One- and two-dimensional search of an equation of state using a newly released 2DRoptimize package

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ABSTRACT

A new package called 2DRoptimize has been released for performing two-dimensional searches of the equation of state (EOS) for rhombohedral, tetragonal, and hexagonal compounds. The package is compatible and available with the WIEN2k package. The 2DRoptimize package performs a convenient volume and **c/a** structure optimization. First, the package finds the best value for **c/a** and the associated energy for each volume. In the second step, it calculates the EoS. The package then finds the equation of the **c/a** ratio vs. volume to calculate the **c/a** ratio at the optimized volume. In the last stage, by using the optimized volume and **c/a** ratio, the 2DRoptimize package calculates **a** and **c** lattice constants for tetragonal and hexagonal compounds, as well as the **a** lattice constant with the **α** angle for rhombohedral compounds. We tested our new package based on several hexagonal, tetragonal, and rhombohedral structures, and the 2D search results for the EOS showed that this method is more accurate than 1D search. Our results agreed very well with the experimental data and they were better than previous theoretical calculations.

1. Introduction

The rapid increase in computational power motivated us to improve the method used for obtaining the equation of state (EOS) for compounds with two degrees of freedom, i.e., tetragonal, hexagonal, and rhombohedral (THR) symmetries (changes in volume and **c/a** ratio). One of the methods for obtaining the EOS for THR compounds involves calculating the EOS based on changes in volume at a constant **c/a** ratio (one-dimensional (1D) search of the EOS). However, the accuracy of the results obtained is inadequate if we do not find the minimum of the **c/a** and the associated energy for each volume in order to obtain the correct EOS. Using the new 2DRoptimize package [1], we aim to perform structural optimization by changing both the volume and **c/a**, i.e., our package first finds the minimum values of **c/a** and the associated energy for each volume, which are then used for obtaining the EOS. Thus, if we try to improve the method for obtaining the EOS for compounds with more than one degree of freedom, such as THR symmetries, we can improve the determination of the lattice parameters, which is a first step toward predicting important properties such as the electronic, optical, and magnetic properties according to the theoretical framework employed (density functional theory (DFT) in this case) [2,3]. It has been proved that DFT is one of the most accurate methods for computing the electronic structures of solids [4–6], especially when using the highly accurate all-electron full-potential (linearized) augmented plane-wave plus local orbital [FP-(L)APW+lo] method. We refer to the new package for two-dimensional (2D) search of the EOS as 2DRoptimize. The results obtained by 2D search of the EOS are better than those produced by 1D search of the EOS. In addition, the accuracy of the calculation is increased compared with 1D search. In our previous study [7], we calculated the cell parameters and bulk modulus (B) for hexagonal MnAs and Mg structure compounds using the old version of this package (2Doptimize) [8], which only supports hexagonal and tetragonal structures. In this study, we performed a detailed comparison of the results obtained based on 1D and 2D searches of the EOS for THR compounds.

2. 2D search

The 2DRoptimize [1] package performs a convenient volume and **c/a** structure optimization for THR compounds. Therefore, several self-consistent calculations are required to obtain the optimized lattice parameters (**a** and **c**). In this package, for each volume, we first select different sets of **c/a** and using the following equation:

$$E = E_0 + a_1 x + \ldots\ldots + a_n x^n \quad n = 2, 3, 4, \tag{1}$$

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where n and x represent the order of fitting and the c/a ratio, respectively, the package finds the best **c/a** ratio for each corresponding volume such that the energy has the minimum value and the best order of fitting. In the next step, we have a set of energies and volumes at the optimized **c/a** ratios, and by using the EOSs supported in the package, i.e., EOS2, Murnaghan, and Brich–Murnaghan, the minimum of the total energy and the equilibrium volume are calculated. Next, in order to find the **c/a** ratio at the equilibrium volume, the 2DRoptimize package fits the optimized **c/a** ratios for each volume according to the polynomial:

$$coa(v) = b_0 + b_1 v + \ldots\ldots + b_n v^n \quad n = 2, 3, 4, \tag{2}$$

where coa and v denote the optimized **c/a** ratio for the volume used and the optimized volume, respectively. Using the resulting fit based on equation (2), the 2DRoptimize package calculates the optimized **c/a** ratio at the optimized volume.

