npj Computational Materials

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Elasticity-based-exfoliability measure for high-throughput computational exfoliation of two-dimensional materials

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Two-dimensional (2D) materials are promising candidates for uses in next-generation electronic and optoelectronic devices. However, only a few high-quality 2D materials have been mechanically exfoliated to date. One of the critical issues is that the exfoliability of 2D materials from their bulk precursors is unknown. To assess the exfoliability of potential 2D materials from their bulk counterparts, we derived an elasticity-based-exfoliability measure based on an exfoliation mechanics model. The proposed measure has a clear physical meaning and is universally applicable to all material systems. We used this measure to calculate the exfoliability of 10,812 crystals having a first-principles calculated elastic tensor. By setting the threshold values for easy and potential exfoliation based on already-exfoliated materials, we predicted 58 easily exfoliable bulk crystals and 90 potentially exfoliable bulk crystals for 2D materials. As evidence, a topology-based algorithm indicates that there is no interlayer bonding topology for 93% predicted exfoliable bulk crystals, and the analysis on packing ratios shows that 99% predicted exfoliable bulk crystals exhibit a relatively low packing ratio value. Moreover, literature survey shows that 34 predicted exfoliable bulk crystals have been experimentally exfoliated into 2D materials. In addition, the characteristics of these predicted 2D materials were discussed for practical use of such materials.

npj Computational Materials (2021)7:211 ; https://doi.org/10.1038/s41524-021-00677-4

INTRODUCTION

Two-dimensional (2D) materials with ultimate thinness are highly promising for applications in next-generation electronic, optoelectronic devices, and macroscopic assemblies, benefiting from their extreme structures and properties[1–7]. However, their rise begins only after high-quality monolayers being successfully isolated. Mechanical exfoliation is one of the most reliable techniques to obtain high-quality 2D materials[8]. A few 2D monolayers have been mechanically exfoliated from their parent layered solids[8–10], in which the most canonical example is the exfoliation of graphene from graphite[8]. It should be noted that the method of mechanical exfoliation also has disadvantages in scalability and doping control. To overcome such limitations, several methods such as the liquid exfoliation[11,12], chemical vapor deposition[13,14], and wet-chemistry synthesis[15], have been developed. These methods also play a significant role in the science of 2D materials. Regardless of different synthesis technologies, the existence of an exfoliable bulk precursor generally indicates a weak interlayer coupling and a relative stability of free-standing 2D monolayers. Therefore, measuring the exfoliability of 2D materials is crucial not only for discovering new 2D materials but also for assessing the stabilities of free-standing 2D materials.

Progress in this field would be accelerated if the family of 2D materials can be greatly extended. However, experimental identification of 2D materials out of their bulk counterparts is a trial-and-error and time-consuming approach, and hence, only a few 2D materials have been successfully exfoliated to date. For parent bulk crystals, the accumulated knowledge of structure-property has been collected in databases such as the Pauling file[16], the Inorganic Crystal Structure Database (ICSD)[17,18], the Crystallographic Open Database (COD)[19], the Computational 2D Materials Database (C2DB)[20], and Materials Project (MP)[21]. The growing crystal structure databases and computational methods have promoted the progress in powerful high-throughput techniques for screening materials before synthesizing them[22,23]. These techniques have been employed in mining 2D materials from three-dimensional crystal databases and remarkable achievements have been made[24–28]. Considering the characteristic of weak interlayer bonding of layered crystals, recent studies searched the ICSD for crystals with a large interlayer spacing[24,25]. They used packing fraction and interlayer gap criteria to successfully identify almost 100 layered solids. Furthermore, topology-scaling algorithms have been developed to search for layered materials, that is, the possible parents of 2D materials[26,27]. These structure-based algorithms and criteria are efficient for the identification of layered crystals. However, it depends on empirical parameters to determine whether two atoms are bonded, and it is noted that layered crystals are not equivalent to exfoliable bulk crystals for 2D materials for the following reasons: (i) Not all exfoliable crystals are layered crystals. For example, if the interlayer of a crystal is loosely or weakly bonded, it can be an exfoliable crystal although it is a non-layered crystal (Fig. 1). (ii) Not all layered crystals are exfoliable crystals. For example, if the in-plane strength of a layered crystal is not strong enough to resist the interlayer interaction, the material's plane will be fractured during the mechanical exfoliation, and hence this layered crystal is not an exfoliable crystal (Fig. 1). Briefly, both layered crystals and non-layered crystals are potentially exfoliable or non-exfoliable, which significantly depends on their interlayer interactions and in-plane resistance.

To assess the exfoliability of bulk crystals (the feasibility of exfoliating 2D materials from their parent bulk crystals), several measures have been proposed from the views of energy and mechanical force, where the interlayer binding energy is a widely

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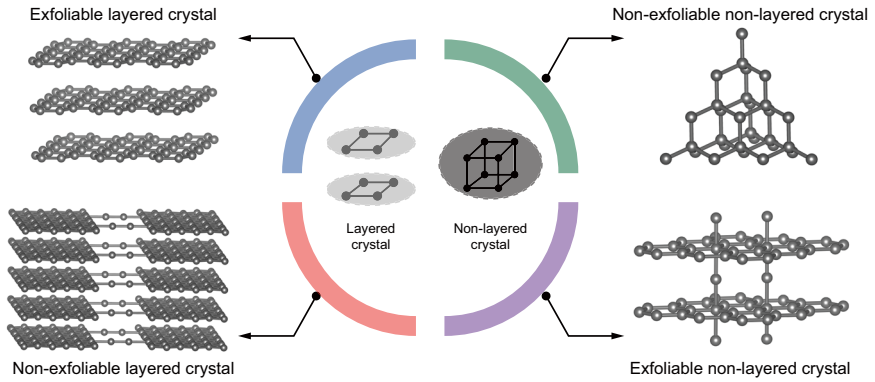

Fig. 1 Illustration of different types of crystals. The exfoliable layered crystal, non-exfoliable layered crystal, non-exfoliable non-layered crystal, and exfoliable non-layered crystal are illustrated.

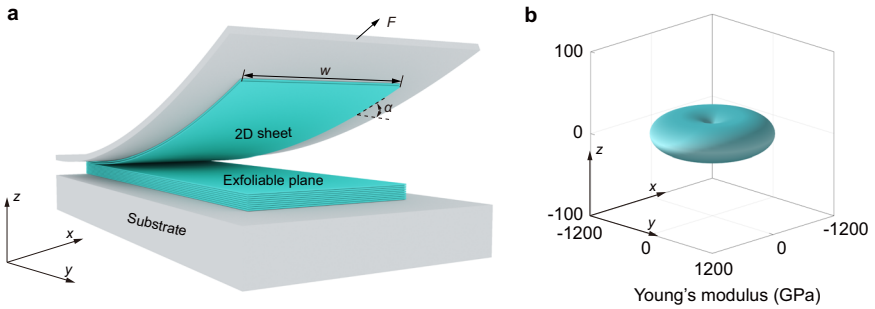

Fig. 2 Mechanical exfoliation model and elastic modulus distribution for an exfoliable crystal. a Model of mechanical exfoliation of 2D materials. **b** Spatial dependence of the Young's moduli for graphite.

used parameter. Intuitively, the lower the binding energy is, the easier the 2D materials can be exfoliated from the bulk counterparts[29]. Yet, this intuition may break down since it does not consider the in-plane mechanical resistance of 2D materials (Fig. 1, the non-exfoliable layered crystal)[30]. Considering the requirement of a high in-plane strength and a weak interlayer interaction for mechanically exfoliable 2D materials, Gao et al.[30] derived a dimensionless measure σ_s/γ based on an exfoliation mechanics model, where σ_s and γ are the in-plane 2D strength (the fracture force divided by the width of 2D sheet) and the interlayer binding energy, respectively. Despite that this measure shows a great reliability for measuring the exfoliability of 2D materials[30], the costly calculations of the in-plane strength and interlayer binding energy limit its uses in high-throughput computational identification of exfoliable 2D materials. Therefore, based on the literature survey, a proper measure of exfoliability which has (i) a clear physical meaning, (ii) a universal applicability, and (iii) is simple and efficient for high-throughput calculations is still missing for 2D materials.

Herein, we derived an elasticity-based-exfoliability measure based on an exfoliation mechanics model, i.e., the maximum ratio of the minimum in-plane Young's modulus to the out-of-plane Young's modulus of crystals over all possible exfoliable planes. This measure has a clear physical meaning and is universally applicable to all material systems. More importantly, it can be efficiently determined from experiments or first-principles calculations, making it attractive for high-throughput identification of exfoliable 2D materials. Using this measure, we evaluated the exfoliability of 10,812 screened crystals having a first-principles calculated elastic tensor from MP crystal structure database. Based on the minimum and median values of elasticity-based-exfoliability measure for 34 already-exfoliated crystals from literature survey, we screened out 58 easily and 90 potentially exfoliable bulk crystals for 2D materials, which have an elasticity-based-exfoliability measure larger than the median value (25.9), and between the minimum (10.5) and median values of already-exfoliated crystals, respectively. Afterward, an extended topology-scaling algorithm shows that 138 (93%) of these exfoliable bulk crystals are layered solids, and the analysis on packing ratios shows that 147 (99%) predicted exfoliable bulk crystals exhibit a relatively low packing ratio value ranging between 0.1 and 0.8, providing further supports to our prediction. Finally, the characteristics of these predicted 2D materials were discussed for practical applications.

RESULTS AND DISCUSSION

Elasticity-based-exfoliability measure based on an exfoliation mechanics model

The mechanical exfoliation of 2D materials can be rationalized into a forced peeling model as illustrated in Fig. 2a (see ref. [30] for details). Based on the Rivlin model[31], the peeling force F can be written as $F(1\text{-}\cos\alpha) = \gamma w$, where α and w are the peeling angle and peeling sheet width (Fig. 2a), respectively, and γ is the cleavage energy density. Then, we define a 2D peeling stress which is the applied peeling force divided by the width of the 2D sheet, that is, $\sigma_{2D} = F/w = \gamma/(1\text{-}\cos\alpha)$. To ensure the in-plane mechanical integrity during mechanical exfoliation, σ_{2D} should be lower than the intrinsic 2D strength of the material (σ_s), that is $\sigma_{2D} = \gamma/(1\text{-}\cos\alpha) < \sigma_s$, since the real strength of 2D materials that usually contain defects can be much lower than σ_s[32–35]. Consequently, a fracture-based-exfoliability measure $\sigma_s/\gamma > C$ can be derived, where C is an exfoliable threshold. First-principles calculations for some already-exfoliated 2D materials show that the values of σ_s/γ for graphene, h-BN, MoS_2, and black phosphorus are 104.4, 191.6, 50.3, and 42.9, respectively, indicating their high exfoliability. This measure considers both in-plane and out-of-plane mechanical properties of 2D materials and shows great reliability[30]. However, both computational and experimental

determinations of in-plane strength and cleavage energy density for bulk crystals are costly, which prevents the fracture-based-exfoliability measure from being widely used for high-throughput identification of exfoliable 2D materials.

