev, Julia Yang, Tina Chen, Stephen T Dacek, Rafael A Sarmiento-Pérez, Maguel AL Marques, Haowei Peng, Gerbrand Ceder, John P Perdew, et al. Efficient first-principles prediction of solid stability: Towards chemical accuracy. npj Computational Materials, 4(1):1–6, 2018.

[40] Anubhav Jain, Shyue Ping Ong, Geoffroy Hautier, Wei Chen, William Davidson Richards, Stephen Dacek, Shreyas Cholia, Dan Gunter, David Skinner, Gerbrand Ceder, and Kristin a. Persson. The Materials Project: A materials genome approach to accelerating materials innovation. APL Materials, 1(1):011002, 2013.

[41] Stefano Curtarolo, Wahyu Setyawan, Shidong Wang, Junkai Xue, Kesong Yang, Richard H Taylor, Lance J Nelson, Gus LW Hart, Stefano Sanvito, Marco Buongiorno-Nardelli, et al. Aflowlib. org: A distributed materials properties repository from high-throughput ab initio calculations. Computational Materials Science, 58:227–235, 2012.

[42] James E Saal, Scott Kirklin, Muratahan Aykol, Bryce Meredig, and Christopher Wolverton. Materials design and discovery with high-throughput density functional theory: the open quantum materials database (oqmd). Jom, 65(11):1501–1509, 2013.

[43] Scott Kirklin, James E Saal, Bryce Meredig, Alex Thompson, Jeff W Doak, Muratahan Aykol, Stephan Rühl, and Chris Wolverton. The open quantum materials database (oqmd): assessing the accuracy of dft formation energies. npj Computational Materials, 1(1):1–15, 2015.

[44] I Levin. Nist inorganic crystal structure database (icsd). National Institute of Standards and Technology, 2018.

9 Appendix

For the structural data of the calculated compounds in the form of the **.struct* files with excluded symmetry operations see the additional **.txt* files.

Table 17: Literature formation energies for the tested transition metals. Sources: The Open Quantum Materials Database [42,43], The Materials Project [40] (*) and the works from Zhang et al. [39] (**).

compound	formation energy in eV / atom
TiS	-1.373
PtO**	-0.37
NiO	-1.242
NbN	-1.218
MoAs*	-0.232
MnSe	-0.889
MnS	-1.11
MnO	-1.996
LaN	-1.572
FeO	-1.415
CuSe	-0.217
CuI	-0.369
Cu_2Se	-0.228
CrO*	-1.605
CoO	-1.233
AgSe*	-0.148
AgF	-1.052

```
------------------------------------------------------------
PBE
------------------------------------------------------------
CoO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.657771  5.657771 27.719699 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Co1       NPT=  781  R0=0.00005000 RMT=    1.8400   Z: 27.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Co2       NPT=  781  R0=0.00005000 RMT=    1.8400   Z: 27.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.5800   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12      NUMBER OF SYMMETRY OPERATIONS
------------------------------------------------------------
SCAN
------------------------------------------------------------
CoO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.752400  5.752400 28.183325 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Co1       NPT=  781  R0=0.00005000 RMT=    1.8400   Z: 27.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Co2       NPT=  781  R0=0.00005000 RMT=    1.8400   Z: 27.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.5800   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12      NUMBER OF SYMMETRY OPERATIONS
------------------------------------------------------------
PBE-EECE
------------------------------------------------------------
```

CoO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS: 3166_R-3m
MODE OF CALC=RELA unit=ang
  5.770956 5.770956 28.274239 90.000000 90.000000120.000000
ATOM -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1   ISPLIT= 4
Co1   NPT= 781 R0=0.00005000 RMT=   1.8400   Z: 27.0
LOCAL ROT MATRIX: 1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1   ISPLIT= 4
Co2   NPT= 781 R0=0.00005000 RMT=   1.8400   Z: 27.0
LOCAL ROT MATRIX: 1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2   ISPLIT= 4
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O   NPT= 781 R0=0.00010000 RMT=   1.5800   Z: 8.0
LOCAL ROT MATRIX: 1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12   NUMBER OF SYMMETRY OPERATIONS

SCAN-EECE

CoO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS: 3166_R-3m
MODE OF CALC=RELA unit=ang
  5.696000 5.696000 27.907000 90.000000 90.000000120.000000
ATOM -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1   ISPLIT= 4
Co1   NPT= 781 R0=0.00005000 RMT=   1.8400   Z: 27.0
LOCAL ROT MATRIX: 1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1   ISPLIT= 4
Co2   NPT= 781 R0=0.00005000 RMT=   1.8400   Z: 27.0
LOCAL ROT MATRIX: 1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2   ISPLIT= 4
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O   NPT= 781 R0=0.00010000 RMT=   1.5800   Z: 8.0
LOCAL ROT MATRIX: 1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12   NUMBER OF SYMMETRY OPERATIONS

PBE-EECE 0.4

CoO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS: 3166_R-3m
MODE OF CALC=RELA unit=ang

```
  5.807715  5.807715 28.454335 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Co1       NPT=  781  R0=0.00005000 RMT=    1.8400   Z: 27.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Co2       NPT=  781  R0=0.00005000 RMT=    1.8400   Z: 27.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
      -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.5800   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE 0.4
-------------------------------------------------------------
CoO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.733723  5.733723 28.091820 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Co1       NPT=  781  R0=0.00005000 RMT=    1.8400   Z: 27.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Co2       NPT=  781  R0=0.00005000 RMT=    1.8400   Z: 27.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
      -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.5800   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE-EECE 0.55
-------------------------------------------------------------
CoO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.844014  5.844014 28.632179 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
```

```
Co1       NPT=  781  R0=0.00005000 RMT=    1.8400   Z: 27.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1         ISPLIT= 4
Co2       NPT=  781  R0=0.00005000 RMT=    1.8400   Z: 27.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2         ISPLIT= 4
       -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.5800   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE 0.55
-------------------------------------------------------------
CoO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
 5.733723  5.733723 28.091820 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1         ISPLIT= 4
Co1       NPT=  781  R0=0.00005000 RMT=    1.8400   Z: 27.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1         ISPLIT= 4
Co2       NPT=  781  R0=0.00005000 RMT=    1.8400   Z: 27.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2         ISPLIT= 4
       -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.5800   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE
-------------------------------------------------------------
CoO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
 5.997828  5.997828  8.481797 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1         ISPLIT=-2
Co1       NPT=  781  R0=0.00005000 RMT= 1.84       Z: 27.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
```

```
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Co2       NPT=  781  R0=0.00005000 RMT= 1.84       Z: 27.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.58       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  8      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
CoO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
 6.080000  6.080000  8.598000 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Co1       NPT=  781  R0=0.00005000 RMT= 1.84       Z: 27.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Co2       NPT=  781  R0=0.00005000 RMT= 1.84       Z: 27.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.58       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  8      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE-EECE
-------------------------------------------------------------
CoO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
 6.199246  6.199246  8.766631 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Co1       NPT=  781  R0=0.00005000 RMT= 1.84       Z: 27.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
```

```
Co2       NPT=  781  R0=0.00005000 RMT= 1.84       Z: 27.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.58       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  8      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
CoO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
  6.120266  6.120266  8.654942 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Co1       NPT=  781  R0=0.00005000 RMT= 1.84       Z: 27.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Co2       NPT=  781  R0=0.00005000 RMT= 1.84       Z: 27.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.58       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  8      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE-EECE 0.4
-------------------------------------------------------------
 CoO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
  6.237992  6.237992  8.821424 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Co1       NPT=  781  R0=0.00005000 RMT= 1.84       Z: 27.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Co2       NPT=  781  R0=0.00005000 RMT= 1.84       Z: 27.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
```

```
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.58       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE 0.4
-------------------------------------------------------------
CoO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
  6.160009  6.160009  8.711145 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Co1       NPT=  781  R0=0.00005000 RMT= 1.84       Z: 27.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Co2       NPT=  781  R0=0.00005000 RMT= 1.84       Z: 27.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.58       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE-EECE 0.55
-------------------------------------------------------------
CoO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
  6.276263  6.276263  8.875544 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Co1       NPT=  781  R0=0.00005000 RMT= 1.84       Z: 27.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Co2       NPT=  781  R0=0.00005000 RMT= 1.84       Z: 27.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
```

```
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1        NPT=  781  R0=0.00010000 RMT= 1.58        Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  8      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE 0.55
-------------------------------------------------------------
CoO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
          RELA
  6.199246  6.199246  8.766631 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
        MULT= 1         ISPLIT=-2
Co1        NPT=  781  R0=0.00005000 RMT= 1.84        Z: 27.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
        MULT= 1         ISPLIT=-2
Co2        NPT=  781  R0=0.00005000 RMT= 1.84        Z: 27.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
        MULT= 2         ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1        NPT=  781  R0=0.00010000 RMT= 1.58        Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  8      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE
-------------------------------------------------------------
FeO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
 5.750000  5.750000 28.168000 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
        MULT= 1         ISPLIT= 4
Fe1        NPT=  781  R0=0.00005000 RMT=    1.8900   Z: 26.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
        MULT= 1         ISPLIT= 4
Fe2        NPT=  781  R0=0.00005000 RMT=    1.8900   Z: 26.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
        MULT= 2         ISPLIT= 4
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
          NPT=  781  R0=0.00010000 RMT=    1.6300   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
```

```
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