In the last stage, using the optimized volume and **c/a** ratio, the 2DRoptimize package calculates the lattice constants **a** and **c** for tetragonal and hexagonal compounds, and the lattice constant **a** with the **α** angle for rhombohedral compounds. The package then checks the sensitivity of the results to the order of fitting by obtaining the equation of **c/a** vs. volume. The 2DRoptimize package converts the calculated **a** and **c** lattice parameters into rhombohedral specifications using the following equations.

$$\alpha_r = 2 \text{Arcsin}(9a^2/(4c^2 + 12a^2))^{0.5} \tag{3}$$

$$a_r = (a/2)\sin(\alpha_r/2) \tag{4}$$

The best strategy involves selecting only 3×3 points and more points can be added in the next step if necessary to check the sensitivity of the results to the order of fitting in equations (1) and (2). If we need to specify the old volume and **c/a** ratio, then these results will be considered automatically without recalculation. Moreover, the 2DRoptimize package allows us to leave out the points that are very far from the minimum (i.e., a volume with different values of **c/a**).

It should be noted that during the calculation of the EOS for THR compounds using 1D search (changes the volume at a constant **c/a** ratio), we must use the same **c/a** ratio for all of the volume changes, whereas the 2D search of the EOS finds the best value of the **c/a** ratio for each value of the volume changes. This is one of the most important features of the new package.

We performed several calculations to test the results obtained by 2D search of the EOS using the 2DRoptimize package. Table 1 shows the relative errors (as percentages) for the **c/a** ratio used in 2D and 1D searches of the EOS. These relative errors with respect to the **c/a** ratio were used in 1D search of the EOS for different percentage volume changes by the tetragonal MnO_2 and SnO_2 compounds using the 2DRoptimize package within Perdew, Burke and Ernzerhof Generalized gradient approximation (PBE) [9]. According to Table 1, the results obtained by 2D search of the EOS using the 2DRoptimize package could be important, and they may be a source of error between the 1D and 2D searches of the EOS. However, these errors may be negligible in some cases, so we performed several tests to assess this hypothesis. For example, we performed 1D and 2D searches of the EOS for Y and Sc within the PBE functional. The results and the experimental data [10] are presented in Table 2. Table 2 shows that the effect of 2D search of the EOS using the 2DRoptimize package is important, where the accuracy of this method is better than that of 1D search of the EOS. Furthermore, we

Table 1
Relative error (percentage) in the c/a ratio when used in 2D and 1D searches of the EOS relative to the c/a ratio used for 1D search of EOS for different percentage volume changes for tetragonal MnO_2 and SnO_2 within the PBE.

Volume change, percentage	−10	−5	0	5	10
MnO_2	0.63	0.08	−0.63	−1.41	−2.37
SnO_2	2.75	1.55	0.40	−0.86	−2.35

Table 2
Effects of 1D and 2D searches of EOS on the optimized values of hexagonal Y and Sc compounds within the PBE.

	V (bohr^3)	B (GPa)	B′	E (Ryd)
Y_{1D}	443.6371	40.73	2.90	−13542.8590
Y_{2D}	443.6268	40.93	3.00	−13542.8591
Exp[a]	446.4639	37		
Sc_{1D}	332.3874	55.20	2.48	−3056.9046
Sc_{2D}	332.2953	54.45	2.05	−3056.9047
Exp[a]	337.8289	44		

[a] Ref. [10].

Table 3
Effects of 1D and 2D searches of EOS on the optimized values and pressure of the induced-phase transition for the CdTe compound within the PBE.

