



First principle studies of structural, magnetic and elastic properties of orthorhombic rare-earth diaurides intermetallics RAu_2 ($\text{R}=\text{La}$, Ce , Pr and Eu)

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HIGHLIGHTS

- First principle calculations of RAu_2 ($\text{R}=\text{La}$, Ce , Pr and Eu) compounds are carried out.
- Their structural, magnetic and elastic properties are investigated.
- These compounds are elastically stable and antiferromagnetic in nature.
- CeAu_2 , EuAu_2 and LaAu_2 are ductile while PrAu_2 is stiffer.
- LaAu_2 , PrAu_2 and EuAu_2 are anisotropic and CeAu_2 is isotropic.

ARTICLE INFO

Article history:

Received 20 November 2016

Received in revised form

13 January 2018

Accepted 8 March 2018

Available online 9 March 2018

Keywords:

Orthorhombic intermetallics

Structural properties

Magnetic and mechanical properties

Elastic constants

Rare-earth diaurides

ABSTRACT

The structural, magnetic and elastic properties of orthorhombic phase of RAu_2 compounds ($\text{R}=\text{La}$, Ce , Pr and Eu) are reported theoretically for the first time using full potential linearized augmented plane waves method within the density functional theory. The structural properties are investigated by treating the exchange and correlation energies with the generalized gradient approximation, PBEsol. Our computed lattice constants are found consistent with the reported experimental results. Our data reveal that they are stable in orthorhombic CeCu_2 type structure. Their mechanical properties such as Young, Shear and bulk moduli, Poisson and anisotropic ratio, Cauchy pressure and B_0/G ratio are explored using the PBEsol to evaluate the importance of these compounds in various types of engineering applications. One of the striking features of their mechanical properties is their ductile nature. Magnetically all these intermetallics are antiferromagnetic.

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1. Introduction

Today's technological applications require the materials which are ductile, stiff, non corrosive, strong at high temperatures and light in weight. Computational science is very helpful in determining valued materials for experimentalists to be applied for high-tech applications [1].

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Many of the greenest technologies of the age, from electric cars and efficient light bulbs to very large wind turbines and future magnetic refrigeration, are made possible by an unusual group of elements: the lanthanides. They possess peculiar electronic structure and delicately changing bonding, due to the presence of inner and interacting d- and f-orbitals. These d- and f-electrons are responsible for their catalytic activities, alloying behaviors, and particular luminescent characteristics [2]. The use of rare earths in corrosion protection as inhibitors is very effective because of their non-toxicity, as compared to the common chromate inhibitors [3]. Furthermore, rare earths are becoming increasingly important due

to their crucial role in permanent magnets, lamp phosphors, catalysts and rechargeable batteries [4]. The lanthanides demonstrate varying magnetism, coordination, oxidation states, and bonding types, as a function of the number and localization of the f-state electrons.

Intermetallics are the compounds consisting of two or more metals having mixed metallic, ionic and covalent bonding. Their physical, chemical, mechanical and magnetic properties are often better than those of the constituent metals [5]. They are characterized by high strength, high melting point, ductility, cracking stiffness, good magnetic properties, striking high temperature mechanical properties and electrical properties which make them suitable for high temperature constructing materials, aerospace applications, electric power generation, engines, boilers, and heat exchangers [6].

One of the interesting subgroup of lanthanide intermetallics is the noble metals (Cu, Ag and Au) based intermetallics [7]. The bond stabilities of lanthanides with these noble metals are in the order of $RAu > RCu > RAg$ (R = lanthanide element) [8,9]. The most stable compounds among them are the compounds with gold and they form compounds because of their electronegativity difference [10]. Similarly, very high relativistic effects in lanthanide-gold (RAu) bond are also responsible for its great stability [8]. They are the first group of atoms containing 4f-orbitals. They have greatly varying crystal structures, magnetic and electrical properties [11]. The high stability of these materials can be judged from their high melting points, high dissociation energies and high heat of formation [9]. The very high stability of the R-Au bond is explained by the Pauling model as given below:

$$D(A-B) = \frac{1}{2} [D(A-A) + D(B-B)] + Q (EN_A - EN_B)^2, \quad (1)$$

where $D(A-B)$ represents the dissociation energy of diatomic bond, EN_A is the Pauling electronegativity of atom A, and Q is constant. This model shows that the 2.4 electronegativity of gold is mainly due to its relativistic effect, that shows high stability of gold compounds [8].