As an alternative, elasticity-based techniques have been widely used to characterize the properties of materials, engineering structures, and biological tissues. These techniques are non-destructive and efficient, as the elastic deformation can be fully recovered after mechanically unloading. A canonical example is ultrasonic testing that utilizes elastic waves to detect cracks and defects in parts and materials. Inspired by the elasticity-based techniques, we extended the aforementioned fracture-based-exfoliability measure (σ_s/γ) into an elasticity-based-exfoliability measure for high-throughput computational identification of exfoliable 2D materials. Under a linear elasticity assumption, the 2D uniaxial tensile strength of a 2D material can be written as $\sigma_s = Y_{in}\varepsilon_{in}d$, where Y_{in}, ε_{in}, and d are the in-plane Young's modulus, strain-to-failure, and interlayer distance, respectively. The cleavage energy density is $\gamma = Y_{out}{\varepsilon_{out}}^2 d/2$, where Y_{out} and ε_{out} are the out-of-plane Young's modulus and strain-to-failure, respectively. Hence, the fracture-based-exfoliability measure can be written as

$$\sigma_s/\gamma = (2\varepsilon_{in}/\varepsilon_{out}^2)(Y_{in}/Y_{out}). \quad (1)$$

As most single crystals would break at a certain strain[32,36], a constant pre-factor $f = 2\varepsilon_{in}/{\varepsilon_{out}}^2$ can be assumed. The justification of this assumption is made as follows. Since the tensile strength and cleavage energy are much more complex than the linear-elastic moduli, it is challenging to screen these properties over all possible exfoliable planes (or directions) by using first-principles calculations for anisotropic materials. As an alternative, the tensile strength and cleavage energy of crystals were correlated with the elastic moduli based on the above-mentioned assumptions for an ideal crystal, Frenkel's model[37] indicates that the tensile strength is about 1/10 of the Young's modulus, that is $\sigma_{th} \approx Y/10$. This is generally consistent with more recent results[38–40], which predict that crystals can break at the stress of Y/15-Y/8. In addition, we calculated the in-plane and out-of-plane mechanical properties for two typical exfoliable crystals (graphite and h-BN, see "Methods" for calculation details). It can be seen that the in-plane and out-of-plane strain-to-failure are 19% and 18% for graphite, and 18% and 16% for h-BN, respectively, resulting in the corresponding pre-factor values of 11.73 and 14.06, respectively. These results indicate a relatively narrow range of pre-factor values. Considering that the elasticity-based-exfoliability measure values for exfoliable crystals are orders of magnitude larger than that of non-exfoliable crystals as discussed below, it is expected that the assumption of constant pre-factor would have relatively insignificant effects on the prediction of exfoliability. Therefore, the ratio of the in-plane Young's modulus to the out-of-plane Young's modulus of crystals is proportional to the fracture-based-exfoliability measure (σ_s/γ)

$$Y_{in}/Y_{out} \propto \sigma_s/\gamma. \quad (2)$$

Notably, this formula is derived for in-plane isotropic sheet crystals that has a definite exfoliable plane. However, for most bulk crystals, the exfoliable plane is unknown and the in-plane property is anisotropic. It is expected that for any plane of a generally anisotropic bulk crystal (xy-plane), there is a minimum in-plane Young's modulus [$\min_{xy}(Y_{in})$], and the most possible exfoliable plane of a bulk crystal is the plane having the maximum value of [$\min_{xy}(Y_{in})$]/Y_{out}. Hence, the maximum ratio of the minimum in-plane Young's modulus to the out-of-plane Young's modulus over all possible exfoliable planes of an unknown bulk crystal can be used to define a measure of exfoliability as

$$E = \max_z \left[\frac{\min_{xy}(Y_{in})}{Y_{out}}\right], \quad (3)$$

where z is the out-of-plane directional vector of an arbitrarily possible exfoliable plane xy. The xy-plane for obtaining E can be seen as the most possible exfoliable plane of the crystal. Notably, the minimum in-plane Young's modulus was adopted for calculating the exfoliability of anisotropic crystals (Eq. (3)). Considering that some materials might be exfoliated along a higher in-plane modulus direction, our measure would provide a conservative prediction on the exfoliability of such materials. The larger of E for a specific crystal is, the easier the 2D material can be mechanically exfoliated from the crystal. Overall, E satisfies all three criteria for a proper measure of exfoliability as specified above: (i) It has a clear physical meaning from an exfoliation mechanics model. (ii) It is universally applicable to all material systems. Although empirical assumptions and threshold values have been adopted in the derivation of this measure, no empirical parameters are needed when calculating the measure from the elastic tensors of crystals by using Eq. (3). Meanwhile, it can correctly filtrate out the crystals having low in-plane mechanical resistance that cannot resist the exfoliating loads by considering the in-plane and out-of-plane mechanical properties of bulk crystals. (iii) It can be calculated from the elastic tensors of crystals that can be conveniently obtained by first-principles calculations or experimental measurements. Since the elastic tensors have been calculated and collected for a large number of crystals in the MP database, this measure can be directly used for high-throughput computational exfoliation of 2D materials.

High-throughput computational identification

The elasticity-based-exfoliability measure can be extracted from the elastic tensor of crystals. We first calculated the Young's moduli of all directions for a crystal (see "Methods" for details). Typical Young's moduli distribution of graphite is shown in Fig. 2b. Afterward, the elasticity-based-exfoliability measure can be obtained based on Eq. (3).

Following the above-mentioned procedures, we calculated the elasticity-based-exfoliability measure for crystals having a first-principles calculated elastic tensor from MP database to identify exfoliable 2D materials. It should be noted that our prediction of the exfoliability depends on the accuracy of calculated data in MP database. Although some data in MP database are found to be incorrectly presented due to the possible processing or calculating errors[41], our previous work[41] indicated that most of the data in the MP database are reliable. By October 1, 2021, MP crystal structure database organizes 144,595 inorganic crystal materials, in which 13,176 crystals have structural information and first-principles calculated elastic tensors. As shown in Fig. 3a, we first extracted these 13,176 crystals from MP database. Before calculating the elasticity-based-exfoliability measure of these crystals, we cleaned the database by filtering out crystals having non-positive definite stiffness tensor (in the processing, the crystals have the minimum eigenvalue of the elastic tensor $\lambda_{min} \leq$ 0.1 GPa were filtrated out). Thus, 11,503 crystals that satisfy the Born criteria of elastic stability were retained. Furthermore, 691 crystals containing radioactive elements were also filtered out. Finally, the elasticity-based-exfoliability measures and the corresponding exfoliable planes of all 10,812 retained crystals were automatically calculated using a developed batch program.

The minimum in-plane Young's modulus [$\min_{xy}(Y_{in})$] and the out-of-plane Young's modulus (Y_{out}) for the most possible exfoliated plane of each crystal were calculated as distributed in Fig. 3b. Approximately 3% (293 crystals), 2% (190 crystals), and 1% (106 crystals) of the total crystals have E values above 5, 10, and 20, respectively. To filtrate out the duplicate crystals, we determined the crystal topologies using a topological approach[42], and then identified duplicate crystal structures

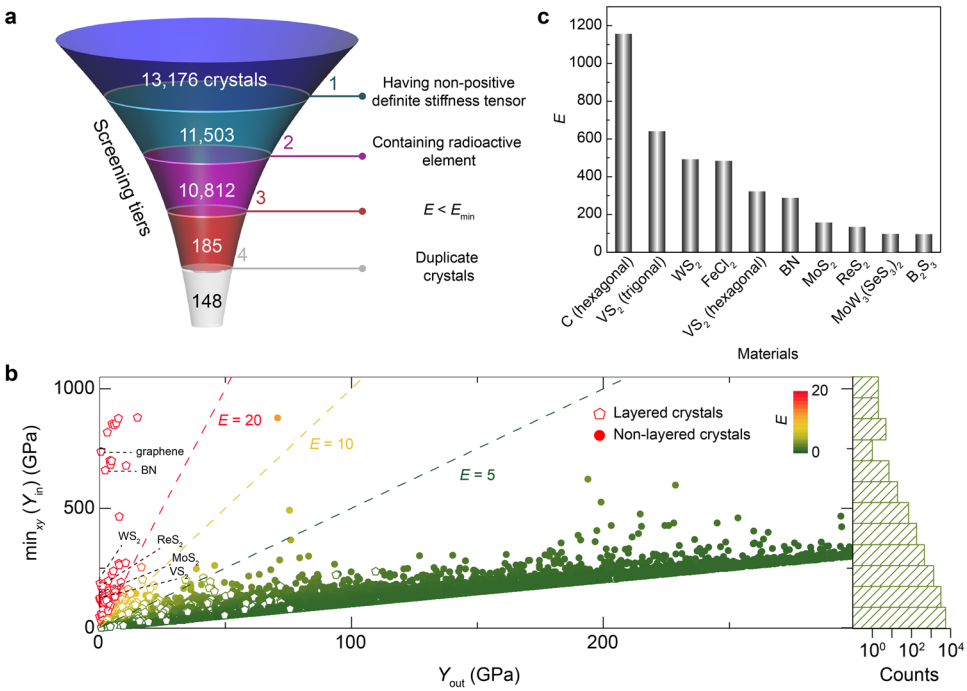

Fig. 3 High-throughput computational identification of exfoliable 2D materials. a Tiered screening pipeline for discovery of easily and potentially exfoliable crystals. Tier 1: Filter out the crystals having non-positive definite stiffness tensor. Tier 2: Filter out the crystals which contain radioactive elements. Tier 3: Filter out the crystals with a measure less than E_{min}. Tier 4: Filter out the duplicate crystals. **b** Distribution of the minimum in-plane Young's modulus [$\min_{xy}(Y_{in})$] and the out-of-plane Young's modulus (Y_{out}) for the most possible exfoliated plane of all 10,812 crystals. **c** Top 10 crystals with the largest elasticity-based-exfoliability measure.

Table 1. Information of top 10 crystals with the largest elasticity-based-exfoliability measure.

Formula	Measure	Density (g/cm^3)	Energy-above-hull (eV/atom)	ID
C[8] (hexagonal)	1156.3	0.756	0.008	mp-990448
VS_2[44] (trigonal)	641.2	3.364	0.003	mp-1013526
WS_2[45]	492.8	6.577	0.000	mp-224
$FeCl_2$	484.6	3.184	0.324	mp-571096
VS_2 (hexagonal)	322.0	3.024	0.000	mp-1013525
BN[46]	288.1	1.825	0.000	mp-7991
MoS_2[47]	157.1	4.306	0.001	mp-1018809
ReS_2[48]	134.9	6.733	0.000	mp-572758
$MoW_3(SeS_3)_2$	97.3	5.069	0.034	mp-1029037
B_2S_3	95.6	1.955	0.105	mp-866066

based on their topologies. After filtering out the duplicate crystals, the crystals having the top 10 values of E were sorted in Fig. 3c, which contains 6 experimentally exfoliated 2D materials, including graphene[8], VS_2[43], WS_2[44], BN[45], MoS_2[46], and ReS_2[47]. Table 1 presents the related information of these 10 materials. Furthermore, we did a literature survey on already-exfoliated 2D crystals and calculated their values of E, and found 34 already-exfoliated 2D crystals with $E \geq 10$ in experiments. The already-exfoliated 2D crystals in experiments have E ranging from 10.5 to 1156.3 (Supplementary Table 1). Herein, the median value and the minimum value of E of already-exfoliated 2D crystals ($E_{med} = 25.9$, $E_{min} = 10.5$) are defined as two exfoliable thresholds for easy and potential exfoliation, there are 58 crystals exhibiting $E \geq E_{med}$ and 90 crystals having $E_{med} > E \geq E_{min}$ (Supplementary Table 1), which are expected to be easily exfoliable 2D crystals and potentially exfoliable 2D crystals, respectively. The typical atomistic views of predicted top 10 exfoliable 2D crystals are shown in Fig. 4a.