CdTe	V (bohr^3/atom)	B (GPa)	B′	E (Ryd/atom)	P (GPa)
1D search	245.6168	35.21	4.41	−12392.896945	11.4
2D search	245.6107	35.25	4.36	−12392.896949	10.6

performed another test related to the pressure of the induced phase transition of the CdTe compound from cubic to hexagonal phases within the PBE, and the results are given in Table 3. According to Table 3, the effect of 2D search of the EOS for the hexagonal phase of the CdTe compound is negligible, but the 2D search of the EOS predicts that the pressure of the induced phase transition is around 0.8 (GPa) lower than that obtained by the 1D search of the EOS for the CdTe compound. Finally, we calculated the EOS for the rhombohedral-Bi within the PBE exchange-correlation based on 2D and 1D searches of the EOS. As shown in Fig. 1, when we changed the search method from 2D to 1D, the effect of 2D search caused the value of the optimized volume to change from 496.96 to 494.96 ($Bohr^3$), and from 463.69 to 465.62 within PBE-sol. Moreover, for Bi, the 2D search predicted a lower bulk modulus (B) and a higher pressure derivative (B′) than those obtained using 1D search. Therefore, these results show clearly that if we can improve the method used to search for the EOS for compounds with more than one degree of freedom, such as THR symmetries, then the accuracy of the calculation method (DFT in this study) will be better than that obtained using 1D search.

3. Details of the calculations

A new and more accurate package called 2DRoptimize has been released for 2D search of the EOS for THR compounds. The old version of this package called 2Doptimize [8] only supports hexagonal and tetragonal structures, whereas the new 2DRoptimize package also supports rhombohedral structure in addition to hexagonal and tetragonal structures. The new package is compatible with the FPLAPW+lo method, as implemented in the WIEN2k package [11]. It should be noted that when using the 2DRoptimize package for calculations, switch 5 is generally used for calculating the volume changes and switch 7 for calculating the **c/a** changes. Therefore, in these calculations, at least 35 self-consistent calculations are needed in order to find the optimized lattice parameters **a** and **c** for each symmetry. Table 4 shows the other critical parameters comprising the **k**-points mesh, number of times of the smallest atomic muffin-tin sphere radius, and the largest K vector ($R_{min\ MT} \times K_{max}$) as a cutoff parameter to check the convergence of the basis set and the maximum angular momentum (l_{max}) for WIEN2k calculations. For compounds with internal coordinates, we minimized the forces (1 mRy/au) acting on each atom.

4. Results and discussion

Using the 2DRoptimize package, we calculated the cell parameters of 21 THR compounds, as shown in Tables S2 and S3 in the supplementary materials. Fig. 2 shows the differences in the optimized energy, volume,
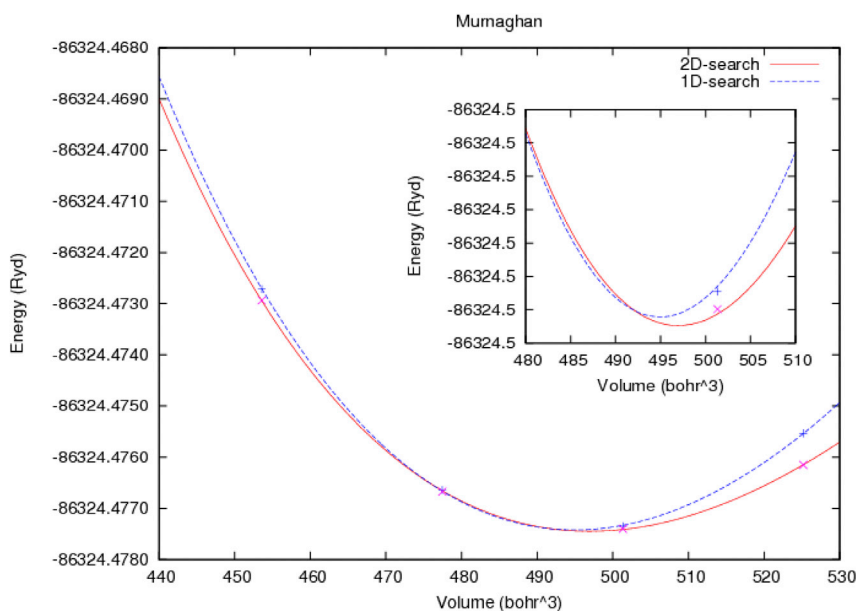
Fig. 1. EOSs for the rhombohedral Bi based on 2D and 1D searches within the PBE.