FeO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.711408  5.711408 27.978947 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Fe1       NPT=  781  R0=0.00005000 RMT=    1.8900   Z: 26.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Fe2       NPT=  781  R0=0.00005000 RMT=    1.8900   Z: 26.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.6300   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE-EECE
-------------------------------------------------------------
FeO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.862774  5.862774 28.720454 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Fe1       NPT=  781  R0=0.00005000 RMT=    1.8900   Z: 26.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Fe2       NPT=  781  R0=0.00005000 RMT=    1.8900   Z: 26.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.6300   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
```

```
------------------------------------------------------------
SCAN-EECE
------------------------------------------------------------
FeO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.788081  5.788081 28.354548 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Fe1       NPT=  781  R0=0.00005000 RMT=    1.8900   Z: 26.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Fe2       NPT=  781  R0=0.00005000 RMT=    1.8900   Z: 26.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.6300   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
------------------------------------------------------------
PBE-EECE 0.4
------------------------------------------------------------
FeO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.899417  5.899417 28.899962 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Fe1       NPT=  781  R0=0.00005000 RMT=    1.8900   Z: 26.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Fe2       NPT=  781  R0=0.00005000 RMT=    1.8900   Z: 26.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.6300   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
------------------------------------------------------------
SCAN-EECE 0.4
------------------------------------------------------------
```

```
FeO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.825667  5.825667 28.538674 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Fe1       NPT=  781  R0=0.00005000 RMT=    1.8900   Z: 26.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Fe2       NPT=  781  R0=0.00005000 RMT=    1.8900   Z: 26.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.6300   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE
-------------------------------------------------------------
FeO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
          RELA
  6.047140  6.047140  8.552213 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Fe1       NPT=  781  R0=0.00005000 RMT= 1.89       Z: 26.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Fe2       NPT=  781  R0=0.00005000 RMT= 1.89       Z: 26.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.63       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
FeO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
          RELA
```

```
  6.088000  6.088000  8.610000 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Fe1       NPT=  781  R0=0.00005000 RMT= 1.89       Z: 26.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Fe2       NPT=  781  R0=0.00005000 RMT= 1.89       Z: 26.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.63       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE-EECE
-------------------------------------------------------------
FeO zincblende AF1
P  LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
          RELA
  6.284521  6.284521  8.887932 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Fe1       NPT=  781  R0=0.00005000 RMT= 1.89       Z: 26.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Fe2       NPT=  781  R0=0.00005000 RMT= 1.89       Z: 26.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.63       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
FeO zincblende AF1
P  LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
          RELA
  6.207403  6.207403  8.778866 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
```

```
Fe1        NPT=  781  R0=0.00005000 RMT= 1.89       Z: 26.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Fe2        NPT=  781  R0=0.00005000 RMT= 1.89       Z: 26.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
       -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1        NPT=  781  R0=0.00010000 RMT= 1.63       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE-EECE 0.4
-------------------------------------------------------------
FeO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
 6.359792  6.359792  8.994384 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Fe1        NPT=  781  R0=0.00005000 RMT= 1.89       Z: 26.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Fe2        NPT=  781  R0=0.00005000 RMT= 1.89       Z: 26.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
       -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1        NPT=  781  R0=0.00010000 RMT= 1.63       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE 0.4
-------------------------------------------------------------
FeO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
 6.246200  6.246200  8.833736 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Fe1        NPT=  781  R0=0.00005000 RMT= 1.89       Z: 26.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
```

```
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Fe2        NPT=  781  R0=0.00005000 RMT= 1.89        Z: 26.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1        NPT=  781  R0=0.00010000 RMT= 1.63        Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  8      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE
-------------------------------------------------------------
MnO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.939314  5.939314 29.096576 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Mn1        NPT=  781  R0=0.00005000 RMT=    1.9800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Mn2        NPT=  781  R0=0.00005000 RMT=    1.9800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O          NPT=  781  R0=0.00010000 RMT=    1.7100   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
 12      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
MnO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.899452  5.899452 28.901291 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Mn1        NPT=  781  R0=0.00005000 RMT=    1.9800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
```

```
Mn2       NPT=  781  R0=0.00005000 RMT=    1.9800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
      -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.7100   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE-EECE
-------------------------------------------------------------
MnO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.978648  5.978648 29.289274 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Mn1       NPT=  781  R0=0.00005000 RMT=    1.9800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Mn2       NPT=  781  R0=0.00005000 RMT=    1.9800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
      -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.7100   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
MnO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.939314  5.939314 29.096576 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Mn1       NPT=  781  R0=0.00005000 RMT=    1.9800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Mn2       NPT=  781  R0=0.00005000 RMT=    1.9800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
```

```
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
      -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.7100   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  12      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE-EECE 0.4
-------------------------------------------------------------
MnO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  6.017472  6.017472 29.479470 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Mn1       NPT=  781  R0=0.00005000 RMT=    1.9800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Mn2       NPT=  781  R0=0.00005000 RMT=    1.9800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
      -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.7100   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  12      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE 0.4
-------------------------------------------------------------
MnO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.978648  5.978648 29.289274 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Mn1       NPT=  781  R0=0.00005000 RMT=    1.9800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Mn2       NPT=  781  R0=0.00005000 RMT=    1.9800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
```

```
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.7100   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE-EECE 0.55
-------------------------------------------------------------
MnO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  6.055801  6.055801 29.667242 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Mn1       NPT=  781  R0=0.00005000 RMT=    1.9800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Mn2       NPT=  781  R0=0.00005000 RMT=    1.9800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.7100   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE 0.55
-------------------------------------------------------------
MnO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
 5.978648  5.978648 29.289274 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Mn1       NPT=  781  R0=0.00005000 RMT=    1.9800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Mn2       NPT=  781  R0=0.00005000 RMT=    1.9800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
          NPT=  781  R0=0.00010000 RMT=    1.7100   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
```

```
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE
-------------------------------------------------------------
MnO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
          RELA
  6.250601  6.250601  8.839685 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
        MULT= 1         ISPLIT=-2
Mn1       NPT=  781  R0=0.00005000 RMT= 1.98       Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
        MULT= 1         ISPLIT=-2
Mn2       NPT=  781  R0=0.00005000 RMT= 1.98       Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
        MULT= 2         ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.71       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
   8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
MnO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
          RELA
  6.250601  6.250601  8.839685 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
        MULT= 1         ISPLIT=-2
Mn1       NPT=  781  R0=0.00005000 RMT= 1.98       Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
        MULT= 1         ISPLIT=-2
Mn2       NPT=  781  R0=0.00005000 RMT= 1.98       Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
        MULT= 2         ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.71       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
   8     NUMBER OF SYMMETRY OPERATIONS
```

```
------------------------------------------------------------
PBE-EECE
------------------------------------------------------------
MnO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
           RELA
  6.373193  6.373193  9.013056 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Mn1       NPT=  781  R0=0.00005000 RMT= 1.98       Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Mn2       NPT=  781  R0=0.00005000 RMT= 1.98       Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.71       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
------------------------------------------------------------
SCAN-EECE
------------------------------------------------------------
MnO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
           RELA
  6.332855  6.332855  8.956010 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Mn1       NPT=  781  R0=0.00005000 RMT= 1.98       Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Mn2       NPT=  781  R0=0.00005000 RMT= 1.98       Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.71       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
------------------------------------------------------------