Supports for the prediction

We then checked whether the predicted exfoliable bulk crystal is a layered crystal and where the cleaved plane locates. To this end, we first extended the topology-scaling algorithm proposed by Ashton et al.[26] to identify layered crystals and the normal vectors of cleaved planes therein. In this algorithm, the bonded clusters of atoms in a crystal cell are first determined, where a bond is formed if the distance between two neighboring atoms is <1.3 times of the sum of their covalent radii (the adopted covalent radii are from refs. [26,48]). Afterward, the original crystal cell is extended into a $n \times n \times n$ supercell, in which the maximum number of atoms in an isolated bonded cluster (m) is counted. If m scales as n^2, it is identified as a layered crystal. Then, a least square method is used for fitting the atoms coordinates in the cluster to obtain the normal vector of the cleaved plane ($\boldsymbol{a}$) for the identified layered crystal. The results show that 55 (95%) of the predicted 58 easily exfoliable crystals and 83 (92%) of the 90 potentially exfoliable

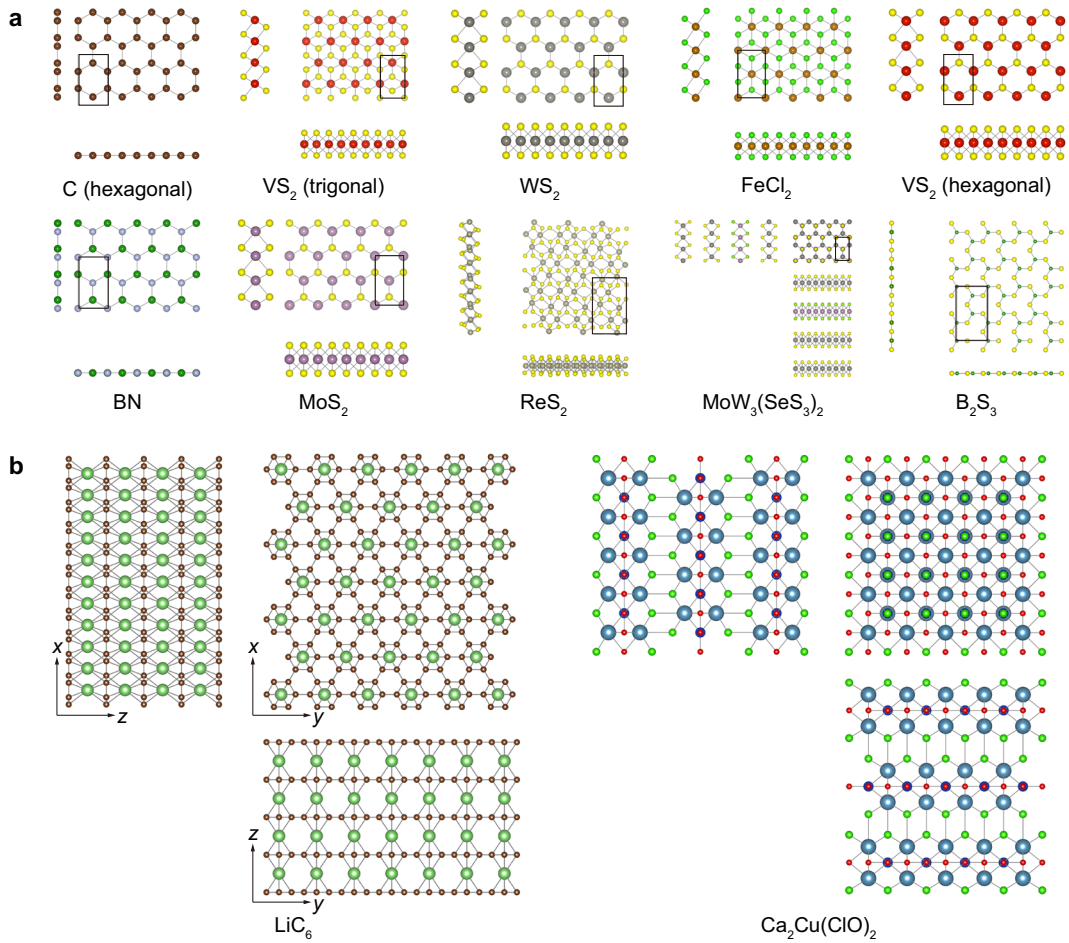

Fig. 4 Structures of typical predicted promising exfoliable crystals. a Crystal structure prototypes of the top 10 crystals with the largest elasticity-based-exfoliability measure. **b** Two typical non-layered crystals with an elasticity-based-exfoliability measure above E_{min}. The *xy*-plane shown in the top view of crystals corresponds to the exfoliation plane.

crystals are layered crystals, and all predicted exfoliable planes are the out-of-planes of these layered crystals, which supports the prediction of exfoliable 2D materials from our measure. Notably, the exfoliable crystals are not equivalent to layered crystals. If a crystal contains material planes that are loosely interlayer bonded, it might be exfoliable, such as LiC_6 and $Ca_2Cu(ClO)_2$ (Fig. 4b). Recent experiments provided supports on that non-layered materials can be exfoliated into 2D materials, such as WO_3[49], PbS[50], Bi[51], and Te[52]. Among these materials, Bi and Te are prepared by hot-pressing their bulk agglomerates, indicating the potential of breaking interfacial bonds by mechanical methods. Furthermore, we found that the percentage of layered crystals increases for crystals having larger *E* (Fig. 5a), which falls within our expectation. These results support our prediction on exfoliable crystals and suggest that non-layered crystals are possible to be exfoliated.

In addition, we calculated the packing ratio of each crystal (Fig. 5b), which is defined as the covalent volume of all atoms divided by the total volume of the crystal cell. Most (99%) predicted exfoliable bulk crystals have packing ratios ranging between 0.1 and 0.8. Figure 5b also shows that the mean value of packing ratio will increase for crystals having smaller *E*. This indicates that our predicted exfoliable crystals generally have a relatively low packing ratio and thus a loosely packed structure, which is consistent with the conclusions in references[25,29] and further supports the prediction of exfoliable 2D crystals from our elasticity-based-exfoliability measure.

Characteristics of exfoliable crystals

Finally, we extracted the characteristics for 148 promising exfoliable crystals (Fig. 6). We first showed the distributions of crystal systems in all crystals from MP database, compared to that of our identified 149 exfoliable crystals (Fig. 6a). The notable difference exists in cubic crystal system, in which there is no promising exfoliable crystals. The results also show that crystals of trigonal crystal system are most promising for mechanical exfoliation. Figure 6b compares the distribution of compositional complexity of identified exfoliable crystals, from which we can find that binary (85) and ternary (54) compounds comprise 94% of all 148 crystals. Furthermore, the stability is significant for using such exfoliable crystals, which can be measured by the value of energy-above-hull[41]. Figure 6c shows the values of energy-above-hull for all 10,812 crystals. The distribution range of energy-above-hull values for crystals with larger *E* values becomes narrow. These results might be attributed to that the number of crystals is rapidly reduced as *E* values increase (Fig. 6c).

In summary, we theoretically derived a simple and universal elasticity-based-exfoliability measure for high-throughput computational identification of exfoliable 2D materials. Based on this measure, we evaluated the feasibility of exfoliating 2D materials from bulk crystals in MP database. By roughly setting the median (25.9) and minimum (10.5) values of the elasticity-based-exfoliability measure for already-exfoliated 2D materials as threshold values for easily and potentially exfoliable materials, respectively, the search yields 58 easily and 90 potentially exfoliable 2D materials. Our predictions are

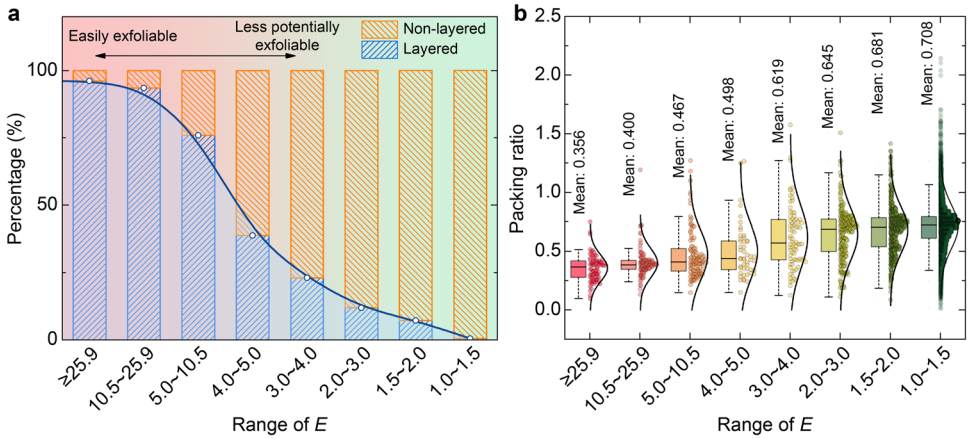

Fig. 5 Supports from topological and structural analysis of a large number of crystals. a Percentage of layered crystals, and **b** box plots and distributions of packing ratios for 10,812 crystals having different ranges of *E*. The dots represent the packing ratio value for each crystal. On each box, the central mark indicates the median, and the bottom and top edges indicate the 25th and 75th percentiles of packing ratio values, respectively.

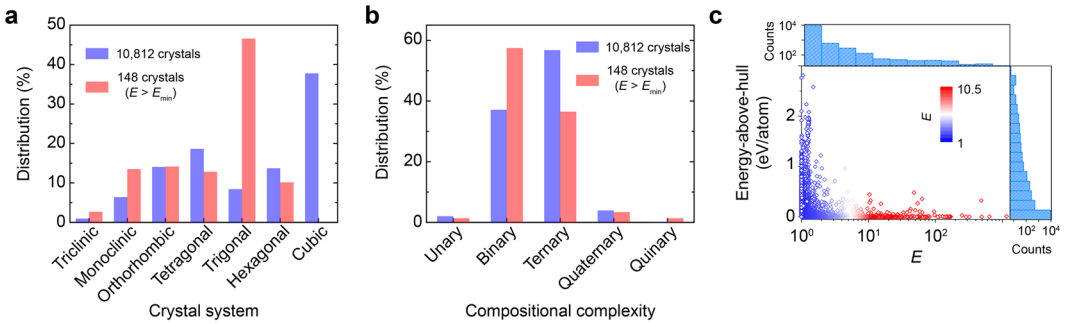

Fig. 6 Characteristics of 149 easily and potentially exfoliable crystals. a Distributions of crystal systems for all 10,812 crystals from MP database and 148 crystals with an elasticity-based-exfoliability measure above 10.5. **b** Distributions of the compositional complexity among 10,812 crystals and 148 exfoliable crystals. **c** Distributions of energy-above-hull values for all 10,812 crystals.

supported by topological and structural analysis of 10,812 crystals, and literature survey of already-exfoliated crystals. In addition, characteristics of predicted exfoliable crystals were discussed. This work not only provides a fundamental measure of exfoliability for the high-throughput computational identification of exfoliable 2D materials, but also extends the scope of potential 2D materials to be explored.

METHODS

First-principles calculations

The density functional theory calculations were conducted via the Vienna ab initio simulation package (VASP)[53]. The Perdew–Burke–Ernzerhof parameterization of the generalized gradient approximation was used for the exchange and correlation interactions[54,55]. The cut-off energy was set as 520 eV in all calculations to ensure the accuracy. To avoid the interaction from periodically repeated images, the vacuum layer of 40 Å was adopted. A Monkhorst-Pack *k*-mesh with densities about 40 Å (the product of each lattice constant and the corresponding number of *k*-points) was adopted. For all calculations, the convergence criteria for energy and force on each atom were 0.1 meV and 0.001 eV/Å, respectively.

Computation of Young's moduli in all directions

The generalized Hooke's law describes the relation between the stress (σ) and strain (ε) for a material, that is, $\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$ or $\varepsilon_{ij} = S_{ijkl}\sigma_{kl}$, where C_{ijkl} is the stiffness tensor and S_{ijkl} is the compliance tensor. For anisotropic materials, the stiffness and compliance tensors are orientation-dependent. With Einstein's summation rule, the transformation for the fourth-order tensor can be described as $S'_{\alpha\beta\gamma\delta} = r_{\alpha i}r_{\beta j}r_{\gamma k}r_{\delta l}S_{ijkl}$, where $r_{\alpha i}$ is the direction cosine between the new (α) and reference (i) coordinates. By defining two angles (θ and φ) in spherical coordinates, a single unit vector $\boldsymbol{a}$ can be used to represent the Young's modulus along a certain direction, that is[56]:

$$\boldsymbol{a} = \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix}, (0 \le \theta \le \pi, 0 \le \varphi \le 2\pi). \quad (4)$$

With the above equation, the Young's modulus in an arbitrary direction is derived as

$$Y = \frac{1}{S'_{1111}} = \frac{1}{r_{1i}r_{1j}r_{1k}r_{1l}S_{ijkl}} = \frac{1}{a_i a_j a_k a_l S_{ijkl}}. \quad (5)$$

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

CODE AVAILABILITY

All codes of this current study are available from the corresponding author upon reasonable request.

Received: 14 July 2021; Accepted: 19 November 2021;
Published online: 20 December 2021

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ACKNOWLEDGEMENTS

This work was supported by the National Natural Science Foundation of China (12172261 and 11902225). X.J. acknowledges the technical assistance from Xiaoang Yuan and Boxue Wang. The numerical calculations in this work have been performed on a supercomputing system in the Supercomputing Center of Wuhan University.

AUTHOR CONTRIBUTIONS

E.G. conceived the idea. C.Q. and K.H. provided advices on this project. Q.S. and Y.X. wrote the program. X.J., R.L, Y.G., Q.S., and E.G. carried out the analysis. All authors wrote the paper. X.J., Q.S., and Y.X. are co-first authors.