bulk modulus, and pressure derivative of the bulk modulus using 2D and 1D searches of the EOS for THR compounds within the PBE. Fig. 2 demonstrates that the effect of 2D search of the EOS can be important where it can influence the optimized values, although this difference may be negligible. Thus, the accuracy of calculations performed using 2D search of the EOS is much better than that of those based on 1D search. Moreover, Fig. 2 shows that the 2D search of the EOS usually predicts an optimized energy lower than that obtained by 1D search of the EOS. The biggest difference between 2D and 1D searches of the EOS is the bulk modulus for TiO$_2$, which is about 15. Therefore, we conclude that the effect of 2D search of the EOS can be important. Fig. 2 also indicates that

the effect of 2D search of the EOS for CuSn is negligible, which can be explained by the negligible effect of finding the minimum of the **c/a** ratio and the corresponding energy for each volume compared with 1D search of the EOS.

The best parameter for illustrating the effect of 2D search of the EOS compared with 1D search is the relative error. Thus, Table S1 (supplementary materials) shows the percentage relative error using 2D search compared with 1D search of the EOS for the optimized values of some THR compounds within the PBE. For AuSn, the predicted values of the optimized volume, bulk modulus, and pressure derivative of bulk modulus were 0.04%, 1.0%, and 0.92% lower using 2D search than 1D search within the PBE, respectively. The effect of 2D search on the optimized volume of CuSn was negligible, but it influenced the pressure derivative of the bulk modulus, which was 0.03% larger than that obtained using 1D search.

For the In compound, the main difference was in the pressure derivative of the bulk modulus calculated using 2D search, which was 16% larger than that obtained with 1D search within the PBE. In addition, 2D search of the EOS calculated the optimized volume of tetragonal MnO$_2$ as 0.129% larger than that obtained by 1D search of the EOS. This effect decreased the bulk modulus and increased its pressure derivative by 3.2% and 5.51%, respectively, compared with 1D search. A convenient volume and **c/a** structure optimization for NiSn predicted a lower optimized volume as well as a larger bulk modulus and pressure derivative of the bulk modulus than those obtained using 1D search. Table S1 (supplementary materials) shows that 2D search decreased the bulk modulus of PtSn by 2.0% compared with 1D search of the EOS.

It should also be noted that the 2D search of the EOS predicted that the bulk modulus of SnO$_2$ and its pressure derivative were 6.5% and 7.54% lower and higher than those obtained by using 1D search, respectively. For TiO$_2$, 2D search predicted that the optimized volume, bulk modulus, and pressure derivative of the bulk modulus were 0.22% larger, 7.5% lower, and 12.0% larger than those obtained by 1D search within the PBE, respectively. The effect of 2D search was negligible on the optimized volume of the B compound, but it influenced the bulk modulus and its pressure derivative, which were 0.58% lower and 2.49% higher than those obtained using 1D search, respectively. Therefore, in order to increase the accuracy of the lattice constant calculations, we
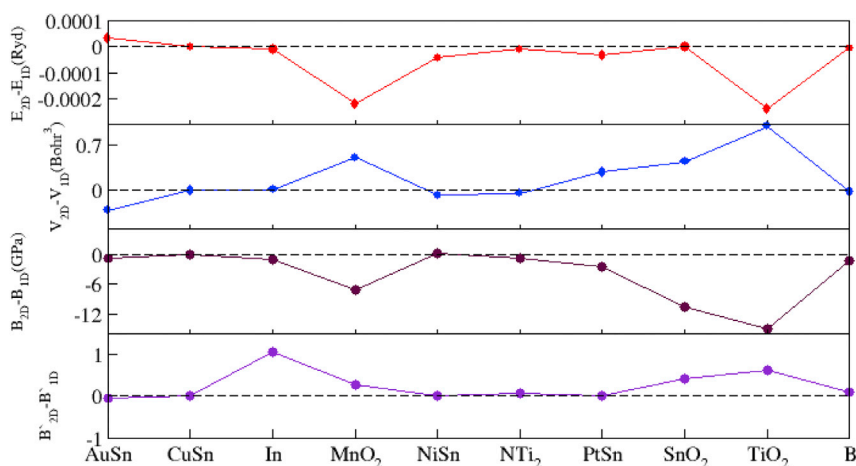
Table 4
K-point mesh and cut-off parameter ($R_{min}^{MT} \times K_{max}$) to check the convergence of the basis set in the interstitial region and the maximum angular momentum (l_{max}) for the radial functions times the spherical harmonics inside the atomic spheres for the compounds considered in this study.