Their high dissociation energies are due to its greater thermal stability, high heat of formation and high melting points. The bond between Au and R is metallic and partly ionic in nature. The phase stability, melting temperatures, and enthalpy of formations of RAu_2 compounds are given in Table 1. $PrAu_2$ exists in two polymorphic forms, i.e., orthorhombic and tetragonal [12].

The RAu_2 (R = La, Ce, Pr and Eu) compounds were synthesized by arc-melting method where appropriate quantity of the elements was taken on a water-cooled copper hearth in an argon atmosphere. The starting materials of La, Ce, Pr, and Eu were 99.9% and Au was 99.99% pure. The samples were heated to 800 °C and then cooled just below their melting temperature for a week. The structures were determined with x-ray powder method [13].

The rare-earth intermetallics studied in the present work are RAu_2 (R = La, Ce, Pr and Eu). Literature survey indicates that, in spite of technological importance of these rare-earth intermetallics, there is still a need for a systematic study of structural, magnetic and mechanical properties of these materials for future

applications. The present study is an attempt in this direction. First principle calculations have been done by the density functional theory (DFT) formalism within full-potential augmented plane waves plus local orbitals (FP-APW+lo) method for the rare earth intermetallics (RAu_2).

2. Computational detail

Density functional theory has become an unchallenging “typical model” because of its impressive predictive role and decisive results with extensive applicability in materials science. It is reliable tool for the theoretical prediction and understanding of the structural, optical, electronic, mechanical and magnetic properties of metals, semimetals, semiconductors, and insulators. Full-potential (linearized) augmented plane waves plus local orbitals (FP-(L) APW+lo) method is the perfect scheme for solving the Kohn–Sham equations [14,15]. This tool is based on the first-principle density-functional theory and can be used by a variety of the exchange-correlation functionals such as the generalized gradient approximation (GGA) [16]. The computations details, formulas and the WIEN2k package are reported elsewhere [15,17]. In these DFT calculations, FP-APW+lo method within the GGA and PBEsol as implemented in the WIEN2k code [18] is utilized to solve Kohn–Sham equations for the RAu_2 compounds. The higher rate of angular momentum $l_{max} = 10$ is taken for the wave function expansion within atomic spheres.

To make sure that no electron is leaked out from the core and exact results are obtained, 2000 k-points and plane waves cut-off value of $R_{MT} K_{max} = 8.00$ basis functions are used. The separation energy among the inner and outer states is 6.0 Ryd. RMT value of 2.5 a.u. is taken for both lanthanide and Au atoms. The charge density is Fourier expanded up to $G_{max} = 12.00$ Ry. The lattice constants for RAu_2 are first optimized to ensure that the calculations were based on equilibrium lattice constants.

Orthorhombic-elastic software [19] and PBEsol exchange correlation are applied to compute the elastic properties of RAu_2 . The energy that separates the valence and core states is considered as -9.0 Ry. The $R_{MT}K_{max}$ parameter that controls the size of the basis was set 7.5 in the elastic calculations. The k-points were kept at 2000. The magnetic properties for single cell calculation are carried out using HF-B3PW91 functional and double cell AFM calculation is carried out with PBEsol functional. For HF-B3PW91 calculations we use the correct exchange potential $\alpha = 0.15$ to 0.25. The PHONON software which has an interface with the WIEN2k code is used to calculate phonon frequency which is 4.0 TZs (133.4 cm^{-1}) at the Γ point.

3. Results and discussion

3.1. Structural properties

Structural properties are very important because they predict other properties like strength, toughness, ductility, hardness, thermal and electrical conductivity, magnetic and optical properties etc. Determination of these properties further utilize for the proper and relevant applications of these materials. Some of the

Table 1
Phase stability, melting temperature and enthalpy of formation of RAu_2 (R = La, Ce, Pr and Eu) compounds.