COMPETING INTERESTS

The authors declare no competing interests.

ADDITIONAL INFORMATION

Supplementary information The online version contains supplementary material available at https://doi.org/10.1038/s41524-021-00677-4.

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Supplementary Information for

Elasticity-Based-Exfoliability Measure for High-Throughput Computational Exfoliation of Two-Dimensional Materials

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Supplementary Table 1 Information of crystals with $E \geq E_{min}$.

Formula	Measure	Band Gap (eV)	Density (g/cm^3)	Energy-above-hull (eV/atom)	Formation energy (eV/atom)	Magnetic Ordering	Tot. Magnetization (μ_B/cell)	ID
C[1] (hexagonal)	1156.3	0.000	0.756	0.008	0.008	NM	0.000	mp-990448
VS_2[2] (trigonal)	641.2	0.000	3.364	0.003	-1.291	FM	0.627	mp-1013526
WS_2[3]	492.8	1.566	6.577	0.000	-1.261	NM	0.000	mp-224
$FeCl_2$	484.6	0.623	3.184	0.324	-0.698	FM	0.000	mp-571096
VS_2 (hexagonal)	322.0	0.000	3.024	0.000	-1.294	NM	0.001	mp-1013525
BN[4]	288.1	4.270	1.825	0.000	-1.473	NM	0.000	mp-7991
MoS_2[5]	157.1	1.336	4.306	0.001	-1.307	NM	0.000	mp-1018809
ReS_2[6]	134.9	1.446	6.733	0.000	-1.011	NM	0.000	mp-572758
$MoW_3(SeS_3)_2$	97.3	1.162	5.069	0.034	-1.102	NM	0.000	mp-1029037
B_2S_3	95.6	1.547	1.955	0.105	-0.727	NM	0.000	mp-866066
$PtSe_2$[5]	81.5	0.674	7.821	0.000	-0.387	NM	0.000	mp-1115
Mo_2SeS_3	77.7	0.758	3.574	0.010	-1.140	NM	0.000	mp-1027890
$Ca_2Cu(BrO)_2$	74.5	0.000	4.171	0.000	-2.114	NM	0.009	mp-545481
NbS_2[7] (hexagonal)	69.0	0.000	4.020	0.000	-1.456	NM	0.007	mp-10033
$TaSe_2$[8] (trigonal)	66.3	0.000	7.759	0.004	-0.814	FM	0.471	mp-7834
$Mo(WSe_3)_2$	63.8	1.240	5.296	0.084	-0.595	NM	0.000	mp-1025575
CN_2	63.4	4.792	2.551	0.358	0.358	NM	0.000	mp-1019086
$NbSe_2$[5] (orthorhombic)	63.1	0.000	3.211	0.011	-0.830	FM	0.975	mp-7007
Te_2Mo (hexagonal)	62.6	1.120	6.928	0.001	-0.274	NM	0.000	mp-602
ZrI_2	58.9	0.298	5.355	0.000	-0.893	NM	0.001	mp-570506
C_3N_4	58.4	2.194	2.337	0.108	0.108	NM	0.000	mp-971683
LiC_{12}	58.1	0.000	2.019	0.000	-0.006	NM	0.000	mp-1021323

SmBrO	56.9	4.524	6.013	0.000	-3.138	NM	0.000	mp-29327
$TiNbS_4$	56.6	0.000	3.656	0.019	-1.567	NM	0.000	mp-34289
$MoSe_2$[5]	55.1	1.481	5.970	0.000	-0.673	NM	0.000	mp-7581
PtS_2[9]	55.1	1.444	6.204	0.000	-0.792	NM	0.000	mp-762
NbS_2 (tetragonal)	54.3	0.000	4.146	0.269	-1.187	NM	0.003	mp-1008860
SnS_2[5]	52.2	1.562	3.670	0.000	-0.823	NM	0.000	mp-1170
$TeMoWSeS_2$	50.1	0.000	5.115	0.130	-0.760	NM	0.001	mp-1027164
SnGe	48.1	0.609	1.531	0.481	0.481	NM	0.000	mp-995181
$AlCl_3$	44.7	5.311	2.215	0.000	-1.951	NM	0.000	mp-25469
Nb_2CS_2	44.6	0.000	4.974	0.022	-1.114	NM	0.000	mp-5745
SnO_2	42.6	2.005	5.755	0.153	-1.970	NM	0.000	mvc-11686
AlClO	42.3	5.597	2.642	0.000	-2.784	NM	0.000	mp-27863
$SrMg_6Ga$	41.4	0.000	2.428	0.116	-0.013	NM	0.030	mp-1016442
WSe_2[5]	39.7	1.677	5.900	0.000	-0.557	NM	0.000	mp-1028698
ZrNCl	39.5	1.756	4.199	0.000	-2.092	NM	0.000	mp-568592
YBr_3	39.0	4.052	3.482	0.000	-1.916	NM	0.000	mp-754815
$Te_2Mo_3W(Se_2S)_2$	37.6	0.397	4.977	0.087	-0.679	NM	0.001	mp-1030827
ZrIN (orthorhombic)	37.6	1.217	4.968	0.000	-1.502	NM	0.000	mp-23052
TmBrO	37.2	4.377	7.072	0.000	-3.191	NM	0.000	mp-754969
PtO_2	34.9	1.542	9.219	0.005	-0.932	NM	0.000	mp-7868
TiIN	33.9	0.015	4.638	0.000	-1.279	NM	0.000	mp-27848
$TiMn_2O_6$	33.2	1.499	3.931	0.085	-2.299	FM	6.000	mp-775831
NbS_2 (trigonal)	33.0	0.000	4.184	0.037	-1.419	NM	0.043	mp-995122
PdS_2	32.2	0.654	4.277	0.000	-0.713	NM	0.000	mp-13682
NdI_2	32.1	0.000	5.590	0.000	-1.295	NM	0.016	mp-28753
$NiCl_2$	31.4	0.000	3.221	0.000	-0.765	FM	0.140	mp-27396

$ScCl_3$	31.2	3.879	2.137	0.000	-2.564	NM	0.000	mp-23309
TiS_2[5] (trigonal)	31.0	0.000	2.865	0.000	-1.715	NM	0.000	mp-2156
Te_2W	29.8	0.000	8.523	0.000	-0.106	NM	0.000	mp-22693
NiS_2	29.0	0.000	4.323	0.022	-0.678	NM	0.000	mp-850131
BiBrO	28.4	2.308	7.294	0.000	-1.384	NM	0.000	mp-23072
SnS[10]	27.5	1.532	2.572	0.046	-0.732	NM	0.000	mp-8781
ZrIN (trigonal)	27.4	1.018	5.816	0.030	-1.472	NM	0.000	mp-580886
$Na_3(CuO_2)_2$	27.0	0.000	3.689	0.042	-1.350	FM	1.005	mp-754483
$MgCl_2$ (trigonal)	26.9	5.674	2.055	0.000	-2.254	NM	0.000	mp-23210
TaS_2[5]	26.5	0.000	6.115	0.000	-1.491	NM	0.013	mp-1984
$Sr_2Cu(BrO)_2$	25.8	0.000	4.735	0.000	-2.139	NM	0.005	mp-546898
LaFeSi	25.7	0.000	6.128	0.000	-0.583	NM	0.077	mp-505332
$MgPSe_3$	25.7	2.296	3.593	0.000	-0.606	NM	0.000	mp-30943
$CrSiTe_3$[5]	25.3	0.000	4.995	0.000	-0.177	FM	0.491	mp-3779
$CrBr_3$[11]	25.2	1.291	3.943	0.000	-0.817	FM	2.992	mp-27734
H_3ClO	24.9	5.390	1.419	0.000	-1.234	NM	0.000	mp-34078
GaS[5]	24.0	1.948	3.392	0.006	-0.977	NM	0.000	mp-9889
$TiGeO_3$	23.8	1.123	3.933	0.040	-2.693	NM	0.000	mp-780260
CrP_2S_7	23.5	0.000	2.131	0.056	-0.689	FM	0.000	mp-768680
VCl_2	23.4	1.260	2.873	0.000	-1.551	FM	3.001	mp-22877
$SmBr_3$	22.8	2.929	4.833	0.000	-1.895	NM	0.000	mp-27976
$Mg_2Al_2Se_5$	22.4	1.985	3.766	0.000	-1.049	NM	0.012	mp-29624
LaI_2	22.4	0.000	5.584	0.000	-1.420	NM	0.010	mp-23194
NdBrO	22.3	4.483	5.810	0.000	-3.111	NM	0.000	mp-23068
Ta_2CS_2	22.1	0.000	8.684	0.007	-1.193	NM	0.000	mp-559976
Nb_3SBr_7	22.1	0.744	4.636	0.000	-1.060	NM	0.000	mp-29057
ZrS_2[5]	21.6	1.042	3.307	0.000	-1.956	NM	0.002	mp-1186

Sc_2NCl_2	21.5	0.000	3.086	0.000	-2.298	NM	0.015	mp-28480
VSe_2[5]	21.4	0.000	5.086	0.000	-0.692	FM	0.731	mp-694
MgI_2	21.3	3.677	3.893	0.000	-1.031	NM	0.000	mp-23205
TiNCl	20.9	0.561	2.961	0.000	-1.861	NM	0.000	mp-27850
$HfSnO_3$	20.6	2.378	6.593	0.069	-3.008	NM	0.001	mp-776083
LaI_3	20.4	2.071	4.888	0.000	-1.547	NM	0.000	mp-27979
Nb_3TeCl_7	19.9	0.703	3.729	0.000	-1.579	NM	0.000	mp-28938
$TePdI_2$	19.9	0.546	5.924	0.016	-0.245	NM	0.000	mp-573321
Nb_3Cl_8	19.9	0.151	3.361	0.000	-1.702	FM	0.991	mp-29950
$ZrCl_2$	19.6	0.861	3.856	0.000	-2.041	NM	0.000	mp-23162
$TaSe_3$	19.2	0.000	7.392	0.000	-0.653	NM	0.000	mp-29652
$Ni(PS_3)_2$	19.0	0.325	2.635	0.093	-0.568	NM	0.000	mp-769218
GaSe[12]	18.5	1.248	4.408	0.000	-0.591	NM	0.000	mp-1943
$NdBr_3$	18.4	2.922	4.632	0.000	-1.910	NM	0.000	mp-27975
NbS_3	18.3	0.376	3.836	0.017	-1.253	NM	0.000	mp-562100
MnS_2	18.1	0.000	2.768	0.000	-0.997	FM	3.000	mvc-14047
$SnSe_2$[5]	17.8	0.800	5.121	0.000	-0.345	NM	0.000	mp-665
SiH	17.7	2.140	1.277	0.030	-0.042	NM	0.000	mp-29803
$DyCl_3$	17.0	3.900	3.904	0.000	-2.698	NM	0.000	mp-28448
HfSiTe	16.8	0.000	8.002	0.000	-0.720	NM	0.000	mp-13963
$MnBr_2$	16.4	1.611	3.826	0.000	-0.813	FM	5.001	mp-28306
Ti_2Te_2P	16.1	0.000	5.513	0.000	-0.915	NM	0.025	mp-12527
$TiSe_2$[5]	16.1	0.000	4.693	0.000	-1.112	NM	0.000	mp-2194
$CoCl_2$	15.9	0.068	3.488	0.024	-0.945	FM	3.000	mp-632413
BiClO	15.9	2.639	7.213	0.000	-1.696	NM	0.000	mp-22939
TiOF	15.4	0.000	3.431	0.069	-3.413	NM	0.000	mp-753059
$CrGeTe_3$[5]	15.3	0.000	5.599	0.260	0.110	FM	0.214	mp-541449