BE-EECE 0.4
------------------------------------------------------------
```

```
MnO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
  6.452371  6.452371  9.125031 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Mn1       NPT=  781  R0=0.00005000 RMT= 1.98       Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Mn2       NPT=  781  R0=0.00005000 RMT= 1.98       Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.71       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE 0.4
-------------------------------------------------------------
MnO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
  6.413026  6.413026  9.069389 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Mn1       NPT=  781  R0=0.00005000 RMT= 1.98       Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Mn2       NPT=  781  R0=0.00005000 RMT= 1.98       Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.71       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE-EECE 0.55
-------------------------------------------------------------
MnO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
```

```
  6.491242  6.491242  9.180002 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Mn1       NPT=  781  R0=0.00005000 RMT= 1.98       Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Mn2       NPT=  781  R0=0.00005000 RMT= 1.98       Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.71       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
   8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE 0.55
-------------------------------------------------------------
MnO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
  6.413026  6.413026  9.069389 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Mn1       NPT=  781  R0=0.00005000 RMT= 1.98       Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Mn2       NPT=  781  R0=0.00005000 RMT= 1.98       Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.71       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
   8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE
-------------------------------------------------------------
NiO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
 5.619975  5.619975 27.531131 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
```

```
Ni1       NPT=  781  R0=0.00005000 RMT=    1.8300   Z: 28.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1         ISPLIT= 4
Ni2       NPT=  781  R0=0.00005000 RMT=    1.8300   Z: 28.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2         ISPLIT= 4
       -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.5700   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
NiO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
 5.583000  5.583000 27.350000 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1         ISPLIT= 4
Ni1       NPT=  781  R0=0.00005000 RMT=    1.8300   Z: 28.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1         ISPLIT= 4
Ni2       NPT=  781  R0=0.00005000 RMT=    1.8300   Z: 28.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2         ISPLIT= 4
       -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.5700   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE-EECE
-------------------------------------------------------------
NiO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
 5.656469  5.656469 27.709910 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1         ISPLIT= 4
Ni1       NPT=  781  R0=0.00005000 RMT=    1.8300   Z: 28.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
```

```
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Ni2       NPT=  781  R0=0.00005000 RMT=    1.8300   Z: 28.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.5700   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  12      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
NiO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.619975  5.619975 27.531131 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Ni1       NPT=  781  R0=0.00005000 RMT=    1.8300   Z: 28.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Ni2       NPT=  781  R0=0.00005000 RMT=    1.8300   Z: 28.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.5700   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  12      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE-EECE 0.4
-------------------------------------------------------------
NiO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.692498  5.692498 27.886411 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Ni1       NPT=  781  R0=0.00005000 RMT=    1.8300   Z: 28.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
```

```
Ni2       NPT=  781  R0=0.00005000 RMT=    1.8300   Z: 28.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
      -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.5700   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE 0.4
-------------------------------------------------------------
NiO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.656469  5.656469 27.709910 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Ni1       NPT=  781  R0=0.00005000 RMT=    1.8300   Z: 28.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Ni2       NPT=  781  R0=0.00005000 RMT=    1.8300   Z: 28.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
      -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.5700   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE
-------------------------------------------------------------
NiO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
 5.952311  5.952311  8.418341 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Ni1       NPT=  781  R0=0.00005000 RMT= 1.83       Z: 28.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Ni2       NPT=  781  R0=0.00005000 RMT= 1.83       Z: 28.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
```

```
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.57       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
NiO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
  5.952311  5.952311  8.418341 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Ni1       NPT=  781  R0=0.00005000 RMT= 1.83       Z: 28.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Ni2       NPT=  781  R0=0.00005000 RMT= 1.83       Z: 28.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.57       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE-EECE
-------------------------------------------------------------
NiO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
  6.064646  6.064646  8.577215 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Ni1       NPT=  781  R0=0.00005000 RMT= 1.83       Z: 28.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Ni2       NPT=  781  R0=0.00005000 RMT= 1.83       Z: 28.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
```

```
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1        NPT=  781  R0=0.00010000 RMT= 1.57       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
NiO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
          RELA
  5.990225  5.990225  8.471963 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
        MULT= 1         ISPLIT=-2
Ni1        NPT=  781  R0=0.00005000 RMT= 1.83       Z: 28.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
        MULT= 1         ISPLIT=-2
Ni2        NPT=  781  R0=0.00005000 RMT= 1.83       Z: 28.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
        MULT= 2         ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1        NPT=  781  R0=0.00010000 RMT= 1.57       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE-EECE 0.4
-------------------------------------------------------------
NiO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
          RELA
  6.101181  6.101181  8.628887 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
        MULT= 1         ISPLIT=-2
Ni1        NPT=  781  R0=0.00005000 RMT= 1.83       Z: 28.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
        MULT= 1         ISPLIT=-2
Ni2        NPT=  781  R0=0.00005000 RMT= 1.83       Z: 28.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
        MULT= 2         ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1        NPT=  781  R0=0.00010000 RMT= 1.57       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
```

```
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE 0.4
-------------------------------------------------------------
NiO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
          RELA
  6.027665  6.027665  8.524914 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
        MULT= 1         ISPLIT=-2
Ni1       NPT=  781  R0=0.00005000 RMT= 1.83       Z: 28.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
        MULT= 1         ISPLIT=-2
Ni2       NPT=  781  R0=0.00005000 RMT= 1.83       Z: 28.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
        MULT= 2         ISPLIT= 8
    -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.57       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
```

```
-------------------------------------------------------------
PBE
-------------------------------------------------------------
CoO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.415981  5.415981 30.249980 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Co1       NPT=  781  R0=0.00005000 RMT=    1.8400   Z: 27.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Co2       NPT=  781  R0=0.00005000 RMT=    1.8400   Z: 27.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.5800   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE
-------------------------------------------------------------
CoO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
  6.038355  6.038355  8.368326 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Co1       NPT=  781  R0=0.00005000 RMT= 1.84       Z: 27.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Co2       NPT=  781  R0=0.00005000 RMT= 1.84       Z: 27.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.58       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  8       NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE
-------------------------------------------------------------
```

```
FeO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.472451  5.472451 31.097683 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Fe1       NPT=  781  R0=0.00005000 RMT=    1.8900   Z: 26.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Fe2       NPT=  781  R0=0.00005000 RMT=    1.8900   Z: 26.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.6300   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE
-------------------------------------------------------------
FeO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
          RELA
  6.310384  6.310384  7.853568 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Fe1       NPT=  781  R0=0.00005000 RMT= 1.89       Z: 26.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Fe2       NPT=  781  R0=0.00005000 RMT= 1.89       Z: 26.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.63       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
   8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE
-------------------------------------------------------------
MnO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
```

```
  6.020685  6.020685 28.315401 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Mn1       NPT=  781  R0=0.00005000 RMT=    1.9800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Mn2       NPT=  781  R0=0.00005000 RMT=    1.9800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
      -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.7100   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE
-------------------------------------------------------------
MnO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
 6.426766  6.426766  8.361715 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Mn1       NPT=  781  R0=0.00005000 RMT= 1.98       Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Mn2       NPT=  781  R0=0.00005000 RMT= 1.98       Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
      -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.71       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
   8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE
-------------------------------------------------------------
NiO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
5.619975  5.619975 27.531132 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
```

```