Compound	Kpoint-mesh	$R_{min}^{MT} \times K_{max}$	l_{max}
AuSn	15*15*10	8	9
CuSn	14*14*10	8	9
In	15*15*15	8	9
MnO$_2$	10*10*16	8	9
NiSn	15*15*10	8	9
NTi$_2$	10*10*16	8	9
PtSn	15*15*10	8	9
SnO$_2$	10*10*15	8	9
TiO$_2$	10*10*16	8	9
B	8*8*8	8	9
Al$_2$O$_3$	8*8*8	7	8
Bi	11*11*11	8	9
AsSb	10*10*10	8	9
CdSe	15*15*8	9	10
CdSe$_{0.75}$Te$_{0.25}$	19*19*5	9	10
CdSe$_{0.5}$Te$_{0.5}$	15*15*8	9	10
CdSe$_{0.25}$Te$_{0.75}$	19*19*5	9	10
CdTe	15*15*8	9	10
Sc	18*18*10	8	9
Y	18*18*10	8	9
Tb	18*18*10	8	9

Fig. 2. Differences in the optimized energy, volume, bulk modulus, and its pressure derivative based on 2D and 1D searches of EOS within the PBE.

calculated the cell parameters of the compounds considered by using 2D search of the EOS within different exchange correlations, as shown in Tables S2 and S3 (supplementary materials), where previous theoretical results [12–17] and the experimental data [10,18–30] are also presented to allow useful comparisons.

We calculated the lattice parameters of the hexagonal AuSn compound within the PBE and local density approximation (LDA) [31], as shown in Table S2 (supplementary materials) alongside the experimental data [18]. Clearly, the results obtained using LDA were better than those obtained with the PBE, and they agreed very well with the experimental data. Thus, we conclude that LDA solved the exchange-correlation for the AuSn compound better than PBE, and we also note that the calculated lattice parameters obtained from the new 2Droptimize package were in very good agreement with the experimental data. The simulated lattice constants obtained for CuSn using FPLAPW-PBE were compared with the experimental measurements [18], where Table S2 shows that the predictions obtained by 2D search of the EOS were in excellent agreement with the experimental data. For the NiSn compound, we calculated the lattice constants within different exchange-correlation potentials comprising PBE, LDA, PBEsol [32], and WC [33], and they were compared with the experimental data [18]. The results obtained by PBE were better than those produced using LDA, PBEsol, and WC. Again, it should be noted that the predictions obtained by 2D search of the EOS were in very good agreement with the experimental data. Moreover, Table S2 shows that the lattice parameters calculated by PBEsol and WC were almost the same for the NiSn compound.

The lattice parameters calculated for the hexagonal PtSn compound within the PBE and LDA are also given in Table S2 alongside the experimental data [18]. Clearly, the results obtained using LDA were in better agreement with the experimental data than those produced with the PBE. Thus, we conclude that LDA solved the exchange-correlation for the PtSn compound better than the PBE. We also found that the lattice parameters calculated by 2D search of the EOS were in very good agreement with the experimental data. Furthermore, our results showed that the lattice constants calculated for tetragonal MnO_2 using convenient the 2D structural optimization process within the PBE functional agreed very well with experimental data [19,20].