Compounds	LaAu ₂	Ce Au ₂	Pr Au ₂	Eu Au ₂
Phase stability	1214 °C [47]	1130 °C [48]	1180 °C [9,49]	1085 °C [23]
Melting point	1487.15 K [50]	1479 K [51]	1415 K [26]	—
Enthalpy formation	−81.5 kJ/mol [52]	−71.3 ± 2.0 kJ/mol of atoms [51]	−97.2 kJ/mol of atoms [49] −64.2 kJ/g atoms [53]	—

structural properties are the arrangement of atoms in space, the type of bonding, the bond length, and bond angles in a crystal. In this subsection, we have determined the structural properties of RAu_2 ($R = \text{La, Ce, Pr and Eu}$) compounds. The f-electrons in rare-earths play a vital role in exploring their structural properties because of their varying occupancy. The Lanthanides in these compounds are in trivalent state.

The ground state structural properties of RAu_2 ($R = \text{La, Ce, Pr, and Eu}$) compounds are computed evaluating the optimized total energy of unit cell of each compound with respect to volume by using Birch–Murnaghan equation of state [20]. The lattice constants for all the compounds are obtained using GGA-PBEsol exchange–correlation functional. The calculated results are presented in Table 2 and are compared with the available experimental results. All these compounds, LaAu_2 , CeAu_2 , PrAu_2 and EuAu_2 , are found in orthorhombic, CeCu_2 type structure having space group, Imma , No. 74, and atomic Wyckoff positions of R and Au atoms, and the angles are [13,21–29].

x	y	z
R = 0.00	0.25	0.3577
Au = 0.00	0.051	0.1648
Angles 90° (α)	90° (β)	90° (γ)

Our calculated lattice constants are in agreement with the experimental results [24]. However, no theoretical work about their structural properties is available in literature for comparison.

3.2. Magnetic properties

The magnetic properties are the intrinsic physical properties which are associated with charged particles because of its orbital angular momentum and spin. To predict the ground state magnetic nature of orthorhombic RAu_2 ($R = \text{La, Ce, Pr and Eu}$) compounds, we optimized the double cell of each compound ferromagnetically, anti-ferromagnetically and non-magnetically. The energy difference for RAu_2 compounds per unit cell is given in Table 3 which shows that all these compounds are stable in the anti-ferromagnetic (AFM) state. In anti-ferromagnetic materials the electron spins associated with the atoms are aligned in opposite directions and are equal in magnitude. They cancel the effect of each other and therefore the net moment is zero. To explore the origin of magnetism in these compounds, spin polarized single cell calculations are performed for all these compounds by HF-B3PW91 functional within the DFT framework and the calculated magnetic moments per lanthanide atom ($R = \text{La, Ce, Pr and Eu}$) of all these

intermetallics are presented in Table 4. The double cell anti-ferromagnetic calculation is carried out with PBEsol functional which shows that all these materials have zero total magnetic moment as presented in Table 4. To the best of our information only the magnetic moment of Eu in EuAu_2 compound is available to which our result is comparable. We believe that our magnetic moment calculations of these compounds will motivate the experimentalists because we have carried out these calculations with the reliable HF-B3PW91 functional and concluded that the net spin magnetic moments in binary intermetallics are due to the following three contributions: one from the lanthanide atoms (R), the other from Au atom and the third from interstitial region. Au atom and the interstitial regions have negligible magnetic moments. In conclusion, the total spin magnetic moment is due to 4f-unpaired electrons of the lanthanide atom [30,31]. The lanthanides can be considered as a cluster of ions, mostly trivalent, with incomplete 4f orbitals, imbedded in a cloud of free electrons. The deep shell 4f electrons play a secondary role in their mechanical and chemical properties but they are the origin of the magnetic moments [32]. As we go from left to right in a period the number of unpaired electrons first increases that results in the increase of magnetic moment. The Lanthanum (La) has no “f” electrons thus have no magnetic moment while the EuAu_2 has the highest magnetic moment among the investigated compounds because Eu has six unpaired electrons.

3.3. Elastic constants and mechanical properties

The elastic constants are the ratio of stress to strain of a material. These are essential for describing the mechanical properties, type of bond, presence of different forces and mechanical stability of the compounds [33,34]. They are also useful in predicting the aging behavior of the materials [35]. Therefore, they have a great role in determining the strength of the crystals. They are also associated with thermodynamic behavior such as thermal expansion, specific heat, melting point and Debye temperature. For orthorhombic type crystals there are 9 independent elastic constants denoted by C_{11} , C_{22} , C_{33} , C_{44} , C_{55} , C_{66} , C_{12} , C_{13} , and C_{23} [36,37].