Ni1       NPT=  781  R0=0.00005000 RMT=    1.8300   Z: 28.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Ni2       NPT=  781  R0=0.00005000 RMT=    1.8300   Z: 28.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
      -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.5700   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE
-------------------------------------------------------------
NiO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
 6.308497  6.308497  7.494559 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Ni1       NPT=  781  R0=0.00005000 RMT= 1.83       Z: 28.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Ni2       NPT=  781  R0=0.00005000 RMT= 1.83       Z: 28.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
      -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.57       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
   8      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
CoO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
5.831210  5.831210 27.426671 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Co1       NPT=  781  R0=0.00005000 RMT=    1.8400   Z: 27.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
```

```
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Co2       NPT=  781  R0=0.00005000 RMT=    1.8400   Z: 27.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.5800   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  12      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
CoO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
  6.039999  6.039999  8.712262 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Co1       NPT=  781  R0=0.00005000 RMT= 1.84        Z: 27.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Co2       NPT=  781  R0=0.00005000 RMT= 1.84        Z: 27.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.58        Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
   8      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
FeO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.467325  5.467325 30.532893 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Fe1       NPT=  781  R0=0.00005000 RMT=    1.8900   Z: 26.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
```

```
Fe2       NPT=  781  R0=0.00005000 RMT=    1.8900   Z: 26.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
      -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.6300   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
FeO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
  6.558100  6.558100  7.419873 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Fe1       NPT=  781  R0=0.00005000 RMT= 1.89       Z: 26.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Fe2       NPT=  781  R0=0.00005000 RMT= 1.89       Z: 26.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
      -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.63       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
 8      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
MnO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
 5.939315  5.939315 28.514645 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Mn1       NPT=  781  R0=0.00005000 RMT=    1.9800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Mn2       NPT=  781  R0=0.00005000 RMT=    1.9800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
```

```
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
      -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.7100   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
MnO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
  6.426766  6.426766  8.361715 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Mn1       NPT=  781  R0=0.00005000 RMT= 1.98        Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Mn2       NPT=  781  R0=0.00005000 RMT= 1.98        Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
      -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.71        Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
NiO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.583000  5.583000 27.350001 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Ni1       NPT=  781  R0=0.00005000 RMT=    1.8300   Z: 28.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Ni2       NPT=  781  R0=0.00005000 RMT=    1.8300   Z: 28.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
```

```
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.5700   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
NiO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
  6.283660  6.283660  7.553922 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1         ISPLIT=-2
Ni1       NPT=  781  R0=0.00005000 RMT= 1.83       Z: 28.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1         ISPLIT=-2
Ni2       NPT=  781  R0=0.00005000 RMT= 1.83       Z: 28.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2         ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.57       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
   8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE-EECE
-------------------------------------------------------------
CoO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
 5.770956  5.770956 28.274241 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1         ISPLIT= 4
Co1       NPT=  781  R0=0.00005000 RMT=    1.8400   Z: 27.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1         ISPLIT= 4
Co2       NPT=  781  R0=0.00005000 RMT=    1.8400   Z: 27.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2         ISPLIT= 4
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
          NPT=  781  R0=0.00010000 RMT=    1.5800   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
```

```
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE-EECE
-------------------------------------------------------------
CoO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
          RELA
  6.241134  6.241134  8.649350 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
        MULT= 1         ISPLIT=-2
Co1       NPT=  781  R0=0.00005000 RMT= 1.84       Z: 27.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
        MULT= 1         ISPLIT=-2
Co2       NPT=  781  R0=0.00005000 RMT= 1.84       Z: 27.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
        MULT= 2         ISPLIT= 8
    -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.58       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE-EECE
-------------------------------------------------------------
FeO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.943096  5.943096 27.949377 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
        MULT= 1         ISPLIT= 4
Fe1       NPT=  781  R0=0.00005000 RMT=    1.8900   Z: 26.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
        MULT= 1         ISPLIT= 4
Fe2       NPT=  781  R0=0.00005000 RMT=    1.8900   Z: 26.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
        MULT= 2         ISPLIT= 4
    -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.6300   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
```

```
-------------------------------------------------------------
PBE-EECE
-------------------------------------------------------------
FeO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
           RELA
  6.660586  6.660586  7.912619 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Fe1        NPT=  781  R0=0.00005000 RMT= 1.89        Z: 26.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Fe2        NPT=  781  R0=0.00005000 RMT= 1.89        Z: 26.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1        NPT=  781  R0=0.00010000 RMT= 1.63        Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE-EECE
-------------------------------------------------------------
MnO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  6.019046  6.019046 28.897439 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Mn1        NPT=  781  R0=0.00005000 RMT=    1.9800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Mn2        NPT=  781  R0=0.00005000 RMT=    1.9800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O          NPT=  781  R0=0.00010000 RMT=    1.7100   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
 12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
BE-EECE
-------------------------------------------------------------
```

```
MnO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
          RELA
  6.506006  6.506006  8.648829 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
        MULT= 1         ISPLIT=-2
Mn1       NPT=  781  R0=0.00005000 RMT= 1.98       Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
        MULT= 1         ISPLIT=-2
Mn2       NPT=  781  R0=0.00005000 RMT= 1.98       Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
        MULT= 2         ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.71       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE-EECE
-------------------------------------------------------------
NiO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.656469  5.656469 27.709912 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
        MULT= 1         ISPLIT= 4
Ni1       NPT=  781  R0=0.00005000 RMT=    1.8300   Z: 28.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
        MULT= 1         ISPLIT= 4
Ni2       NPT=  781  R0=0.00005000 RMT=    1.8300   Z: 28.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
        MULT= 2         ISPLIT= 4
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.5700   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
 12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
PBE-EECE
-------------------------------------------------------------
MnO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
          RELA
```

```
  6.281422  6.281422  7.995421 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Ni1       NPT=  781  R0=0.00005000 RMT= 1.83        Z: 28.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Ni2       NPT=  781  R0=0.00005000 RMT= 1.83        Z: 28.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.57        Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
CoO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
 5.696000  5.696000 27.907002 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Co1       NPT=  781  R0=0.00005000 RMT=    1.8400   Z: 27.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Co2       NPT=  781  R0=0.00005000 RMT=    1.8400   Z: 27.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.5800   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
 12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
CoO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
          RELA
6.161621  6.161621  8.539155 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
```

```
Co1       NPT=  781  R0=0.00005000 RMT= 1.84       Z: 27.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1         ISPLIT=-2
Co2       NPT=  781  R0=0.00005000 RMT= 1.84       Z: 27.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2         ISPLIT= 8
      -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.58       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
FeO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
 5.867380  5.867380 27.593296 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1         ISPLIT= 4
Fe1       NPT=  781  R0=0.00005000 RMT=    1.8900   Z: 26.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1         ISPLIT= 4
Fe2       NPT=  781  R0=0.00005000 RMT=    1.8900   Z: 26.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2         ISPLIT= 4
      -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.6300   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
 12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
FeO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
          RELA
 6.686723  6.686723  7.565398 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1         ISPLIT=-2
Fe1       NPT=  781  R0=0.00005000 RMT= 1.89       Z: 26.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
```

```
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Fe2        NPT=  781  R0=0.00005000 RMT= 1.89        Z: 26.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1        NPT=  781  R0=0.00010000 RMT= 1.63        Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  8      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
MnO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.979446  5.979446 28.707318 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Mn1        NPT=  781  R0=0.00005000 RMT=    1.9800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Mn2        NPT=  781  R0=0.00005000 RMT=    1.9800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O          NPT=  781  R0=0.00010000 RMT=    1.7100   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