Table S2 (supplementary materials) shows that lattice constants calculated for the tetragonal SnO_2 by the 2Droptimize package within the LDA were closer to the experimental data [21] than those obtained within the PBE. Thus, LDA solved the exchange-correlation for SnO_2 better than the PBE. For the tetragonal TiO_2 compound, the predicted lattice parameters obtained by 2D search of the EOS within the PBE were very similar to the experimental data [22]. The simulated lattice

constants obtained for tetragonal NTi2 using FPLAPW-PBE are given in Table S2, where they are compared with the experimental data [23]. Clearly, the predictions obtained by 2D search of the EOS were in excellent agreement with the experimental data.

For the tetragonal In compound, we calculated the lattice parameters using different exchange-correlation potentials comprising PBE, LDA, PBEsol, and WC, and the results obtained were compared with previous theoretical calculations [12] and experimental data [24]. The results calculated using WC were better than those obtained with the PBE, LDA, and PBEsol. It should be noted that the predictions obtained by 2D search of the EOS were in very good agreement with the experimental data and better than the previously reported theoretical calculations. The lattice parameters calculated within the PBEsol and WC were almost the same for the In compound, as shown in Table S2. For the hexagonal Y and Sc compounds, the results obtained by 2D search of the EOS within the PBE functional agreed well with the experimental data [10] and they were much better than the previous calculations [13]. Furthermore, we calculated the lattice parameters for hexagonal $CdSe_xTe_{1-x}$ (x = 0.00, 0.25, 0.5, 0.75, 1) alloys by 2D search of the EOS within the PBE. The results obtained as well as the previous calculations [14] and experimental data [25,26] are given in Table S2.

Moreover, we used the 2Droptimize package to calculate the structural properties of the Tb compound using PBE+U (Hubbard U parameter), PBE+U+SO (spin–orbit coupling), LDA-EECE [34] (onsite hybrid functional), and the hybrid B3PW91 approach [35,36] as well as the standard semi-local functionals (LDA, WC, PBEsol, and PBE) in order to overcome the weaknesses of DFT for compounds with localized electrons. The effective Hubbard U parameter calculated for the Tb compound was 0.25 Ryd. Table S2 shows that the calculated lattice parameters predicted using the 2Droptimize package within the LDA, WC, and PBEsol were more distant from the experimental data [5] compared with the PBE exchange-correlation, and the PBE predicted the smallest bulk modulus value for the Tb compound. According to Table S2 (Tb compound), the PBE+U and PBE+U+SO approximations improved the lattice parameters compared to the experimental data. However, the lattice parameters calculated within the PBE+U and PBE+U+SO were overestimated with respect to the experimental values and the PBE calculations. The results (lattice parameters) obtained within the PBE, PBE+U, and PBE+U+SO were in better agreement with the experimental data compared with the standard semi-local functionals. Thus, the effects of the Hubbard U parameter and SO coupling were important for the Tb compound. Table S2 shows that the lattice parameters and bulk modulus calculated using PBE+U were identical to the experimental data [5,30]. However, the PBE did not predict the bulk modulus well compared with the PBE+U

and PBE+U+SO. Thus, the PBE+U calculated with the effective Hubbard U parameter could describe the structural properties of the Tb compound very well. The results showed that the lattice parameters (bulk modulus) predicted within the PBE+U+SO were larger (lower) than those with the PBE+U.