The stability criteria for orthorhombic crystal is given as [38]:

$$C_{11} > 0, C_{22} > 0, C_{33} > 0, C_{44} > 0, C_{55} > 0, C_{66} > 0, [C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23})] > 0,$$

$$(C_{11} + C_{22} - 2C_{12}) > 0, (C_{11} + C_{33} - 2C_{13}) > 0 \text{ and } (C_{22} + C_{33} - 2C_{23}) > 0 \quad (2)$$

Due to the special importance of the Young, shear and bulk moduli, Pugh's ratio, Cauchy pressure, anisotropy and Poisson's ratio for high-tech applications, we computed them from elastic constants. Our calculated results given in Table 5 obey the Born stability criteria for orthorhombic structures [39] and reveal the mechanically stable nature of orthorhombic RAu_2 compounds.

The ratio of stress to strain that determines the stiffness of materials is called Young's modulus, greater its value stiffer will be the material and vice versa. It measures the ability of a material to withstand changes in length under a given amount of stress. It is given by the equation [40]:

$$Y = \frac{9BG}{3B + G} \quad (3)$$

The Young's moduli as indicated in Table 5 are high for PrAu_2 , LaAu_2 and EuAu_2 than CeAu_2 which indicate that these compounds are comparatively stiffer than CeAu_2 . The CeAu_2 , EuAu_2 , LaAu_2 and PrAu_2 are in the order of increasing stiffness and decreasing

Table 2
Calculated lattice constants by GGA-PBEsol compared with the experimental results of orthorhombic RAu_2 ($R = \text{La, Ce, Pr and Eu}$).

Compound	Lattice constant, (Exp) [24,54] (Å)	This work (Å)
LaAu_2	a = 4.700	a = 4.813
	b = 7.295	b = 7.121
	c = 8.155	c = 8.007
CeAu_2	a = 4.528	a = 4.709
	b = 7.203	b = 6.971
	c = 8.068	c = 7.906
PrAu_2	a = 4.672	a = 4.655
	b = 7.040	b = 7.007
	c = 8.178	c = 8.081
EuAu_2	a = 4.670	a = 4.670
	b = 7.330	b = 7.208
	c = 8.140	c = 8.072

Table 3Ground state energies calculated for orthorhombic RAu₂ (R = La, Ce, Pr and Eu).

Compound	E _{NM} (Ry)	E _{FM} (Ry)	E _{AFM} (Ry)	Expt.	This Work
LaAu ₂	−186319.06729	−186319.09363	−745276.370	—	AFM
CeAu ₂	−187789.55083	−187789.55077	−751158.204	—	AFM
PrAu ₂	−189298.80417	−189298.89155	−757195.558	—	AFM
EuAu ₂	−195735.24454	−195736.38415	−758954.153	AFM	AFM

ductility as indicated from their Young's moduli and B_0/G ratios, respectively. The CeAu₂ is the least stiff and good ductile, while PrAu₂ is the least ductile and good stiffer.

Poisson's ratio measures the compressibility of a crystal [35]. It is defined as the ratio of lateral to longitudinal strain. The materials will be incompressible when $\nu = 0.5$ and will be compressible if $\nu = 0.2$ to 0.49 [38]. In our study, the measured Poisson's ratios of RAu₂ compounds vary from 0.265 to 0.353, as presented in Table 5, which indicate that these materials are compressible. The value of this quantity also determines the nature of the bond. Its values for covalent, ionic and metallic bonds in a crystal are 0.1, 0.25 and 0.33, respectively [41]. In this context, our compounds are ionic/metallic crystals according to the calculated Poisson's ratio and there is no covalent character at all. Poisson's ratio may also be used for determining the central forces in solids. For an isotropic compound Poisson's ratio ν is calculated from the following relation [40]:

$$\nu = \frac{3B - 2G}{2(3B + G)} \quad (4)$$

For central forces in crystals, the limits of Poisson's ratio are 0.5 to 0.25 [35]. The value of the calculated Poisson's ratio in the

compounds under consideration remains between these two limits which reveals the predominance of the central inter atomic forces.