 12      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
MnO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
  6.464828  6.464828  8.594089 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Mn1        NPT=  781  R0=0.00005000 RMT= 1.98        Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
```

```
Mn2       NPT=  781  R0=0.00005000 RMT= 1.98       Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.71       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  8      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
NiO rock-salt AF2
R   LATTICE,NONEQUIV.ATOMS:  3166_R-3m
MODE OF CALC=RELA unit=ang
  5.619975  5.619975 27.531132 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Ni1       NPT=  781  R0=0.00005000 RMT=    1.8300   Z: 28.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
Ni2       NPT=  781  R0=0.00005000 RMT=    1.8300   Z: 28.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 4
     -3: X=0.75000000 Y=0.75000000 Z=0.75000000
O         NPT=  781  R0=0.00010000 RMT=    1.5700   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
 12      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
NiO zincblende AF1
P   LATTICE,NONEQUIV.ATOMS:  3 115 P-4m2
            RELA
 6.250992  6.250992  7.779873 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Ni1       NPT=  781  R0=0.00005000 RMT= 1.83       Z: 28.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=-2
Ni2       NPT=  781  R0=0.00005000 RMT= 1.83       Z: 28.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
```

```
                0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT= 8
      -3: X=0.50000000 Y=0.00000000 Z=0.75000000
O 1         NPT=  781  R0=0.00010000 RMT= 1.57        Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
   8      NUMBER OF SYMMETRY OPERATIONS
```

```
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
AgF_exp
F   LATTICE,NONEQUIV.ATOMS:  2 225 Fm-3m
MODE OF CALC=RELA unit=bohr
  9.265074  9.265074  9.265074 90.000000 90.000000 90.000000
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
Ag1       NPT=  781  R0=0.00001000 RMT= 2.27       Z: 47.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM   2: X=0.50000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
F 1       NPT=  781  R0=0.00010000 RMT= 2.05       Z:  9.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  48     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
AgF_exp
F   LATTICE,NONEQUIV.ATOMS:  2 225 Fm-3m
MODE OF CALC=RELA unit=bohr
  9.202890  9.202890  9.202890 90.000000 90.000000 90.000000
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
Ag1       NPT=  781  R0=0.00001000 RMT= 2.27       Z: 47.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM   2: X=0.50000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
F 1       NPT=  781  R0=0.00010000 RMT= 2.05       Z:  9.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  48     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
AgF_0
CXY LATTICE,NONEQUIV.ATOMS:  2 63 Cmcm
MODE OF CALC=RELA unit=bohr
 5.908800 18.275700  7.015200 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.61337000 Z=0.25000000
          MULT= 2          ISPLIT= 8
       -1: X=0.00000000 Y=0.38663000 Z=0.75000000
Ag1       NPT=  781  R0=0.00001000 RMT= 2.27       Z: 47.0
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
ATOM  -2: X=0.00000000 Y=0.13103000 Z=0.75000000
          MULT= 2          ISPLIT= 8
       -2: X=0.00000000 Y=0.86897000 Z=0.25000000
```

```
F 1        NPT=  781  R0=0.00010000 RMT= 2.05        Z:  9.0
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
  8      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
AgF_0
CXY LATTICE,NONEQUIV.ATOMS:  2 63 Cmcm
MODE OF CALC=RELA unit=bohr
  5.878900 18.140700  6.953700 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.61337000 Z=0.25000000
          MULT= 2         ISPLIT= 8
     -1: X=0.00000000 Y=0.38663000 Z=0.75000000
Ag1        NPT=  781  R0=0.00001000 RMT= 2.27        Z: 47.0
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
ATOM  -2: X=0.00000000 Y=0.13103000 Z=0.75000000
          MULT= 2         ISPLIT= 8
     -2: X=0.00000000 Y=0.86897000 Z=0.25000000
F 1        NPT=  781  R0=0.00010000 RMT= 2.05        Z:  9.0
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
  8      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
AgF_3
P   LATTICE,NONEQUIV.ATOMS:  2 221 Pm-3m
MODE OF CALC=RELA unit=bohr
  5.603632  5.603632  5.603632 90.000000 90.000000 90.000000
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1         ISPLIT= 2
Ag1        NPT=  781  R0=0.00001000 RMT= 2.27        Z: 47.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM   2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1         ISPLIT= 2
F 1        NPT=  781  R0=0.00010000 RMT= 2.05        Z:  9.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
 48      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
AgF_3
P   LATTICE,NONEQUIV.ATOMS:  2 221 Pm-3m
MODE OF CALC=RELA unit=bohr
  5.566023  5.566023  5.566023 90.000000 90.000000 90.000000
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1         ISPLIT= 2
Ag1        NPT=  781  R0=0.00001000 RMT= 2.27        Z: 47.0
```

```
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM   2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 2
F 1       NPT=  781  R0=0.00010000 RMT= 2.05       Z:  9.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  48     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
AgF_5
H   LATTICE,NONEQUIV.ATOMS:  2 187 P-6m2
MODE OF CALC=RELA unit=bohr
  5.903100  5.903100  6.301300 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Ag1       NPT=  781  R0=0.00001000 RMT= 2.27       Z: 47.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.33333333 Y=0.66666667 Z=0.50000000
          MULT= 1          ISPLIT= 4
F 1       NPT=  781  R0=0.00010000 RMT= 2.05       Z:  9.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
AgF_5
H   LATTICE,NONEQUIV.ATOMS:  2 187 P-6m2
MODE OF CALC=RELA unit=bohr
  5.927200  5.927200  6.162300 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Ag1       NPT=  781  R0=0.00001000 RMT= 2.27       Z: 47.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.33333333 Y=0.66666667 Z=0.50000000
          MULT= 1          ISPLIT= 4
F 1       NPT=  781  R0=0.00010000 RMT= 2.05       Z:  9.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
AgSe_exp
B   LATTICE,NONEQUIV.ATOMS:  2 216 F-43m
MODE OF CALC=RELA unit=bohr
 11.106863 11.106863 11.106863 90.000000 90.000000 90.000000
```

```
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
Ag1       NPT=  781  R0=0.00001000 RMT= 2.33        Z: 47.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM   2: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 1          ISPLIT= 2
Se1       NPT=  781  R0=0.00005000 RMT= 2.21        Z: 34.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  24     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
AgSe_exp
F   LATTICE,NONEQUIV.ATOMS:  2 216 F-43m
MODE OF CALC=RELA unit=bohr
 11.106863 11.106863 11.106863 90.000000 90.000000 90.000000
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
Ag1       NPT=  781  R0=0.00001000 RMT= 2.33        Z: 47.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM   2: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 1          ISPLIT= 2
Se1       NPT=  781  R0=0.00005000 RMT= 2.21        Z: 34.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  24     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
AgSe_2
F   LATTICE,NONEQUIV.ATOMS:  2 225 Fm-3m
MODE OF CALC=RELA unit=bohr
 10.312720 10.312720 10.312720 90.000000 90.000000 90.000000
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
Ag1       NPT=  781  R0=0.00001000 RMT= 2.33        Z: 47.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM   2: X=0.50000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
Se1       NPT=  781  R0=0.00005000 RMT= 2.21        Z: 34.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  48     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
AgSe_2
```

```
F   LATTICE,NONEQUIV.ATOMS:  2 225 Fm-3m
MODE OF CALC=RELA unit=bohr
 10.312720 10.312720 10.312720 90.000000 90.000000 90.000000
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
Ag1        NPT=  781  R0=0.00001000 RMT= 2.33        Z: 47.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM   2: X=0.50000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
Se1        NPT=  781  R0=0.00005000 RMT= 2.21        Z: 34.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  48     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
AgSe_4
H   LATTICE,NONEQUIV.ATOMS:  2 194 P63/mmc
MODE OF CALC=RELA unit=bohr
 7.645600  7.645600 11.136600 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.50000000
          MULT= 2          ISPLIT= 4
     -1: X=0.00000000 Y=0.00000000 Z=0.00000000
Ag1        NPT=  781  R0=0.00001000 RMT= 2.33000     Z: 47.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.33333333 Y=0.66666667 Z=0.75000000
          MULT= 2          ISPLIT= 4
     -2: X=0.66666667 Y=0.33333333 Z=0.25000000
Se1        NPT=  781  R0=0.00005000 RMT= 2.21        Z: 34.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  24     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
AgSe_4
H   LATTICE,NONEQUIV.ATOMS:  2 194 P63/mmc
MODE OF CALC=RELA unit=bohr
 7.639700  7.639700 11.095100 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.50000000
          MULT= 2          ISPLIT= 4
     -1: X=0.00000000 Y=0.00000000 Z=0.00000000
Ag1        NPT=  781  R0=0.00001000 RMT= 2.33000     Z: 47.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.33333333 Y=0.66666667 Z=0.75000000
          MULT= 2          ISPLIT= 4
     -2: X=0.66666667 Y=0.33333333 Z=0.25000000
e1         NPT=  781  R0=0.00005000 RMT= 2.21        Z: 34.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
```

```
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  24     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
AgSe_5
H   LATTICE,NONEQUIV.ATOMS:  2 187 P-6m2
MODE OF CALC=RELA unit=bohr
  7.877500  7.877500  5.524300 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
        MULT= 1         ISPLIT= 4
Ag1       NPT=  781  R0=0.00001000 RMT= 2.33000     Z: 47.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.33333333 Y=0.66666667 Z=0.50000000
        MULT= 1         ISPLIT= 4
Se1       NPT=  781  R0=0.00005000 RMT= 2.21        Z: 34.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
AgSe_5
H   LATTICE,NONEQUIV.ATOMS:  2 187 P-6m2
MODE OF CALC=RELA unit=bohr
  7.905400  7.905400  5.477700 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
        MULT= 1         ISPLIT= 4
Ag1       NPT=  781  R0=0.00001000 RMT= 2.33000     Z: 47.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.33333333 Y=0.66666667 Z=0.50000000
        MULT= 1         ISPLIT= 4
Se1       NPT=  781  R0=0.00005000 RMT= 2.21        Z: 34.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
CrO_exp
F   LATTICE,NONEQUIV.ATOMS   2  225 Fm-3m
MODE OF CALC=RELA unit=bohr
  8.212219  8.212219  8.212219 90.000000 90.000000 90.000000
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
        MULT= 1         ISPLIT= 2
Cr2+      NPT=  781  R0=.000050000 RMT= 1.86        Z:  24.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM   2: X=0.50000000 Y=0.50000000 Z=0.50000000
```

```
        MULT= 1         ISPLIT= 2
O 2-       NPT=  781  R0=.000100000 RMT= 1.68       Z:   8.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  48     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
CrO_exp
F   LATTICE,NONEQUIV.ATOMS   2  225 Fm-3m
MODE OF CALC=RELA unit=bohr
  8.353836  8.353836  8.353836 90.000000 90.000000 90.000000
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
        MULT= 1         ISPLIT= 2
Cr2+       NPT=  781  R0=.000050000 RMT= 1.86       Z:  24.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM   2: X=0.50000000 Y=0.50000000 Z=0.50000000
        MULT= 1         ISPLIT= 2
O 2-       NPT=  781  R0=.000100000 RMT= 1.68       Z:   8.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  48     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
CrO_0
CXY LATTICE,NONEQUIV.ATOMS:  2 66 Cccm
MODE OF CALC=RELA unit=bohr
 7.943300  7.921300 10.031300 90.000000 90.000000 90.000000
ATOM  -1: X=0.25000000 Y=0.75000000 Z=0.50000000
        MULT= 2         ISPLIT= 8
     -1: X=0.75000000 Y=0.75000000 Z=0.00000000