The calculations of the structural properties of the hexagonal Tb compound using the LDA-EECE method with various values for α showed that this method was not very successful at predicting the experimental lattice constants and bulk modulus for the Tb compound. Therefore, in the next step, we evaluated the accuracy of the B3PW91 hybrid functional. According to the results presented in Table S2, the lattice parameters and bulk modulus obtained for the Tb compound within the B3PW91 exchange-correlation functional with the optimized Becke value of $\alpha = 0.2$ [35] were in agreement with the experimental data. The lattice parameters calculated with $\alpha = 0.15$ were in excellent agreement with the experimental lattice parameters. However, the bulk modulus predicted using $\alpha = 0.15$ was lower than the experimental data. Finally, it should be noted that 1D and 2D searches of the EOS using the B3PW91 ($\alpha = 0.15$) predicted bulk modulus and optimized volumes for Tb of 30.26 and 30.25 GPa, respectively, and 432.5636 and 432.5381 bohr^3.

We also calculated the rhombohedral specifications for Al_2O_3, Bi, B, and AsSb compounds by 2D search of the EOS, as shown in Table S3 (supplementary materials) with the previous theoretical calculations [15–17] and experimental data [27–29]. Table S3 shows that the lattice parameter and α angle calculated for the rhombohedral Al_2O_3 compound by 2D search of the EOS within the PBE functional were in very good agreement with the experimental data [27]. The lattice parameter and **α** angle calculated for the rhombohedral B compound by convenient structural optimization within the PBE functional as well as the experimental data [28] and the theoretical calculations [15,16] are presented in Table S3. Our results were in better agreement with the experimental data than the previous theoretical calculations. For the rhombohedral Bi compound, we calculated the lattice parameter and α angle within different exchange-correlation potentials, i.e., PBE, LDA, PBEsol, and WC, and the results obtained were compared with the experimental data [29]. The results calculated within PBEsol were in better agreement with the experimental data than those obtained using the PBE, LDA, and WC. However, the results obtained using PBEsol and WC were almost the same. These results also confirm that 2D search of the EOS is a more accurate method than 1D search of the EOS. It should be noted that our calculations for the rhombohedral Bi compound were performed at 0.0 K, whereas the experimental data were obtained at 4.2 K.

Finally, we calculated the rhombohedral specifications of stibarsen (AsSb), which has the same crystal structure (space group $R3m$, No = 166) as arsenic and antimony, where the lattice parameters of stibarsen are intermediate between those of As and Sb. The lattice parameters of stibarsen were obtained by least-squares refinement and using X-ray powder diffraction data, which were refined in the space group $R3m$ are $a_r = 4.2954$ Å and $\alpha = 55.88°$ [17]. This motivated us to predict the lattice parameter and **α** angle for stibarsen by using the previously reported data [17] and the 2DRoptimize package within different exchange-correlations. The results and the experimental data [17] are given in Table S3.

5. Conclusions

In this study, we assessed a new package called 2DRoptimize for performing 2D searches of the EOSs for THR compounds. The cell parameters of 21 THR compounds were calculated using the 2DRoptimize package. We investigated the differences in the optimized energy, volume, bulk modulus, and pressure derivative of the bulk modulus based on 2D and 1D searches of the EOS for some THR compounds within the PBE. The effects of 2D search of the EOS may be important and it can influence the optimized values and pressure of the induced-phase transition. Thus, the accuracy of calculations based on 2D search of the EOS is much better than that of those obtained by 1D search. Moreover, 2D

search of the EOS usually predicts a lower optimized energy compared with that obtained based on 1D search of the EOS. Furthermore, in order to increase the accuracy of the lattice constant calculations, we calculated the cell parameters for some THR compounds by 2D search of the EOS within different exchange-correlations, which we compared with previous theoretical results and experimental data. Our comparison of the results obtained using the 2DRoptimize package with the available experimental and theoretical data showed that the 2DRoptimize results were in very good agreement with the experimental data and they were better than the previous theoretical calculations, including the results obtained by 1D search of the EOS. Therefore, we conclude that the results obtained using the newly released package for several THR structures within different exchange and correlation potentials exhibited better accuracy than those produced based on 1D search of the EOS.

Appendix A. Supplementary data

Supplementary data related to this article can be found at https://doi.org/10.1016/j.jpcs.2018.01.034.

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