Bulk modulus (B_0) is one of the most important parameters of the engineering materials. It is the measure of resistance to volume change by applied pressure [42]. It gives information about the nature of bond and cohesive and binding energies of the material [43]. Bulk modulus for orthorhombic compounds is determined from the elastic constants by using the following relation [35]:

$$B_0 = \frac{1}{9}(C_{11} + C_{22} + C_{33}) + \frac{2}{9}(C_{12} + C_{13} + C_{23}) \quad (5)$$

The computed values of the Bulk moduli for these compounds are tabulated in Table 5. The results indicate that the bonding type in these materials is ionic/metallic. The large values of Bulk moduli for these compounds also confirm that RAu₂ compounds have high melting points.

The criterion for brittleness or ductility of a material is the value of the Pugh's ratio, B_0/G . The lesser and higher values of the B_0/G ratio than 1.75 reflect the brittle and ductile natures of the material, respectively [44]. The B_0/G ratio calculated for CeAu₂, EuAu₂ and LaAu₂ are 3.0, 2.0, and 1.8, respectively. Thus, all these compounds are ductile in nature, while B_0/G is almost equal to 1.75 for PrAu₂ compound and therefore its ductility is comparatively lower. The computed values of Pugh's ratio are given in Table 5.

Shear modulus is another important mechanical property which determines the resistance toward reversible deformations resulting from shear stress. The harder a substance is, the higher the shear modulus value becomes. It describes hardness of a material better than bulk modulus. The shear modulus is given by this relation [35]:

$$G_V = \frac{1}{15}(C_{11} + C_{22} + C_{33}) - \frac{1}{15}(C_{12} + C_{13} + C_{23}) + \frac{1}{15}(C_{44} + C_{55} + C_{66}). \quad (6)$$

The computed shear modulus for PrAu₂ is the highest which is 50.2 GPa and lowest for CeAu₂ which is 20.7 GPa. Thus, PrAu₂ is the hardest and CeAu₂ is the softest among these understudy compounds. The shear modulus values of these compounds are indicated in Table 5.

The knowledge of elastic anisotropy has important applications in high-tech materials, because it predicts the chance of micro cracks in crystals and determined the durability of a material. It is the measure of intensity of a property in different directions. In different crystallographic planes, shear anisotropy gives a measure of the level of anisotropy in atomic bonding in different planes. Furthermore, it gives information regarding stiffness, mechanical stability, hardness, brittleness, ductile and binding behavior between neighboring atomic planes. Therefore, the determination of the elastic anisotropy of a material is crucial to understand its behaviors and to find means for improving their hardness and durability. That is why we have predicted the elastic anisotropy of RAu₂, as given in Table 7, by the anisotropic factor. For the shear planes (1 0 0) which are perpendicular to the x-axis between <011> and <010> directions, it is defined as follows [40,46,47]:

Table 4Calculated and experimental spin magnetic moments (μ) per R (R = La, Ce, Pr and Eu) atom by HF-B3PW91 with [U] and (α) values and double cell AFM total magnetic moment (μ_{tot}) of RAu₂ compounds in the unit of Bohr magneton (μ_B).

Compound	Caltd. μ per R atom HF-B3PW91 [U] (α)	μ_{tot} AFM HF-B3PW91	Expt. [55] μ per R atom
LaAu ₂	0.0000 [2eV] (0.25)	0.0000	—
CeAu ₂	1.1434 [2eV] (0.15)	0.0000	—
PrAu ₂	2.7195 [2eV] (0.25)	0.0000	—
EuAu ₂	6.9138 [2eV] (0.25)	0.0000	7.59

Table 5Calculated values of elastic constants C_{11} , C_{22} , C_{33} , C_{44} , C_{55} , C_{66} , C_{12} , C_{13} , C_{23} , bulk modulus B_0 , shear modulus G and Young's modulus Y (in GPa), Poisson's ratio ν (in GPa) and B_0/G ratio of orthorhombic RAu₂ (R = La, Ce, Pr and Eu) intermetallics.