$CuTeO_4$	15.2	0.000	5.073	0.017	-1.218	FM	0.228	mp-755455
Rb_2O	15.2	0.484	3.226	0.000	-1.138	NM	0.001	mp-753746
$CdCl_2$	15.1	3.595	3.611	0.000	-1.489	NM	0.000	mp-22881
InSe[5] (monoclinic)	14.6	1.076	5.390	0.036	-0.474	NM	0.000	mp-21405
$MnCl_2$	14.6	1.797	2.673	0.000	-1.482	FM	5.000	mp-28233
$TiSnO_3$	14.5	1.108	4.572	0.000	-2.767	NM	0.000	mp-754246
Nb_3TeI_7	14.4	0.480	5.728	0.002	-0.541	NM	0.000	mp-567713
$Mg(AlSe_2)_2$	14.4	1.072	3.579	0.021	-0.953	NM	0.000	mp-9479
Cu_2WS_4	14.4	1.620	4.299	0.003	-0.838	NM	0.000	mp-8976
$TaSe_2$[5] (hexagonal)	14.1	0.000	7.840	0.013	-0.801	NM	0.003	mp-501
Ga_2NiS_4	14.1	0.000	3.752	0.066	-0.894	NM	0.030	mp-6959
Ta_2Se	14.0	0.000	12.220	0.000	-0.445	NM	0.000	mp-8732
$ZnBr_2$	14.0	3.308	4.049	0.086	-0.826	NM	0.000	mp-569960
BiIO	13.4	1.484	7.379	0.000	-1.215	NM	0.000	mp-22987
NiI_2	13.2	0.000	5.585	0.000	-0.023	NM	0.026	mp-27638
TiClO	13.0	0.000	3.092	0.038	-2.716	NM	0.006	mp-22992
CdI_2	13.0	2.405	5.057	0.001	-0.591	NM	0.002	mp-570437
TiBrO	12.9	0.000	4.142	0.019	-2.365	FM	0.321	mp-23002
InSe (hexagonal)	12.9	0.459	5.078	0.003	-0.507	NM	0.000	mp-20485
$Mg(AlS_2)_2$	12.8	2.017	2.214	0.030	-1.540	NM	0.000	mp-16755
HfS_3	12.8	1.136	5.092	0.000	-1.694	NM	0.000	mp-9922
BiO_2	12.8	1.083	8.946	0.000	-1.471	NM	0.000	mp-557993
$AlSiTe_3$	12.5	1.343	4.573	0.000	-0.268	NM	0.000	mp-31220
BiTeBr	12.4	1.297	6.082	0.000	-0.505	NM	0.000	mp-33723
LiC_6	12.4	0.000	2.164	0.002	-0.003	NM	0.003	mp-1001581
$PdSe_2$[5]	12.3	0.009	5.937	0.000	-0.283	NM	0.000	mp-2418

CuI	12.3	1.647	5.687	0.001	-0.152	NM	0.000	mp-570081
NbI_2O	12.1	0.843	5.133	0.000	-1.436	NM	0.000	mp-549720
Te_2Mo (monoclinic)	12.0	0.000	6.764	0.015	-0.261	NM	0.000	mp-7459
ZnSe	12.0	1.967	4.681	0.160	-0.556	NM	0.000	mp-569679
$HfSe_3$	12.0	0.611	6.660	0.000	-1.013	NM	0.000	mp-15622
Br	12.0	1.327	3.373	0.000	0.000	NM	0.000	mp-23154
$Ca_2Cu(ClO)_2$	11.7	0.000	3.554	0.019	-2.408	NM	0.013	mp-23143
$Mg_3Si_4(HO_6)_2$	11.7	5.232	2.694	0.000	-3.000	NM	0.000	mp-696497
TiBrN	11.6	0.555	3.940	0.000	-1.508	NM	0.000	mp-27849
Bi_2Se_3[5]	11.5	0.543	7.056	0.000	-0.388	NM	0.000	mp-541837
ZrSiTe	11.5	0.000	6.063	0.000	-0.800	NM	0.000	mp-19917
PbI_2[13]	11.5	2.413	5.461	0.003	-0.665	NM	0.001	mp-540789
$ZrSe_2$[14]	11.3	0.343	4.935	0.000	-1.329	NM	0.000	mp-2076
ScHCl	11.2	0.000	2.742	0.000	-1.609	NM	0.000	mp-24081
GaTe[15]	11.0	1.035	5.008	0.003	-0.361	NM	0.000	mp-542812
$TaTe_4Ir$	10.9	0.000	8.616	0.000	-0.367	NM	0.001	mp-17287
$MoCl_3$	10.9	0.146	3.211	0.083	-1.226	NM	0.000	mp-22853
GaGeTe	10.8	0.284	4.989	0.008	-0.235	NM	0.000	mp-8211
GeAs	10.6	0.639	4.813	0.002	-0.031	NM	0.000	mp-9548
$NbTe_2$[5]	10.5	0.000	6.804	0.036	-0.425	NM	0.011	mp-1018150

Structure information of crystals with $E \geq E_{min}$.

1. C (P6/mmm)

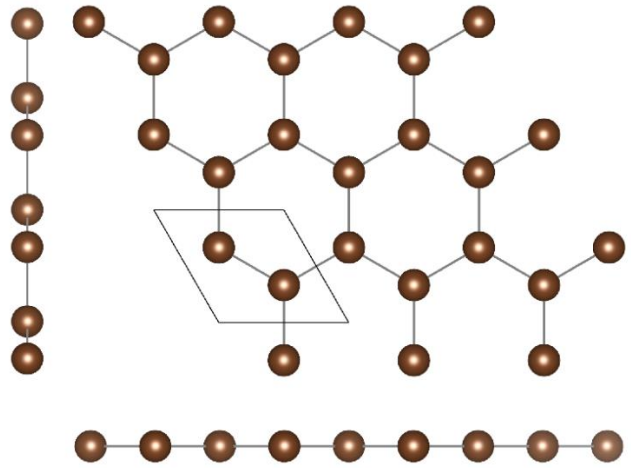
Formula	C	**ID**	mp-990448
Measure	1156.3	**Symbol**	P6/mmm
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	0.756	**Energy-Above-Hull / Atom (eV)**	0.008
Formation Energy / Atom (eV)	0.008	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of C in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.23421000	-2.13771000	0.00000000
a_2	1.23421000	2.13771000	0.00000000
a_3	0.00000000	0.00000000	9.99906000

	x (Å)	*y* (Å)	*z* (Å)
C	1.23420000	-0.71260000	0.00000000
C	1.23420000	0.71260000	0.00000000



Orthographic projections: views of C as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

2. VS_2 ($R\bar{3}m$)

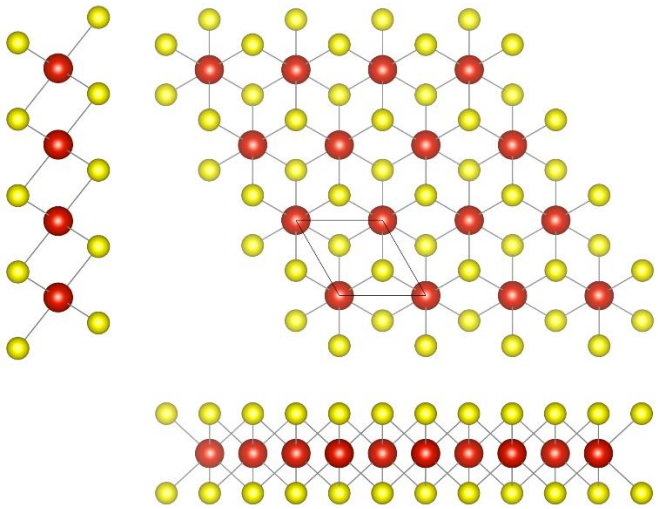
Formula	VS_2	**ID**	mp-1013526
Measure	641.2	**Symbol**	$R\bar{3}m$
Magnetic Ordering	FM	**Tot. Magnetization (μ_B/cell)**	0.627
Density (g/cm^3)	3.364	**Energy-Above-Hull / Atom (eV)**	0.003
Formation Energy / Atom (eV)	-1.291	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of VS_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.59682000	-2.76578000	0.00000000
a_2	1.59682000	2.76578000	0.00000000
a_3	0.00000000	0.00000000	19.29011000

	x (Å)	*y* (Å)	*z* (Å)
V	0.00000000	0.00000000	0.00000000
V	1.59680000	-0.92190000	6.43000000
V	1.59680000	0.92190000	12.86010000
S	1.59680000	-0.92190000	1.46510000
S	0.00000000	0.00000000	4.96490000
S	1.59680000	0.92190000	7.89510000
S	1.59680000	-0.92190000	11.39500000
S	0.00000000	0.00000000	14.32520000
S	1.59680000	0.92190000	17.82500000



Orthographic projections: views of VS_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

3. WS_2 ($P6_3/mmc$)

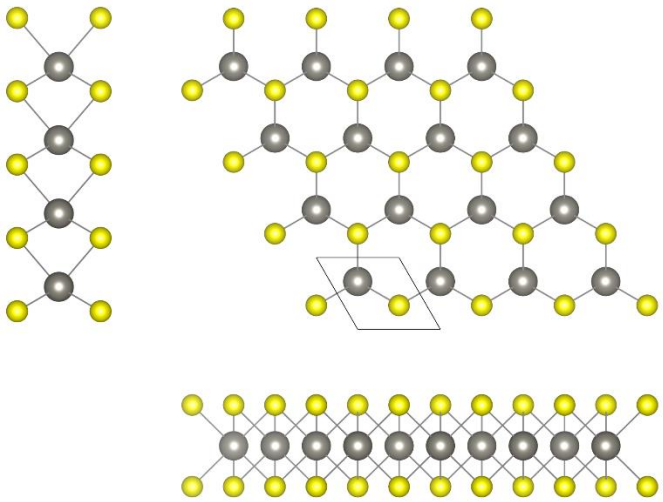
Formula	WS_2	**ID**	mp-224
Measure	492.8	**Symbol**	$P6_3/mmc$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	6.577	**Energy-Above-Hull / Atom (eV)**	0.000
Formation Energy / Atom (eV)	-1.261	**Band Gap (eV)**	1.566

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of WS_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.59537000	-2.76325000	0.00000000
a_2	1.59537000	2.76325000	0.00000000
a_3	0.00000000	0.00000000	14.20240000

	x (Å)	*y* (Å)	*z* (Å)
W	1.59540000	-0.92110000	10.65180000
W	1.59540000	0.92110000	3.55060000
S	1.59540000	-0.92110000	1.97760000
S	1.59540000	0.92110000	9.07880000
S	1.59540000	-0.92110000	5.12360000
S	1.59540000	0.92110000	12.22480000



Orthographic projections: views of WS_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

4. $FeCl_2$ ($P\bar{3}m1$)

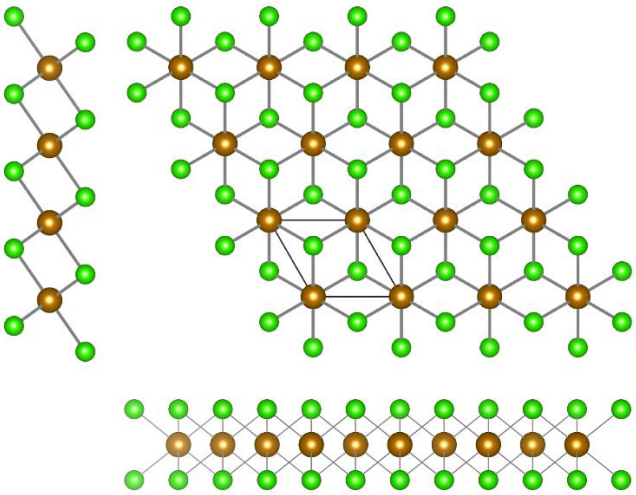
Formula	$FeCl_2$	**ID**	mp-571096
Measure	484.6	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	FM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	3.184	**Energy-Above-Hull (eV / atom)**	0.324
Formation Energy / Atom (eV)	0.698	**Band Gap (eV)**	0.623

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $FeCl_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.75708000	-3.04335000	0.00000000
a_2	1.75708000	3.04335000	0.00000000
a_3	0.00000000	0.00000000	6.18113000

	x (Å)	*y* (Å)	*z* (Å)
Fe	0.00000000	0.00000000	0.00000000
Cl	1.75710000	-1.01450000	4.77560000
Cl	1.75710000	1.01450000	1.40550000



Orthographic projections: views of $FeCl_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