Cr1        NPT=  781  R0=0.00005000 RMT= 1.86       Z: 24.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.00000000 Y=0.00000000 Z=0.25000000
        MULT= 2         ISPLIT= 8
     -2: X=0.00000000 Y=0.00000000 Z=0.75000000
O 1        NPT=  781  R0=0.00010000 RMT= 1.68       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
   8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
CrO_0
CXY LATTICE,NONEQUIV.ATOMS:  2 66 Cccm
MODE OF CALC=RELA unit=bohr
 8.113700  8.119600 10.106400 90.000000 90.000000 90.000000
ATOM  -1: X=0.25000000 Y=0.75000000 Z=0.50000000
        MULT= 2         ISPLIT= 8
```

```
     -1: X=0.75000000 Y=0.75000000 Z=0.00000000
Cr1       NPT=  781  R0=0.00005000 RMT= 1.86       Z: 24.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.00000000 Y=0.00000000 Z=0.25000000
          MULT= 2         ISPLIT= 8
     -2: X=0.00000000 Y=0.00000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.68       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  8      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
CrO_16
P   LATTICE,NONEQUIV.ATOMS:  2 123 P4/mmm
MODE OF CALC=RELA unit=bohr
  5.393500  5.393500  7.061900 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1         ISPLIT=-2
Cr1       NPT=  781  R0=0.00005000 RMT= 1.86       Z: 24.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.00000000
          MULT= 1         ISPLIT=-2
O 1       NPT=  781  R0=0.00010000 RMT= 1.68       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
 16      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
CrO_16
P   LATTICE,NONEQUIV.ATOMS:  2 123 P4/mmm
MODE OF CALC=RELA unit=bohr
  5.427500  5.427500  6.960100 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1         ISPLIT=-2
Cr1       NPT=  781  R0=0.00005000 RMT= 1.86       Z: 24.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.00000000
          MULT= 1         ISPLIT=-2
O 1       NPT=  781  R0=0.00010000 RMT= 1.68       Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
 16      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
Cu2Se_exp
```

```
F   LATTICE,NONEQUIV.ATOMS:  2 225 Fm-3m
MODE OF CALC=RELA unit=bohr
 10.874998 10.874998 10.874998 90.000000 90.000000 90.000000
ATOM   1: X=0.75000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 2
       1: X=0.25000000 Y=0.75000000 Z=0.75000000
Cu1        NPT=  781  R0=0.00005000 RMT= 2.05        Z: 29.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM   2: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
Se1        NPT=  781  R0=0.00005000 RMT= 1.95        Z: 34.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  48     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
Cu2Se_exp
F   LATTICE,NONEQUIV.ATOMS:  2 225 Fm-3m
MODE OF CALC=RELA unit=bohr
 10.874998 10.874998 10.874998 90.000000 90.000000 90.000000
ATOM   1: X=0.75000000 Y=0.25000000 Z=0.25000000
          MULT= 2          ISPLIT= 2
       1: X=0.25000000 Y=0.75000000 Z=0.75000000
Cu1        NPT=  781  R0=0.00005000 RMT= 2.05        Z: 29.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM   2: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
Se1        NPT=  781  R0=0.00005000 RMT= 1.95        Z: 34.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  48     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
Cu2Se_1
P   LATTICE,NONEQUIV.ATOMS:  3 78 P43
MODE OF CALC=RELA unit=bohr
  8.048500  8.048500 20.154200 90.000000 90.000000 90.000000
ATOM  -1: X=0.10659500 Y=0.07720000 Z=0.08087000
          MULT= 4          ISPLIT= 8
      -1: X=0.89340500 Y=0.92280000 Z=0.58087000
      -1: X=0.92280000 Y=0.10659500 Z=0.83087000
      -1: X=0.07720000 Y=0.89340500 Z=0.33087000
Cu1        NPT=  781  R0=0.00005000 RMT= 2.05        Z: 29.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.39340500 Y=0.57720000 Z=0.16913000
          MULT= 4          ISPLIT= 8
      -2: X=0.60659500 Y=0.42280000 Z=0.66913000
```

```
     -2: X=0.42280000 Y=0.39340500 Z=0.91913000
     -2: X=0.57720000 Y=0.60659500 Z=0.41913000
 Cu2       NPT=  781  R0=0.00005000 RMT= 2.05       Z: 29.0
 LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                      0.0000000 1.0000000 0.0000000
                      0.0000000 0.0000000 1.0000000
 ATOM  -3: X=0.09476500 Y=0.59477000 Z=0.75000000
         MULT= 4         ISPLIT= 8
     -3: X=0.90523500 Y=0.40523000 Z=0.25000000
     -3: X=0.40523000 Y=0.09476500 Z=0.50000000
     -3: X=0.59477000 Y=0.90523500 Z=0.00000000
 Se1       NPT=  781  R0=0.00005000 RMT= 1.95       Z: 34.0
 LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                      0.0000000 1.0000000 0.0000000
                      0.0000000 0.0000000 1.0000000
   4     NUMBER OF SYMMETRY OPERATIONS
 -------------------------------------------------------------
 SCAN-EECE
 -------------------------------------------------------------
 Cu2Se_1
 P   LATTICE,NONEQUIV.ATOMS:  3 78 P43
 MODE OF CALC=RELA unit=bohr
  8.008700  8.008700 20.370100 90.000000 90.000000 90.000000
 ATOM  -1: X=0.10659500 Y=0.07720000 Z=0.08087000
         MULT= 4         ISPLIT= 8
     -1: X=0.89340500 Y=0.92280000 Z=0.58087000
     -1: X=0.92280000 Y=0.10659500 Z=0.83087000
     -1: X=0.07720000 Y=0.89340500 Z=0.33087000
 Cu1       NPT=  781  R0=0.00005000 RMT= 2.05       Z: 29.0
 LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                      0.0000000 1.0000000 0.0000000
                      0.0000000 0.0000000 1.0000000
 ATOM  -2: X=0.39340500 Y=0.57720000 Z=0.16913000
         MULT= 4         ISPLIT= 8
     -2: X=0.60659500 Y=0.42280000 Z=0.66913000
     -2: X=0.42280000 Y=0.39340500 Z=0.91913000
     -2: X=0.57720000 Y=0.60659500 Z=0.41913000
 Cu2       NPT=  781  R0=0.00005000 RMT= 2.05       Z: 29.0
 LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                      0.0000000 1.0000000 0.0000000
                      0.0000000 0.0000000 1.0000000
 ATOM  -3: X=0.09476500 Y=0.59477000 Z=0.75000000
         MULT= 4         ISPLIT= 8
     -3: X=0.90523500 Y=0.40523000 Z=0.25000000
     -3: X=0.40523000 Y=0.09476500 Z=0.50000000
     -3: X=0.59477000 Y=0.90523500 Z=0.00000000
 Se1       NPT=  781  R0=0.00005000 RMT= 1.95       Z: 34.0
 LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                      0.0000000 1.0000000 0.0000000
                      0.0000000 0.0000000 1.0000000
   4     NUMBER OF SYMMETRY OPERATIONS
 -------------------------------------------------------------
 SCAN
 -------------------------------------------------------------
 CuI_exp
   LATTICE,NONEQUIV.ATOMS:  2 216 F-43m
 MODE OF CALC=RELA unit=bohr
```

```
 11.322109 11.322109 11.322109 90.000000 90.000000 90.000000
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
        MULT= 1         ISPLIT= 2
Cu1       NPT=  781  R0=0.00005000 RMT= 2.07       Z: 29.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM   2: X=0.25000000 Y=0.25000000 Z=0.25000000
        MULT= 1         ISPLIT= 2
I 1       NPT=  781  R0=0.00001000 RMT= 2.07       Z: 53.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  24     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
CuI_exp
F   LATTICE,NONEQUIV.ATOMS:  2 216 F-43m
MODE OF CALC=RELA unit=bohr
 11.322109 11.322109 11.322109 90.000000 90.000000 90.000000
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
        MULT= 1         ISPLIT= 2
Cu1       NPT=  781  R0=0.00005000 RMT= 2.07       Z: 29.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM   2: X=0.25000000 Y=0.25000000 Z=0.25000000
        MULT= 1         ISPLIT= 2
I1        NPT=  781  R0=0.00001000 RMT= 2.07       Z: 53.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  24     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
CuI_0
P   LATTICE,NONEQUIV.ATOMS:  2 11 P21/m
MODE OF CALC=RELA unit=bohr
 12.425100  7.655000  7.668500 90.000000 90.000000 90.234084
ATOM  -1: X=0.00132000 Y=0.25566000 Z=0.25000000
        MULT= 2         ISPLIT= 8
     -1: X=0.99868000 Y=0.74434000 Z=0.75000000
Cu1       NPT=  781  R0=0.00005000 RMT= 2.07       Z: 29.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.25681000 Y=0.24729000 Z=0.75000000
        MULT= 2         ISPLIT= 8
     -2: X=0.74319000 Y=0.75271000 Z=0.25000000
I1        NPT=  781  R0=0.00001000 RMT= 2.07       Z: 53.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  4     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
```

```
SCAN-EECE
-------------------------------------------------------------
CuI_0
P   LATTICE,NONEQUIV.ATOMS:  2 11 P21/m
MODE OF CALC=RELA unit=bohr
 12.277300  7.723100  7.736300 90.000000 90.000000 90.234084
ATOM  -1: X=0.00132000 Y=0.25566000 Z=0.25000000
          MULT= 2          ISPLIT= 8
      -1: X=0.99868000 Y=0.74434000 Z=0.75000000
Cu1        NPT=  781  R0=0.00005000 RMT= 2.07        Z: 29.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.25681000 Y=0.24729000 Z=0.75000000
          MULT= 2          ISPLIT= 8
      -2: X=0.74319000 Y=0.75271000 Z=0.25000000
I 1        NPT=  781  R0=0.00001000 RMT= 2.07        Z: 53.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
   4     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
CuSe_exp
CXY LATTICE,NONEQUIV.ATOMS   4   63 Cmcm
MODE OF CALC=RELA unit=bohr
 7.472400 13.028200 32.838200 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.36700000 Z=0.75000000
          MULT= 2          ISPLIT= 8
      -1: X=0.00000000 Y=0.63300000 Z=0.25000000
Cu2+       NPT=  781  R0=.000050000 RMT= 1.92        Z:  29.00000
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
ATOM  -2: X=0.00000000 Y=0.34200000 Z=0.10620000
          MULT= 4          ISPLIT= 8
      -2: X=0.00000000 Y=0.65800000 Z=0.89380000
      -2: X=0.00000000 Y=0.34200000 Z=0.39380000
      -2: X=0.00000000 Y=0.65800000 Z=0.60620000
Cu1+       NPT=  781  R0=.000050000 RMT= 1.92        Z:  29.00000
LOCAL ROT MATRIX:    0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
ATOM  -3: X=0.00000000 Y=0.30500000 Z=0.25000000
          MULT= 2          ISPLIT= 8
      -3: X=0.00000000 Y=0.69500000 Z=0.75000000
Se2-       NPT=  781  R0=.000050000 RMT= 1.83        Z:  34.00000
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
ATOM  -4: X=0.00000000 Y=0.00500000 Z=0.06800000
          MULT= 4          ISPLIT= 8
      -4: X=0.00000000 Y=0.99500000 Z=0.93200000
      -4: X=0.00000000 Y=0.00500000 Z=0.43200000
      -4: X=0.00000000 Y=0.99500000 Z=0.56800000
Se1-       NPT=  781  R0=.000050000 RMT= 1.83        Z:  34.00000
```

```
LOCAL ROT MATRIX:    0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
CuSe_exp
CXY LATTICE,NONEQUIV.ATOMS   4   63 Cmcm
MODE OF CALC=RELA unit=bohr
  7.485300 13.056600 32.755900 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.36700000 Z=0.75000000
          MULT= 2          ISPLIT= 8
     -1: X=0.00000000 Y=0.63300000 Z=0.25000000
Cu2+       NPT=  781  R0=.000050000 RMT= 1.92        Z:  29.00000
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
ATOM  -2: X=0.00000000 Y=0.34200000 Z=0.10620000
          MULT= 4          ISPLIT= 8
     -2: X=0.00000000 Y=0.65800000 Z=0.89380000
     -2: X=0.00000000 Y=0.34200000 Z=0.39380000
     -2: X=0.00000000 Y=0.65800000 Z=0.60620000
Cu1+       NPT=  781  R0=.000050000 RMT= 1.92        Z:  29.00000
LOCAL ROT MATRIX:    0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
ATOM  -3: X=0.00000000 Y=0.30500000 Z=0.25000000
          MULT= 2          ISPLIT= 8
     -3: X=0.00000000 Y=0.69500000 Z=0.75000000
Se2-       NPT=  781  R0=.000050000 RMT= 1.83        Z:  34.00000
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
ATOM  -4: X=0.00000000 Y=0.00500000 Z=0.06800000
          MULT= 4          ISPLIT= 8
     -4: X=0.00000000 Y=0.99500000 Z=0.93200000
     -4: X=0.00000000 Y=0.00500000 Z=0.43200000
     -4: X=0.00000000 Y=0.99500000 Z=0.56800000
Se1-       NPT=  781  R0=.000050000 RMT= 1.83        Z:  34.00000
LOCAL ROT MATRIX:    0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
CuSe_0
F   LATTICE,NONEQUIV.ATOMS:  2 216 F-43m
MODE OF CALC=RELA unit=bohr
 10.243956 10.243956 10.243956 90.000000 90.000000 90.000000
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
Cu1        NPT=  781  R0=0.00005000 RMT= 1.92        Z: 29.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
```

```
ATOM   2: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 1          ISPLIT= 2
Se1       NPT=  781  R0=0.00005000 RMT= 1.83       Z: 34.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  24     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
CuSe_0
F   LATTICE,NONEQUIV.ATOMS:  2 216 F-43m
MODE OF CALC=RELA unit=bohr
 10.243956 10.243956 10.243956 90.000000 90.000000 90.000000
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