Compounds	LaAu ₂	CeAu ₂	PrAu ₂	EuAu ₂
C_{11}	314.69	171	65.8	133.4
C_{22}	94.318	55	172.7	154.2
C_{33}	143.69	113.6	106.6	193
C_{44}	11.7	5.60	11.3	69.0
C_{55}	173.3	109.5	280.7	108.95
C_{66}	18.6	7.75	27.0	22.0
C_{12}	48.65	42	41.4	89.8
C_{13}	87.2	131.8	28	7.67
C_{23}	29.7	32	88.1	108.8
B_0	84.433	63.722	63.42	88.2
G	46.845	20.7	50.24	43.4
Y	118.6	56	119	111.84
ν	0.265	0.353	0.186	0.288
B_0/G	1.80	3.00	1.26	2.00

$$A_1 = \frac{4C_{44}}{C_{11} + C_{33} - 2C_{13}}. \quad (7)$$

For shear planes (0 1 0) which are perpendicular to the y-axis between <101> and <001> directions, it is:

$$A_2 = \frac{4C_{55}}{C_{22} + C_{33} - 2C_{23}}. \quad (8)$$

And for the shear planes (0 0 1) which are perpendicular to the z-axis between [110] and [010] directions, it is

$$A_3 = \frac{4C_{66}}{C_{11} + C_{22} - 2C_{12}}. \quad (9)$$

The obtained anisotropic factors for RAu_2 compounds are given in Table 5. The values of A_1 , A_2 and A_3 for an isotropic material is equal to 1, otherwise it is an anisotropic material [36,39,45]. Our results for LaAu_2 , PrAu_2 and EuAu_2 show strong anisotropic behavior in all directions while for CeAu_2 show isotropic behavior along x-axis and anisotropic behavior along y- and z-axes. The anisotropic values for all the four compounds indicate that the elastic anisotropic values for LaAu_2 , PrAu_2 and EuAu_2 in (010) shear planes between [101] and [001] directions are higher than that of (100) shear planes between [011] and [010] directions and (001) shear planes between the [110] and [010] directions. In the case of CeAu_2 , it is isotropic in (100) shear planes between [011] and [010] directions, because A_1 is equal to unity and the anisotropy along the (010) shear planes between [101] and [001] directions is higher than in (001) shear planes between [110] and [010] directions.

Resistance to linear compression in directions a, b, and c are measured from elastic constants C_{11} , C_{22} , and C_{33} , respectively. The calculated C_{22} are lower than the C_{11} and C_{33} for LaAu_2 , CeAu_2 and EuAu_2 . Therefore, these compounds are more compressible across the b-axis in comparison to a-axis and c-axis, while PrAu_2 is more compressible through a-axis than b- and c-axes.

In orthorhombic compounds, we define the Cauchy's pressure in three different directions as: $p_x^{\text{Cauchy}} = C_{23} - C_{44}$, $p_y^{\text{Cauchy}} = C_{13} - C_{55}$ and $p_z^{\text{Cauchy}} = C_{12} - C_{66}$, see Table 6. The Cauchy's pressure gives information about the type of bonding and the ductile behavior of a material. The material will be ductile having metallic bonds, if the value of this expression is positive. On the other hand, if its value is negative, the material will be brittle having directional bonds (covalent). The ionic crystals have a large Cauchy's pressure either positive or negative [28]. All of our compounds have positive Cauchy's pressure in x- and z-axes, while they have negative values in y-axis. It means that these compounds are harder in x- and z-directions than in y-direction. No experimental or theoretical studies of mechanical properties of these compounds are available in literature for comparison. However, our calculation can serve as a tool for future research work. In future experimental work if any will verify our investigations.

3.4. Phonon dispersion curves

To further investigate the dynamical stability of these

Table 6
Calculated values of Cauchy pressure (in GPa) of orthorhombic RAu_2 (R = La, Ce, Pr and Eu) compounds in x-, y- and z-directions.

Compounds	LaAu_2	CeAu_2	PrAu_2	EuAu_2
$p_x^{\text{Cauchy}} = C_{23} - C_{44}$	18	26.4	77	40
$p_y^{\text{Cauchy}} = C_{13} - C_{55}$	-86	22	-252.7	-101
$p_z^{\text{Cauchy}} = C_{12} - C_{66}$	30	34	14.4	68

Table 7
Anisotropic factors, A_1 , A_2 and A_3 of orthorhombic RAu_2 (R = La, Ce, Pr and Eu).