5. VS_2 ($P6_3/mmc$)

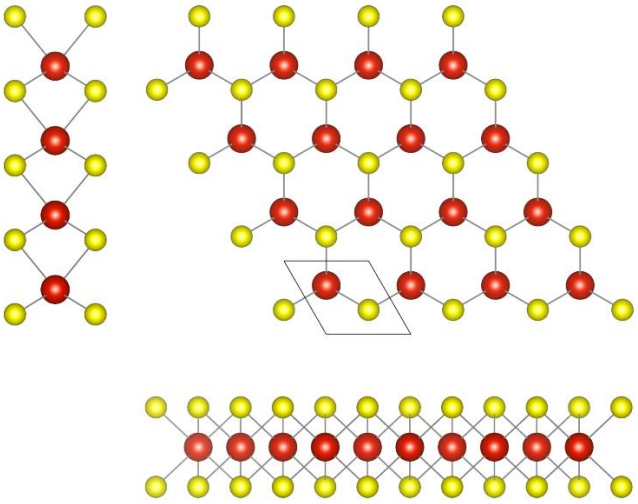
Formula	VS_2	**ID**	mp-1013525
Measure	322.0	**Symbol**	$P6_3/mmc$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.001
Density (g/cm^3)	3.024	**Energy-Above-Hull (eV / atom)**	0.000
Formation Energy (eV / atom)	-1.294	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of VS_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.59013000	-2.75418000	0.00000000
a_2	1.59013000	2.75418000	0.00000000
a_3	0.00000000	0.00000000	14.42964000

	x (Å)	*y* (Å)	*z* (Å)
V	1.59010000	0.91810000	3.60740000
V	1.59010000	-0.91810000	10.82220000
S	1.59010000	-0.91810000	5.09920000
S	1.59010000	0.91810000	12.31410000
S	1.59010000	-0.91810000	2.11560000
S	1.59010000	0.91810000	9.33040000



Orthographic projections: views of VS_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

6. BN ($P6_3/mmc$)

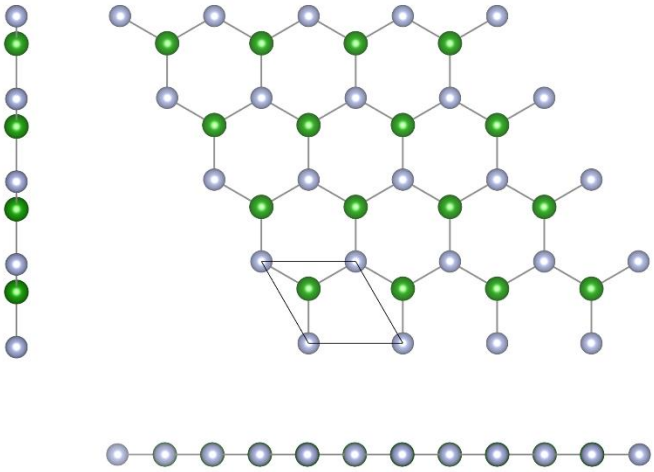
Formula	BN	**ID**	mp-7991
Measure	288.1	**Symbol**	$P6_3/mmc$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	1.825	**Energy-Above-Hull (eV / atom)**	0.000
Formation Energy (eV / atom)	-1.473	**Band Gap (eV)**	4.270

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of BN in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.25580000	-2.17511000	0.00000000
a_2	1.25580000	2.17511000	0.00000000
a_3	0.00000000	0.00000000	8.26780000

	x (Å)	*y* (Å)	*z* (Å)
B	1.25580000	-0.72500000	6.20080000
B	1.25580000	0.72500000	2.06690000
N	0.00000000	0.00000000	6.20080000
N	0.00000000	0.00000000	2.06690000



Orthographic projections: views of BN as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

7. MoS_2 ($P6_3/mmc$)

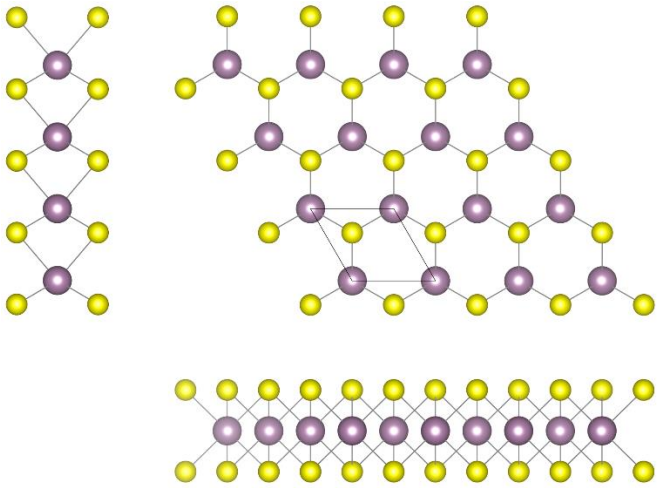
Formula	MoS_2	**ID**	mp-1018809
Measure	157.1	**Symbol**	$P6_3/mmc$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	4.306	**Energy-Above-Hull (eV / atom)**	0.001
Formation Energy (eV / atom)	-1.307	**Band Gap (eV)**	1.336

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of MoS_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.59646000	-2.76515000	0.00000000
a_2	1.59646000	2.76515000	0.00000000
a_3	0.00000000	0.00000000	13.98277000

	x (Å)	*y* (Å)	*z* (Å)
Mo	0.00000000	0.00000000	10.48710000
Mo	0.00000000	0.00000000	3.49570000
S	1.59650000	-0.92170000	12.05330000
S	1.59650000	0.92170000	1.92950000
S	1.59650000	0.92170000	5.06190000
S	1.59650000	-0.92170000	8.92090000



Orthographic projections: views of MoS_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

8. ReS_2 ($P\bar{1}$)

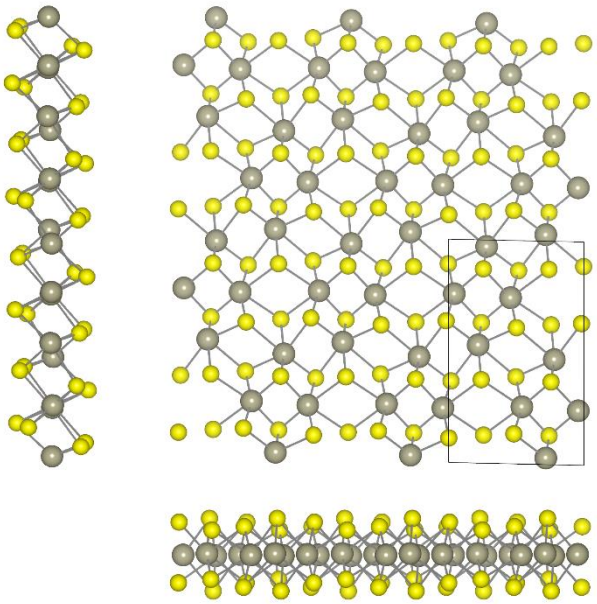
Formula	ReS_2	**ID**	mp-572758
Measure	134.9	**Symbol**	$P\bar{1}$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	6.733	**Energy-Above-Hull (eV / atom)**	0.000
Formation Energy (eV / atom)	-1.011	**Band Gap (eV)**	1.446

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of ReS_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	6.41910000	0.00000000	0.00000000
a_2	-3.14616000	5.71419000	0.00000000
a_3	-1.70119000	-1.18638000	6.73244000

	x (Å)	*y* (Å)	*z* (Å)
Re	3.01170000	3.33700000	3.42060000
Re	-1.44000000	1.19080000	3.31190000
Re	0.18800000	3.48660000	3.38030000
Re	1.38380000	1.04120000	3.35210000
S	3.23460000	-0.04450000	4.55030000
S	3.14600000	1.67090000	1.79620000
S	-0.12020000	-0.21540000	4.71920000
S	0.03810000	1.92600000	1.61660000
S	1.53370000	2.60180000	5.11580000
S	1.69200000	4.74320000	2.01320000
S	-1.66280000	4.57230000	2.18210000
S	-1.57420000	2.85690000	4.93630000



Orthographic projections: views of ReS_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

9. $MoW_3(SeS_3)_2$ (P3m1)

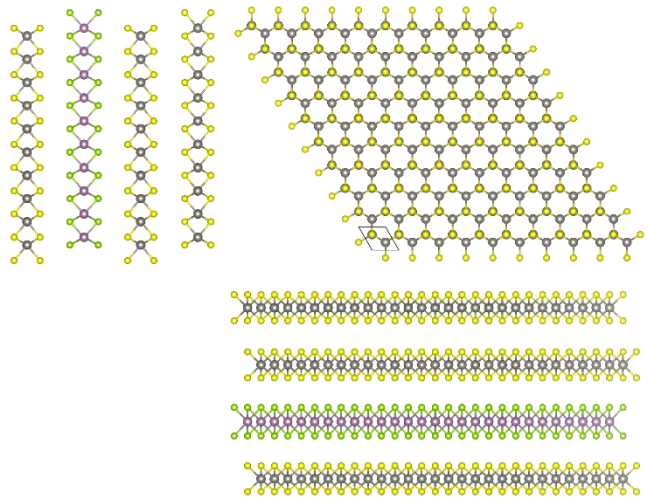
Formula	$MoW_3(SeS_3)_2$	**ID**	mp-1029037
Measure	97.3	**Symbol**	P3m1
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	5.069	**Energy-Above-Hull (eV / atom)**	0.034
Formation Energy (eV / atom)	-1.102	**Band Gap (eV)**	1.162

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $MoW_3(SeS_3)_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.60994000	-2.78850000	0.00000000
a_2	1.60994000	2.78850000	0.00000000
a_3	0.00000000	0.00000000	36.40680000

	x (Å)	*y* (Å)	*z* (Å)
Mo	0.00000000	0.00000000	10.25900000
W	1.60990000	-0.92950000	3.41880000
W	1.60990000	-0.92950000	17.09910000
W	0.00000000	0.00000000	23.93900000
Se	1.60990000	-0.92950000	11.97000000
Se	1.60990000	-0.92950000	8.54850000
S	1.60990000	-0.92950000	25.50260000
S	0.00000000	0.00000000	1.85550000
S	0.00000000	0.00000000	15.53610000
S	0.00000000	0.00000000	4.98260000
S	0.00000000	0.00000000	18.66250000
S	1.60990000	-0.92950000	22.37540000



Orthographic projections: views of $MoW_3(SeS_3)_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

10. B_2S_3 ($R\bar{3}c$)

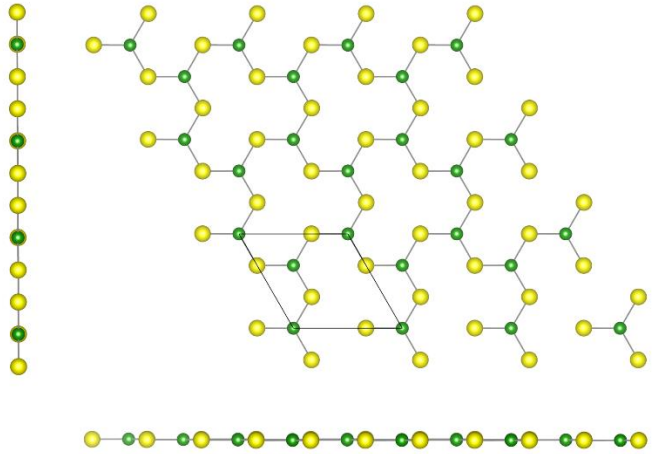
Formula	B_2S_3	**ID**	mp-866066
Measure	95.6	**Symbol**	$R\bar{3}c$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	1.955	**Energy-Above-Hull (eV / atom)**	0.105
Formation Energy (eV / atom)	-0.727	**Band Gap (eV)**	1.547