Cu1       NPT=  781  R0=0.00005000 RMT= 1.92       Z: 29.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM   2: X=0.25000000 Y=0.25000000 Z=0.25000000
          MULT= 1          ISPLIT= 2
Se1       NPT=  781  R0=0.00005000 RMT= 1.83       Z: 34.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  24     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
LaN_exp
F   LATTICE,NONEQUIV.ATOMS:  2 225 Fm-3m
MODE OF CALC=RELA unit=bohr
 9.997515  9.997515  9.997515 90.000000 90.000000 90.000000
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
La1       NPT=  781  R0=0.00001000 RMT= 2.26       Z: 57.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM   2: X=0.50000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
N 1       NPT=  781  R0=0.00010000 RMT= 1.85       Z:  7.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  48     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
LaN_exp
F   LATTICE,NONEQUIV.ATOMS:  2 225 Fm-3m
MODE OF CALC=RELA unit=bohr
10.063726 10.063726 10.063726 90.000000 90.000000 90.000000
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
La1       NPT=  781  R0=0.00001000 RMT= 2.26       Z: 57.0
```

```
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM   2: X=0.50000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
N 1       NPT=  781  R0=0.00010000 RMT= 1.85       Z:  7.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  48     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
LaN_0
P   LATTICE,NONEQUIV.ATOMS:  2 59 Pmmn
MODE OF CALC=RELA unit=bohr
  7.122900  9.962100  7.117400 90.000000 90.000000 90.000000
ATOM  -1: X=0.25000000 Y=0.25000000 Z=0.24162584
          MULT= 2          ISPLIT= 8
     -1: X=0.75000000 Y=0.75000000 Z=0.75837416
La1       NPT=  781  R0=0.00001000 RMT= 2.26       Z: 57.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.25000000 Y=0.75000000 Z=0.20478952
          MULT= 2          ISPLIT= 8
     -2: X=0.75000000 Y=0.25000000 Z=0.79521048
N 1       NPT=  781  R0=0.00010000 RMT= 1.85       Z:  7.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
LaN_0
P   LATTICE,NONEQUIV.ATOMS:  2 59 Pmmn
MODE OF CALC=RELA unit=bohr
  7.155000  9.998800  7.140500 90.000000 90.000000 90.000000
ATOM  -1: X=0.25000000 Y=0.25000000 Z=0.24162584
          MULT= 2          ISPLIT= 8
     -1: X=0.75000000 Y=0.75000000 Z=0.75837416
La1       NPT=  781  R0=0.00001000 RMT= 2.26       Z: 57.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.25000000 Y=0.75000000 Z=0.20478952
          MULT= 2          ISPLIT= 8
     -2: X=0.75000000 Y=0.25000000 Z=0.79521048
N 1       NPT=  781  R0=0.00010000 RMT= 1.85       Z:  7.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
CAN
-------------------------------------------------------------
```

```
MnS_exp
F   LATTICE,NONEQUIV.ATOMS   2  225 Fm-3m
MODE OF CALC=RELA unit=bohr
  9.929699  9.929699  9.929699 90.000000 90.000000 90.000000
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
Mn2+       NPT=  781  R0=.000050000 RMT= 2.17        Z:  25.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM   2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 2
S 2-       NPT=  781  R0=.000100000 RMT= 1.86        Z:  16.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  48     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
MnS_exp
F   LATTICE,NONEQUIV.ATOMS   2  225 Fm-3m
MODE OF CALC=RELA unit=bohr
  9.929699  9.929699  9.929699 90.000000 90.000000 90.000000
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
Mn2+       NPT=  781  R0=.000050000 RMT= 2.17        Z:  25.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM   2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 2
S 2-       NPT=  781  R0=.000100000 RMT= 1.86        Z:  16.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  48     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
MnS_0
B   LATTICE,NONEQUIV.ATOMS:  2 119 I-4m2
MODE OF CALC=RELA unit=bohr
  7.571000  7.571000 10.722300 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Mn1        NPT=  781  R0=0.00005000 RMT= 2.17        Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 1          ISPLIT=-2
S 1        NPT=  781  R0=0.00010000 RMT= 1.86        Z: 16.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
   8     NUMBER OF SYMMETRY OPERATIONS
```

```
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
MnS_0
B   LATTICE,NONEQUIV.ATOMS:  2 119 I-4m2
MODE OF CALC=RELA unit=bohr
  7.623200  7.623200 10.771200 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Mn1       NPT=  781  R0=0.00005000 RMT= 2.17        Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 1          ISPLIT=-2
S 1       NPT=  781  R0=0.00010000 RMT= 1.86        Z: 16.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
   8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
MnS_1
P                    4
          RELA
 7.545900  7.574600 12.290300 90.000000 90.000000120.299992
ATOM  -1: X=0.16328000 Y=0.33131000 Z=0.50000000
          MULT= 1          ISPLIT= 8
Mn1       NPT=  781  R0=0.00005000 RMT=    2.1700   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.83672000 Y=0.66869000 Z=0.00000000
          MULT= 1          ISPLIT= 8
Mn2       NPT=  781  R0=0.00005000 RMT=    2.1700   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.16752000 Y=0.33423667 Z=0.87500000
          MULT= 1          ISPLIT= 8
S 3       NPT=  781  R0=0.00010000 RMT=    1.8600   Z: 16.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -4: X=0.83333334 Y=0.66671667 Z=0.37500000
          MULT= 1          ISPLIT= 8
S 4       NPT=  781  R0=0.00010000 RMT=    1.8600   Z: 16.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  1     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
MnS_1
P                    4
```

```
          RELA
  7.628900  7.656800 12.427600 90.000000 90.000000120.299992
ATOM  -1: X=0.16328000 Y=0.33131000 Z=0.50000000
        MULT= 1         ISPLIT= 8
Mn1       NPT=  781  R0=0.00005000 RMT=    2.1700   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.83672000 Y=0.66869000 Z=0.00000000
        MULT= 1         ISPLIT= 8
Mn2       NPT=  781  R0=0.00005000 RMT=    2.1700   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.16752000 Y=0.33423667 Z=0.87500000
        MULT= 1         ISPLIT= 8
S 3       NPT=  781  R0=0.00010000 RMT=    1.8600   Z: 16.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -4: X=0.83333334 Y=0.66671667 Z=0.37500000
        MULT= 1         ISPLIT= 8
S 4       NPT=  781  R0=0.00010000 RMT=    1.8600   Z: 16.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
   1     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
MnSe_exp
P   LATTICE,NONEQUIV.ATOMS   2  225 Fm-3m
MODE OF CALC=RELA unit=bohr
 10.390042 10.390042 10.390042 90.000000 90.000000 90.000000
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
        MULT= 1         ISPLIT= 2
Mn2+      NPT=  781  R0=.000050000 RMT= 2.18       Z:  25.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM   2: X=0.50000000 Y=0.50000000 Z=0.50000000
        MULT= 1         ISPLIT= 2
Se2-      NPT=  781  R0=.000050000 RMT= 2.07       Z:  34.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  48     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
MnSe_exp
P   LATTICE,NONEQUIV.ATOMS   2  225 Fm-3m
MODE OF CALC=RELA unit=bohr
 10.390042 10.390042 10.390042 90.000000 90.000000 90.000000
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
        MULT= 1         ISPLIT= 2
Mn2+      NPT=  781  R0=.000050000 RMT= 2.18       Z:  25.00000
```

```
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM   2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 2
Se2-       NPT=  781  R0=.000050000 RMT= 2.07        Z:  34.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  48     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
MnSe_0
B   LATTICE,NONEQUIV.ATOMS:  2 119 I-4m2
MODE OF CALC=RELA unit=bohr
  7.930500  7.930500 11.189500 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Mn1        NPT=  781  R0=0.00005000 RMT= 2.18        Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 1          ISPLIT=-2
Se1        NPT=  781  R0=0.00005000 RMT= 2.07        Z: 34.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
   8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
MnSe_0
B   LATTICE,NONEQUIV.ATOMS:  2 119 I-4m2
MODE OF CALC=RELA unit=bohr
  7.988500  7.988500 11.277400 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
Mn1        NPT=  781  R0=0.00005000 RMT= 2.18        Z: 25.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 1          ISPLIT=-2
Se1        NPT=  781  R0=0.00005000 RMT= 2.07        Z: 34.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
   8     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
MnSe_1
                     4
          RELA
  7.887800  7.870900 12.893100 90.000000 90.000000119.438591
```

```
ATOM  -1: X=0.16541500 Y=0.33133500 Z=0.50024000
          MULT= 1         ISPLIT= 8
Mn1       NPT=  781  R0=0.00005000 RMT=    2.1800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.83458500 Y=0.66866500 Z=0.00000000
          MULT= 1         ISPLIT= 8
Mn2       NPT=  781  R0=0.00005000 RMT=    2.1800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.16977500 Y=0.33527500 Z=0.12548000
          MULT= 1         ISPLIT= 8
Se3       NPT=  781  R0=0.00005000 RMT=    2.0700   Z: 34.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -4: X=0.83022500 Y=0.66472500 Z=0.62548000
          MULT= 1         ISPLIT= 8
Se4       NPT=  781  R0=0.00005000 RMT=    2.0700   Z: 34.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  1     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
MnSe_1
P                   4
          RELA
 7.974700  7.957100 13.041700 90.000000 90.000000119.438591
ATOM  -1: X=0.16541500 Y=0.33133500 Z=0.50024000
          MULT= 1         ISPLIT= 8
Mn1       NPT=  781  R0=0.00005000 RMT=    2.1800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.83458500 Y=0.66866500 Z=0.00000000
          MULT= 1         ISPLIT= 8
Mn2       NPT=  781  R0=0.00005000 RMT=    2.1800   Z: 25.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.16977500 Y=0.33527500 Z=0.12548000
          MULT= 1         ISPLIT= 8
Se3       NPT=  781  R0=0.00005000 RMT=    2.0700   Z: 34.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -4: X=0.83022500 Y=0.66472500 Z=0.62548000
          MULT= 1         ISPLIT= 8
Se4       NPT=  781  R0=0.00005000 RMT=    2.0700   Z: 34.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  1     NUMBER OF SYMMETRY OPERATIONS
```

```
------------------------------------------------------------
SCAN
------------------------------------------------------------
MoAs_exp
P   LATTICE,NONEQUIV.ATOMS:  2 62 Pnma
MODE OF CALC=RELA unit=bohr
 11.315700  6.328800 12.034400 90.000000 90.000000 90.000000
ATOM  -1: X=0.98550000 Y=0.25000000 Z=0.18162000
          MULT= 4          ISPLIT= 8
     -1: X=0.51450000 Y=0.75000000 Z=0.68162000
     -1: X=0.01450000 Y=0.75000000 Z=0.81838000
     -1: X=0.48550000 Y=0.25000000 Z=0.31838000
Mo1       NPT=  781  R0=0.00001000 RMT= 2.14       Z: 42.0
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
ATOM  -2: X=0.81500000 Y=0.25000000 Z=0.56851000
          MULT= 4          ISPLIT= 8
     -2: X=0.68500000 Y=0.75000000 Z=0.06851000
     -2: X=0.18500000 Y=0.75000000 Z=0.43149000
     -2: X=0.31500000 Y=0.25000000 Z=0.93149000
As1       NPT=  781  R0=0.00005000 RMT= 2.14       Z: 33.0
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
------------------------------------------------------------
SCAN-EECE
------------------------------------------------------------
MoAs_exp
P   LATTICE,NONEQUIV.ATOMS:  2 62 Pnma
MODE OF CALC=RELA unit=bohr
 11.397600  6.371700 12.064800 90.000000 90.000000 90.000000
ATOM  -1: X=0.98550000 Y=0.25000000 Z=0.18162000
          MULT= 4          ISPLIT= 8
     -1: X=0.51450000 Y=0.75000000 Z=0.68162000
     -1: X=0.01450000 Y=0.75000000 Z=0.81838000
     -1: X=0.48550000 Y=0.25000000 Z=0.31838000
Mo1       NPT=  781  R0=0.00001000 RMT= 2.14       Z: 42.0
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
ATOM  -2: X=0.81500000 Y=0.25000000 Z=0.56851000
          MULT= 4          ISPLIT= 8
     -2: X=0.68500000 Y=0.75000000 Z=0.06851000
     -2: X=0.18500000 Y=0.75000000 Z=0.43149000
     -2: X=0.31500000 Y=0.25000000 Z=0.93149000
As1       NPT=  781  R0=0.00005000 RMT= 2.14       Z: 33.0
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
  8     NUMBER OF SYMMETRY OPERATIONS
------------------------------------------------------------
SCAN
------------------------------------------------------------
MoAs_0
H   LATTICE,NONEQUIV.ATOMS:  2 187 P-6m2
```

```
MODE OF CALC=RELA unit=bohr