Compounds	A_1	A_2	A_3
LaAu_2	0.165	3.88	0.239
CeAu_2	1.000	4.20	0.220
PrAu_2	0.388	10.89	0.694
EuAu_2	0.887	3.360	0.814

compounds, we have calculated the phonon frequencies of LaAu_2 compound in orthorhombic phase using the PHONON code [46]. This code calculates the force constant matrices and phonon frequencies using "Small Displacement Method". The phonon dispersion curves have been calculated in high symmetry directions. The obtained results along the high symmetry directions are plotted in Fig. 1. The absence of the negative frequencies in the phonon dispersion curves strongly supports the dynamical stability of this compound in orthorhombic phase and agrees well with the energy and mechanical stability as we have discussed in the previous sections.

To the best of our knowledge no experimental or theoretical work has been reported investigating the lattice dynamics of this compound. Hence, this work can be considered as a first attempt in this respect.

4. Conclusions

It is concluded that RAu_2 (R = La, Ce, Pr and Eu) compounds have orthorhombic geometry. They obey Born stability criteria and therefore they are elastically stable. That is why they can be efficiently used in technology where materials which can regain its original shape after releasing the stress are required. They are hard and their melting points are very high which can be inferred from their high bulk and shear's moduli. They are dynamically stable as

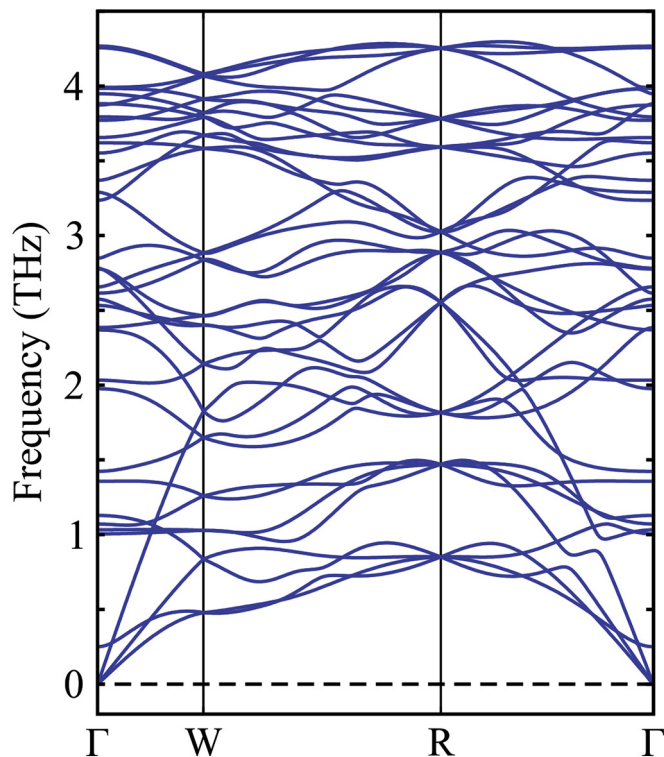


Fig. 1. Phonon dispersion curve for LaAu_2 compound in orthorhombic phase.

confirmed by the phonon dispersion curve. Therefore, they can be used in technologies such as heat engine, automobiles, aerospace and steam turbine where thermally stable and strong materials are required. CeAu₂, EuAu₂ and LaAu₂ are ductile while PrAu₂ is stiffer. This is revealed by their Pugh's ratios and Young's moduli. The compounds LaAu₂, PrAu₂ and EuAu₂ show strong anisotropic behaviors in all directions while CeAu₂ shows isotropic behavior along the x-axis and anisotropic behavior along the y- and z-axes. The anisotropic nature of these materials made them to be used in the fields where heat conduction or magnetic field *etc.* is required in a specific direction. The positive values of their Cauchy's pressures reveal that the bonding type in these intermetallics is metallic/ionic. The Cauchy's pressures also show that all these compounds are harder in the x- and z-directions than in the y-direction. From the elastic constants C_{11} , C_{22} , and C_{33} it is concluded that LaAu₂, CeAu₂ and EuAu₂ compounds are more compressible along the b-axis as compared to a- and c-axes. These promising mechanical properties verify that they are high temperature structural materials. The magnetic properties of these intermetallics show that all these compounds are antiferromagnetic. We hope that our computation will motivate experimentalists to confirm our predictions.

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