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of B_2S_3 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	2.72829000	-4.72553000	0.00000000
a_2	2.72829000	4.72553000	0.00000000
a_3	0.00000000	0.00000000	23.28635000

	x (Å)	*y* (Å)	*z* (Å)
B	2.72830000	-1.57520000	5.81570000
B	2.72830000	1.57520000	5.82750000
B	2.72830000	1.57520000	1.93460000
B	0.00000000	0.00000000	1.94650000
B	2.72830000	1.57520000	13.57780000
B	0.00000000	0.00000000	13.58960000
B	0.00000000	0.00000000	9.69670000
B	2.72830000	-1.57520000	9.70860000
B	0.00000000	0.00000000	21.33990000
B	2.72830000	-1.57520000	21.35180000
B	2.72830000	-1.57520000	17.45880000
B	2.72830000	1.57520000	17.47070000
S	0.90490000	1.56730000	5.82160000
S	3.64680000	0.00000000	5.82160000
S	0.90490000	-1.56730000	5.82160000
S	1.82340000	-0.00790000	1.94050000
S	4.53800000	-1.57520000	1.94050000
S	1.82340000	-3.14250000	1.94050000
S	3.63320000	-0.00790000	13.58370000
S	0.91850000	-1.57520000	13.58370000
S	3.63320000	-3.14250000	13.58370000
S	1.82340000	3.14250000	9.70260000
S	4.53800000	1.57520000	9.70260000
S	1.82340000	0.00790000	9.70260000
S	3.63320000	3.14250000	21.34580000
S	0.91850000	1.57520000	21.34580000
S	3.63320000	0.00790000	21.34580000
S	1.82340000	-3.15820000	17.46480000
S	1.80980000	0.00000000	17.46480000
S	1.82340000	3.15820000	17.46480000



Orthographic projections: views of B_2S_3 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

11. $PtSe_2$ ($P\bar{3}m1$)

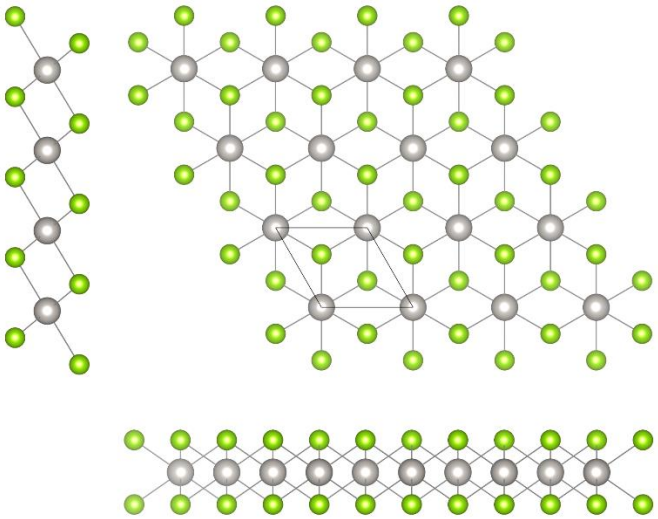
Formula	$PtSe_2$	**ID**	mp-1115
Measure	81.5	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	7.821	**Energy-Above-Hull (eV / atom)**	0.000
Formation Energy (eV / atom)	-0.387	**Band Gap (eV)**	0.674

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $PtSe_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.88051000	-3.25714000	0.00000000
a_2	1.88051000	3.25714000	0.00000000
a_3	0.00000000	0.00000000	6.11797000

	x (Å)	*y* (Å)	*z* (Å)
Pt	0.00000000	0.00000000	0.00000000
Se	1.88050000	-1.08570000	4.81130000
Se	1.88050000	1.08570000	1.30670000



Orthographic projections: views of $PtSe_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

12. Mo_2SeS_3 (P3m1)

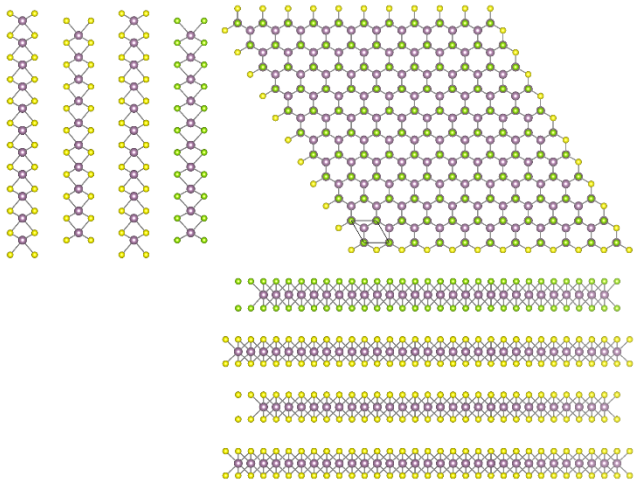
Formula	Mo_2SeS_3	**ID**	mp-1027890
Measure	77.7	**Symbol**	P3m1
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	3.574	**Energy-Above-Hull (eV / atom)**	0.010
Formation Energy / Atom(eV)	-1.140	**Band Gap (eV)**	0.758

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Mo_2SeS_3 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.61197000	-2.79201000	0.00000000
a_2	1.61197000	2.79201000	0.00000000
a_3	0.00000000	0.00000000	37.88841000

	x (Å)	*y* (Å)	*z* (Å)
Mo	0.00000000	0.00000000	3.52140000
Mo	0.00000000	0.00000000	17.75180000
Mo	1.61200000	0.93070000	10.67990000
Mo	1.61200000	0.93070000	24.98930000
Se	0.00000000	0.00000000	26.70080000
Se	0.00000000	0.00000000	23.27880000
S	0.00000000	0.00000000	12.23630000
S	1.61200000	0.93070000	1.96520000
S	1.61200000	0.93070000	16.19500000
S	1.61200000	0.93070000	5.07750000
S	1.61200000	0.93070000	19.30880000
S	0.00000000	0.00000000	9.12470000



Orthographic projections: views of Mo_2SeS_3 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

13. $Ca_2Cu(BrO)_2$ (I4/mmm)

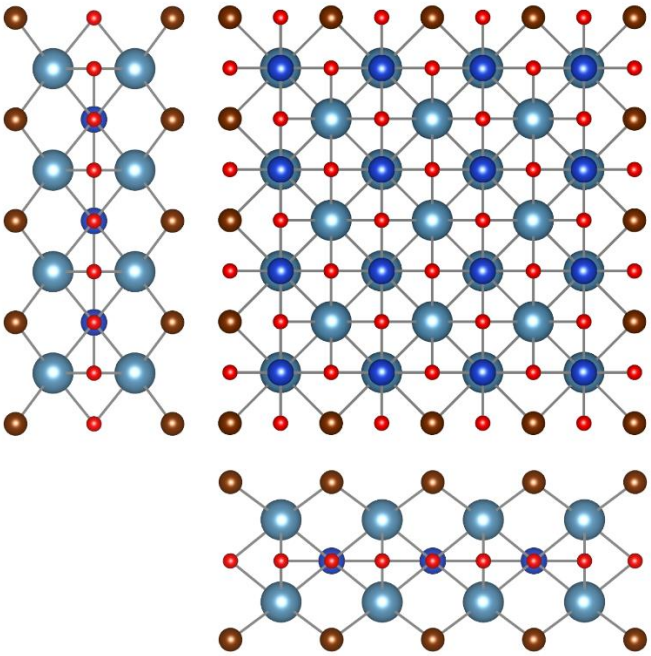
Formula	$Ca_2Cu(BrO)_2$	**ID**	mp-545481
Measure	74.5	**Symbol**	I4/mmm
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.009
Density (g/cm^3)	4.171	**Energy-Above-Hull (eV / atom)**	0.000
Formation Energy / Atom(eV)	-2.114	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $Ca_2Cu(BrO)_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.88490000	0.00000000	0.00000000
a_2	0.00000000	3.88490000	0.00000000
a_3	0.00000000	0.00000000	17.69836000

	x (Å)	*y* (Å)	*z* (Å)
Ca	0.00000000	0.00000000	7.27620000
Ca	1.94240000	1.94240000	1.57300000
Ca	1.94240000	1.94240000	16.12540000
Ca	0.00000000	0.00000000	10.42220000
Cu	0.00000000	0.00000000	0.00000000
Cu	1.94240000	1.94240000	8.84920000
Br	1.94240000	1.94240000	5.83450000
Br	0.00000000	0.00000000	3.01470000
Br	0.00000000	0.00000000	14.68370000
Br	1.94240000	1.94240000	11.86380000
O	1.94240000	0.00000000	0.00000000
O	0.00000000	1.94240000	0.00000000
O	0.00000000	1.94240000	8.84920000
O	1.94240000	0.00000000	8.84920000



Orthographic projections: views of $Ca_2Cu(BrO)_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

14. NbS_2 ($P6_3/mmc$)

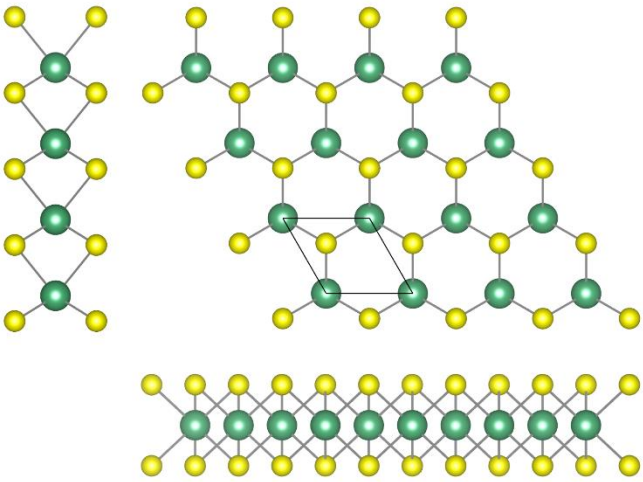
Formula	NbS_2	**ID**	mp-10033
Measure	69.0	**Symbol**	$P6_3/mmc$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.007
Density (g/cm^3)	4.020	**Energy-Above-Hull (eV / atom)**	0.000
Formation Energy (eV / atom)	-1.456	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of NbS_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.68138000	-2.91223000	0.00000000
a_2	1.68138000	2.91223000	0.00000000
a_3	0.00000000	0.00000000	13.24900000

	x (Å)	*y* (Å)	*z* (Å)
Nb	0.00000000	0.00000000	9.93670000
Nb	0.00000000	0.00000000	3.31220000
S	1.68140000	-0.97070000	11.50330000
S	1.68140000	0.97070000	1.74570000
S	1.68140000	0.97070000	4.87880000
S	1.68140000	-0.97070000	8.37020000



Orthographic projections: views of NbS_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

15. $TaSe_2$ (R3m)

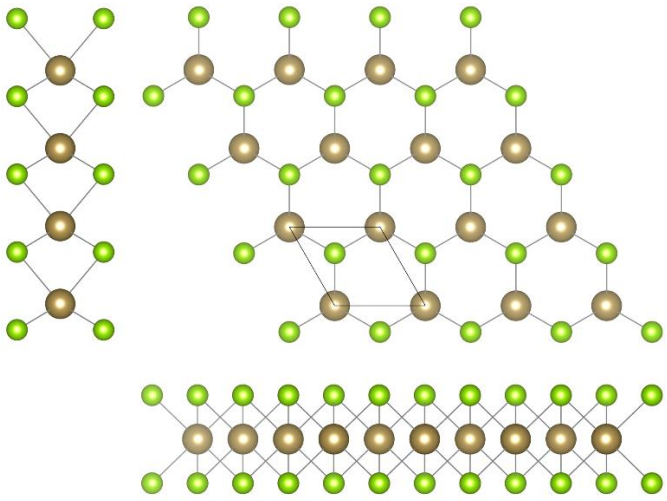
Formula	$TaSe_2$	**ID**	mp-7834
Measure	66.3	**Symbol**	R3m
Magnetic Ordering	FM	**Tot. Magnetization (μ_B/cell)**	0.471
Density (g/cm^3)	7.759	**Energy-Above-Hull (eV/atom)**	0.004
Formation Energy (eV/atom)	-0.814	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $TaSe_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.73968000	-3.01322000	0.00000000
a_2	1.73968000	3.01322000	0.00000000
a_3	0.00000000	0.00000000	20.75216000

	x (Å)	*y* (Å)	*z* (Å)
Ta	0.00000000	0.00000000	0.00510000
Ta	1.73970000	-1.00440000	6.92250000
Ta	1.73970000	1.00440000	13.83990000
Se	0.00000000	0.00000000	5.23720000
Se	1.73970000	1.00440000	1.68200000
Se	1.73970000	-1.00440000	12.15460000
Se	0.00000000	0.00000000	8.59930000
Se	1.73970000	1.00440000	19.07200000
Se	1.73970000	-1.00440000	15.51670000



Orthographic projections: views of $TaSe_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

16. $Mo(WSe_3)_2$ ($P\bar{6}m2$)