  6.280600  6.280600  6.268200 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Mo1       NPT=  781  R0=0.00001000 RMT= 2.14       Z: 42.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.33333333 Y=0.66666667 Z=0.50000000
          MULT= 1          ISPLIT= 4
As1       NPT=  781  R0=0.00005000 RMT= 2.14       Z: 33.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
MoAs_0
H   LATTICE,NONEQUIV.ATOMS:  2 187 P-6m2
MODE OF CALC=RELA unit=bohr
  6.307600  6.307600  6.323000 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Mo1       NPT=  781  R0=0.00001000 RMT= 2.14       Z: 42.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.33333333 Y=0.66666667 Z=0.50000000
          MULT= 1          ISPLIT= 4
As1       NPT=  781  R0=0.00005000 RMT= 2.14       Z: 33.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
NbN_exp
H   LATTICE,NONEQUIV.ATOMS:  2 194 P63/mmc
MODE OF CALC=RELA unit=bohr
  5.609900  5.609900 10.534200 90.000000 90.000000120.000000
ATOM  -1: X=0.33333333 Y=0.66666667 Z=0.75000000
          MULT= 2          ISPLIT= 4
            -1: X=0.66666667 Y=0.33333333 Z=0.25000000
Nb1       NPT=  781  R0=0.00001000 RMT= 2.02       Z: 41.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.00000000 Y=0.00000000 Z=0.50000000
          MULT= 2          ISPLIT= 4
            -2: X=0.00000000 Y=0.00000000 Z=0.00000000
N  1      NPT=  781  R0=0.00010000 RMT= 1.74       Z:  7.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  24     NUMBER OF SYMMETRY OPERATIONS
```

```
------------------------------------------------------------
SCAN-EECE
------------------------------------------------------------
NbN_exp
H   LATTICE,NONEQUIV.ATOMS:  2 194 P63/mmc
MODE OF CALC=RELA unit=bohr
  5.635100  5.635100 10.605100 90.000000 90.000000120.000000
ATOM  -1: X=0.33333333 Y=0.66666667 Z=0.75000000
          MULT= 2          ISPLIT= 4
     -1: X=0.66666667 Y=0.33333333 Z=0.25000000
Nb1       NPT=  781  R0=0.00001000 RMT= 2.02       Z: 41.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.00000000 Y=0.00000000 Z=0.50000000
          MULT= 2          ISPLIT= 4
     -2: X=0.00000000 Y=0.00000000 Z=0.00000000
N 1       NPT=  781  R0=0.00010000 RMT= 1.74       Z:  7.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  24     NUMBER OF SYMMETRY OPERATIONS
------------------------------------------------------------
SCAN
------------------------------------------------------------
NbN_0
H   LATTICE,NONEQUIV.ATOMS:  2 187 P-6m2
MODE OF CALC=RELA unit=bohr
  5.576700  5.576700  5.434800 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Nb1       NPT=  781  R0=0.00001000 RMT= 2.02       Z: 41.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.33333333 Y=0.66666667 Z=0.50000000
          MULT= 1          ISPLIT= 4
N 1       NPT=  781  R0=0.00010000 RMT= 1.74       Z:  7.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
------------------------------------------------------------
SCAN-EECE
------------------------------------------------------------
NbN_0
H   LATTICE,NONEQUIV.ATOMS:  2 187 P-6m2
MODE OF CALC=RELA unit=bohr
  5.601300  5.601300  5.474500 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Nb1       NPT=  781  R0=0.00001000 RMT= 2.02       Z: 41.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.33333333 Y=0.66666667 Z=0.50000000
          MULT= 1          ISPLIT= 4
```

```
N 1       NPT=  781  R0=0.00010000 RMT= 1.74       Z:  7.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
NbN_1
H   LATTICE,NONEQUIV.ATOMS:  2 187 P-6m2
MODE OF CALC=RELA unit=bohr
  5.576700  5.576700  5.434800 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Nb1       NPT=  781  R0=0.00001000 RMT= 2.02       Z: 41.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.33333333 Y=0.66666667 Z=0.50000000
          MULT= 1          ISPLIT= 4
N 1       NPT=  781  R0=0.00010000 RMT= 1.74       Z:  7.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
NbN_1
H   LATTICE,NONEQUIV.ATOMS:  2 187 P-6m2
MODE OF CALC=RELA unit=bohr
  5.601300  5.601300  5.474500 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Nb1       NPT=  781  R0=0.00001000 RMT= 2.02       Z: 41.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.33333333 Y=0.66666667 Z=0.50000000
          MULT= 1          ISPLIT= 4
N 1       NPT=  781  R0=0.00010000 RMT= 1.74       Z:  7.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
PtO_exp
P   LATTICE,NONEQUIV.ATOMS:  2 131 P42/mmc
MODE OF CALC=RELA unit=bohr
  5.865900  5.865900  9.994400 90.000000 90.000000 90.000000
ATOM  -1: X=0.50000000 Y=0.00000000 Z=0.50000000
          MULT= 2          ISPLIT= 8
            -1: X=0.00000000 Y=0.50000000 Z=0.00000000
Pt1       NPT=  781  R0=0.00000500 RMT= 1.84       Z: 78.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
```

```
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT=-2
     -2: X=0.50000000 Y=0.50000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.51       Z:  8.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
  16     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
PtO_exp
P   LATTICE,NONEQUIV.ATOMS:  2 131 P42/mmc
MODE OF CALC=RELA unit=bohr
  5.888300  5.888300  9.953700 90.000000 90.000000 90.000000
ATOM  -1: X=0.50000000 Y=0.00000000 Z=0.50000000
          MULT= 2          ISPLIT= 8
     -1: X=0.00000000 Y=0.50000000 Z=0.00000000
Pt1       NPT=  781  R0=0.00000500 RMT= 1.84       Z: 78.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT=-2
     -2: X=0.50000000 Y=0.50000000 Z=0.75000000
O 1       NPT=  781  R0=0.00010000 RMT= 1.51       Z:  8.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                0.7071068 0.7071068 0.0000000
                0.0000000 0.0000000 1.0000000
  16     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
PtO_0
P   LATTICE,NONEQUIV.ATOMS:  2 62 Pnma
MODE OF CALC=RELA unit=bohr
 12.776000  6.349800  7.984800 90.000000 90.000000 90.000000
ATOM  -1: X=0.43145000 Y=0.25000000 Z=0.19192000
          MULT= 4          ISPLIT= 8
     -1: X=0.06855000 Y=0.75000000 Z=0.69192000
     -1: X=0.56855000 Y=0.75000000 Z=0.80808000
     -1: X=0.93145000 Y=0.25000000 Z=0.30808000
Pt1       NPT=  781  R0=0.00000500 RMT= 1.84       Z: 78.0
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
                1.0000000 0.0000000 0.0000000
ATOM  -2: X=0.66440000 Y=0.25000000 Z=0.50144000
          MULT= 4          ISPLIT= 8
     -2: X=0.83560000 Y=0.75000000 Z=0.00144000
     -2: X=0.33560000 Y=0.75000000 Z=0.49856000
     -2: X=0.16440000 Y=0.25000000 Z=0.99856000
O 1       NPT=  781  R0=0.00010000 RMT= 1.51       Z:  8.0
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                0.0000000 0.0000000 1.0000000
                1.0000000 0.0000000 0.0000000
```

```
  8      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
PtO_0
P   LATTICE,NONEQUIV.ATOMS:  2 62 Pnma
MODE OF CALC=RELA unit=bohr
 12.808300  6.354600  7.987500 90.000000 90.000000 90.000000
ATOM  -1: X=0.43145000 Y=0.25000000 Z=0.19192000
          MULT= 4          ISPLIT= 8
     -1: X=0.06855000 Y=0.75000000 Z=0.69192000
     -1: X=0.56855000 Y=0.75000000 Z=0.80808000
     -1: X=0.93145000 Y=0.25000000 Z=0.30808000
Pt1       NPT=  781  R0=0.00000500 RMT= 1.84       Z: 78.0
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
ATOM  -2: X=0.66440000 Y=0.25000000 Z=0.50144000
          MULT= 4          ISPLIT= 8
     -2: X=0.83560000 Y=0.75000000 Z=0.00144000
     -2: X=0.33560000 Y=0.75000000 Z=0.49856000
     -2: X=0.16440000 Y=0.25000000 Z=0.99856000
O 1       NPT=  781  R0=0.00010000 RMT= 1.51       Z:  8.0
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
  8      NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
TiS_exp
R   LATTICE,NONEQUIV.ATOMS:  4 166 R-3m
MODE OF CALC=RELA unit=bohr
 6.514200  6.514200 49.984700 90.000000 90.000000120.000000
ATOM  -1: X=0.11877000 Y=0.11877000 Z=0.11877000
          MULT= 2          ISPLIT= 4
     -1: X=0.88123000 Y=0.88123000 Z=0.88123000
Ti1       NPT=  781  R0=0.00005000 RMT= 2.09       Z: 22.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Ti2       NPT=  781  R0=0.00005000 RMT= 2.09       Z: 22.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
S 1       NPT=  781  R0=0.00010000 RMT= 1.89       Z: 16.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -4: X=0.27656000 Y=0.27656000 Z=0.27656000
          MULT= 2          ISPLIT= 4
     -4: X=0.72344000 Y=0.72344000 Z=0.72344000
S 2       NPT=  781  R0=0.00010000 RMT= 1.89       Z: 16.0
```

```
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
TiS_exp
R   LATTICE,NONEQUIV.ATOMS:  4 166 R-3m
MODE OF CALC=RELA unit=bohr
  6.536700  6.536700 50.395000 90.000000 90.000000120.000000
ATOM  -1: X=0.11877000 Y=0.11877000 Z=0.11877000
          MULT= 2          ISPLIT= 4
     -1: X=0.88123000 Y=0.88123000 Z=0.88123000
Ti1       NPT=  781  R0=0.00005000 RMT= 2.09        Z: 22.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Ti2       NPT=  781  R0=0.00005000 RMT= 2.09        Z: 22.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 4
S 1       NPT=  781  R0=0.00010000 RMT= 1.89        Z: 16.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -4: X=0.27656000 Y=0.27656000 Z=0.27656000
          MULT= 2          ISPLIT= 4
     -4: X=0.72344000 Y=0.72344000 Z=0.72344000
S 2       NPT=  781  R0=0.00010000 RMT= 1.89        Z: 16.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
TiS_0
H   LATTICE,NONEQUIV.ATOMS:  2 187 P-6m2
MODE OF CALC=RELA unit=bohr
  6.162300  6.162300  6.064000 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Ti1       NPT=  781  R0=0.00005000 RMT= 2.09        Z: 22.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.66666666 Y=0.33333334 Z=0.50000000
          MULT= 1          ISPLIT= 4
S 1       NPT=  781  R0=0.00010000 RMT= 1.89        Z: 16.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
```

```
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
TiS_0
H   LATTICE,NONEQUIV.ATOMS:  2 187 P-6m2
MODE OF CALC=RELA unit=bohr
  6.183300  6.183300  6.117500 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Ti1       NPT=  781  R0=0.00005000 RMT= 2.09       Z: 22.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.66666666 Y=0.33333334 Z=0.50000000
          MULT= 1          ISPLIT= 4
S 1       NPT=  781  R0=0.00010000 RMT= 1.89       Z: 16.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
TiS_1
H   LATTICE,NONEQUIV.ATOMS:  2 187 P-6m2
MODE OF CALC=RELA unit=bohr
  6.162200  6.162200  6.064000 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Ti1       NPT=  781  R0=0.00005000 RMT= 2.09       Z: 22.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.33333333 Y=0.66666667 Z=0.50000000
          MULT= 1          ISPLIT= 4
S 1       NPT=  781  R0=0.00010000 RMT= 1.89       Z: 16.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
TiS_1
H   LATTICE,NONEQUIV.ATOMS:  2 187 P-6m2
MODE OF CALC=RELA unit=bohr
  6.183300  6.183300  6.117400 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Ti1       NPT=  781  R0=0.00005000 RMT= 2.09       Z: 22.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.33333333 Y=0.66666667 Z=0.50000000
          MULT= 1          ISPLIT= 4
S 1       NPT=  781  R0=0.00010000 RMT= 1.89       Z: 16.0
```

```
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN
-------------------------------------------------------------
TiS_5
H   LATTICE,NONEQUIV.ATOMS:  2 194 P63/mmc
MODE OF CALC=RELA unit=bohr
  6.154800  6.154800 12.143300 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.50000000
          MULT= 2          ISPLIT= 4
      -1: X=0.00000000 Y=0.00000000 Z=0.00000000
Ti1       NPT=  781  R0=0.00005000 RMT= 2.09        Z: 22.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.33333333 Y=0.66666667 Z=0.75000000
          MULT= 2          ISPLIT= 4
      -2: X=0.66666667 Y=0.33333333 Z=0.25000000
S 1       NPT=  781  R0=0.00010000 RMT= 1.89        Z: 16.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  24     NUMBER OF SYMMETRY OPERATIONS
-------------------------------------------------------------
SCAN-EECE
-------------------------------------------------------------
TiS_5
H   LATTICE,NONEQUIV.ATOMS:  2 194 P63/mmc
MODE OF CALC=RELA unit=bohr
  6.154900  6.154900 12.315100 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.50000000
          MULT= 2          ISPLIT= 4
      -1: X=0.00000000 Y=0.00000000 Z=0.00000000
Ti1       NPT=  781  R0=0.00005000 RMT= 2.09        Z: 22.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.33333333 Y=0.66666667 Z=0.75000000
          MULT= 2          ISPLIT= 4
      -2: X=0.66666667 Y=0.33333333 Z=0.25000000
S 1       NPT=  781  R0=0.00010000 RMT= 1.89        Z: 16.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  24     NUMBER OF SYMMETRY OPERATIONS
```