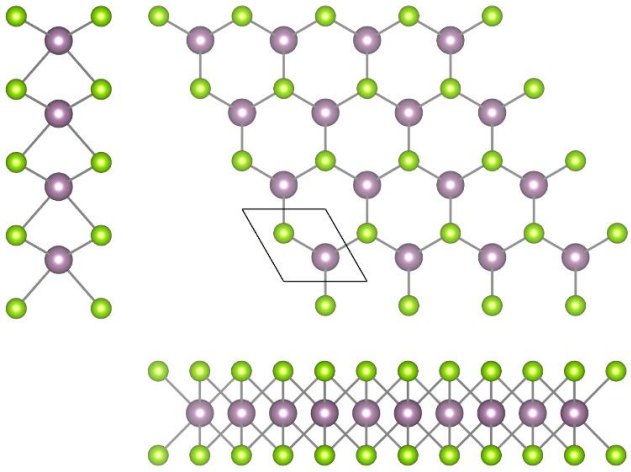
Formula	$Mo(WSe_3)_2$	**ID**	mp-1025575
Measure	63.8	**Symbol**	$P\bar{6}m2$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	5.296	**Energy-Above-Hull (eV/atom)**	0.084
Formation Energy (eV/atom)	-0.595	**Band Gap (eV)**	1.240

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $Mo(WSe_3)_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.66134000	-2.87753000	0.00000000
a_2	1.66134000	2.87753000	0.00000000
a_3	0.00000000	0.00000000	30.74080000

	x (Å)	*y* (Å)	*z* (Å)
Mo	1.66130000	-0.95920000	0.00000000
W	1.66130000	0.95920000	23.62930000
W	1.66130000	0.95920000	7.11150000
Se	1.66130000	0.95920000	1.67630000
Se	1.66130000	-0.95920000	21.94500000
Se	1.66130000	-0.95920000	5.42700000
Se	1.66130000	-0.95920000	25.31380000
Se	1.66130000	-0.95920000	8.79580000
Se	1.66130000	0.95920000	29.06450000



Orthographic projections: views of $Mo(WSe_3)_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

17. CN_2 ($P\bar{4}2_1m$)

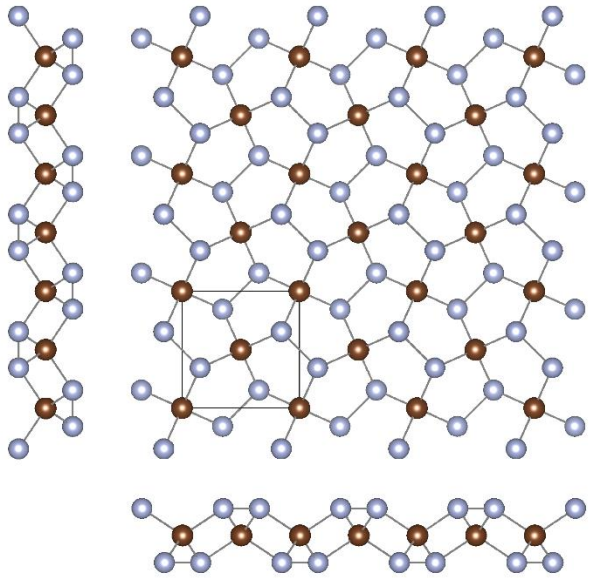
Formula	CN_2	**ID**	mp-1019086
Measure	63.4	**Symbol**	$P\bar{4}2_1m$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	2.551	**Energy-Above-Hull (eV/atom)**	0.358
Formation Energy (eV/atom)	0.358	**Band Gap (eV)**	4.792

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CN_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.31300000	0.00000000	0.00000000
a_2	0.00000000	3.31300000	0.00000000
a_3	0.00000000	0.00000000	4.74800000

	x (Å)	*y* (Å)	*z* (Å)
C	1.65650000	1.65650000	0.00000000
C	0.00000000	0.00000000	0.00000000
N	0.51160000	1.14490000	0.76350000
N	1.14490000	2.80140000	3.98450000
N	2.80140000	2.16810000	0.76350000
N	2.16810000	0.51160000	3.98450000



Orthographic projections: views of CN_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

18. $NbSe_2$ (Fmm2)

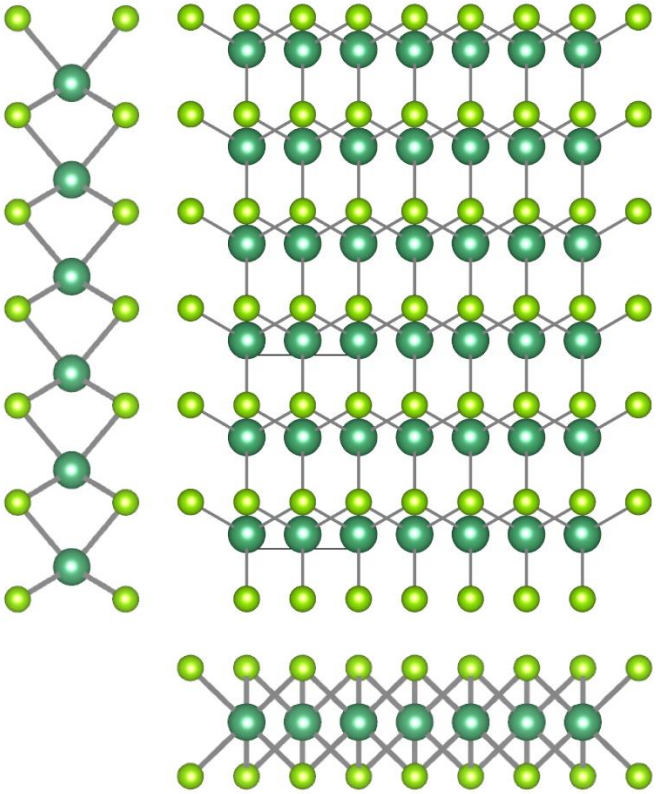
Formula	$NbSe_2$	**ID**	mp-7007
Measure	63.1	**Symbol**	Fmm2
Magnetic Ordering	FM	**Tot. Magnetization (μ_B/cell)**	0.975
Density (g/cm^3)	3.211	**Energy-Above-Hull (eV/atom)**	0.011
Formation Energy (eV/atom)	-0.830	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $NbSe_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.48291000	0.00000000	0.00000000
a_2	0.00000000	6.03693000	0.00000000
a_3	0.00000000	0.00000000	24.67796000

	x (Å)	*y* (Å)	*z* (Å)
Nb	1.74150000	3.47270000	0.00000000
Nb	1.74150000	0.45420000	12.33900000
Nb	0.00000000	0.45420000	0.00000000
Nb	0.00000000	3.47270000	12.33900000
Se	1.74150000	4.47870000	10.65580000
Se	0.00000000	4.47870000	1.68310000
Se	1.74150000	1.46020000	22.99480000
Se	0.00000000	1.46020000	14.02210000
Se	0.00000000	1.46020000	10.65580000
Se	1.74150000	1.46020000	1.68310000
Se	0.00000000	4.47870000	22.99480000
Se	1.74150000	4.47870000	14.02210000



Orthographic projections: views of $NbSe_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

19. Te_2Mo ($P6_3/mmc$)

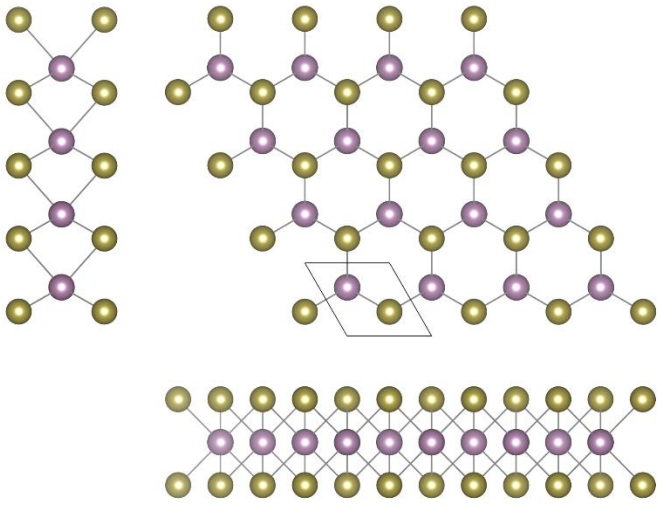
Formula	Te_2Mo	**ID**	mp-602
Measure	62.6	**Symbol**	$P6_3/mmc$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	6.928	**Energy-Above-Hull (eV/atom)**	0.001
Formation Energy (eV/atom)	-0.274	**Band Gap (eV)**	1.120

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Te_2Mo in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.77936000	-3.08193000	0.00000000
a_2	1.77936000	3.08193000	0.00000000
a_3	0.00000000	0.00000000	15.34665000

	x (Å)	*y* (Å)	*z* (Å)
Te	1.77940000	-1.02730000	2.02700000
Te	1.77940000	1.02730000	9.70030000
Te	1.77940000	1.02730000	13.31970000
Te	1.77940000	-1.02730000	5.64630000
Mo	1.77940000	-1.02730000	11.51000000
Mo	1.77940000	1.02730000	3.83670000



Orthographic projections: views of Te_2Mo as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

20. ZrI_2 ($Pmn2_1$)

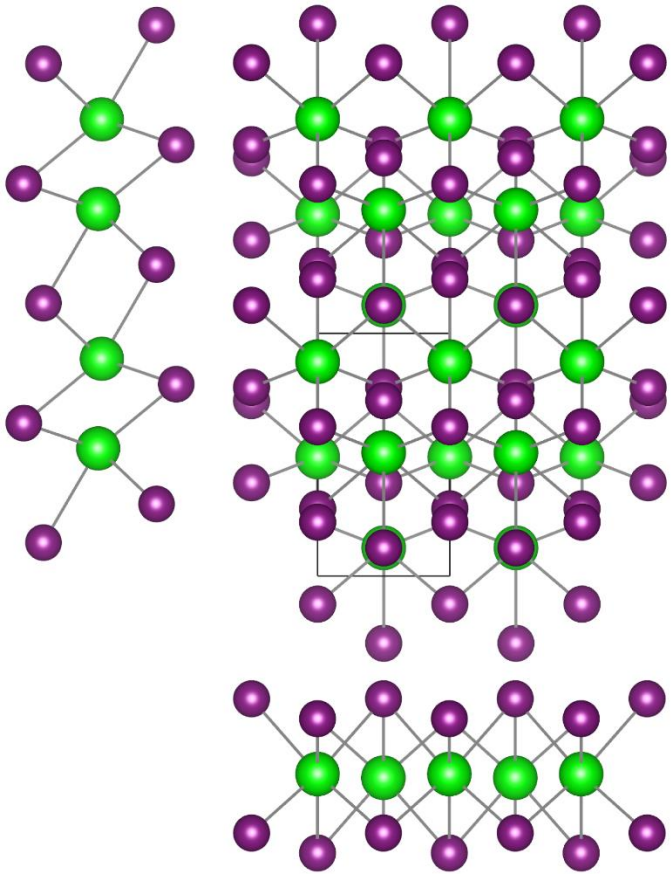
Formula	ZrI_2	**ID**	mp-570506
Measure	58.9	**Symbol**	$Pmn2_1$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.001
Density (g/cm^3)	5.355	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.893	**Band Gap (eV)**	0.298

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of ZrI_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.77641000	0.00000000	0.00000000
a_2	0.00000000	6.92474000	0.00000000
a_3	0.00000000	0.00000000	16.36434000

	x (Å)	*y* (Å)	*z* (Å)
Zr	0.00000000	3.39900000	0.11410000
Zr	0.00000000	6.11840000	8.19010000
Zr	1.88820000	0.80630000	0.00790000
Zr	1.88820000	3.52580000	8.29620000
I	0.00000000	6.12300000	1.69660000
I	1.88820000	5.38590000	6.03670000
I	0.00000000	1.53880000	14.21890000
I	1.88820000	5.00680000	14.78900000
I	1.88820000	0.80180000	9.87880000
I	1.88820000	2.66380000	2.26720000
I	0.00000000	1.91800000	6.60680000
I	0.00000000	4.26100000	10.44930000



Orthographic projections: views of ZrI_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

21. C_3N_4 ($P3_1$)

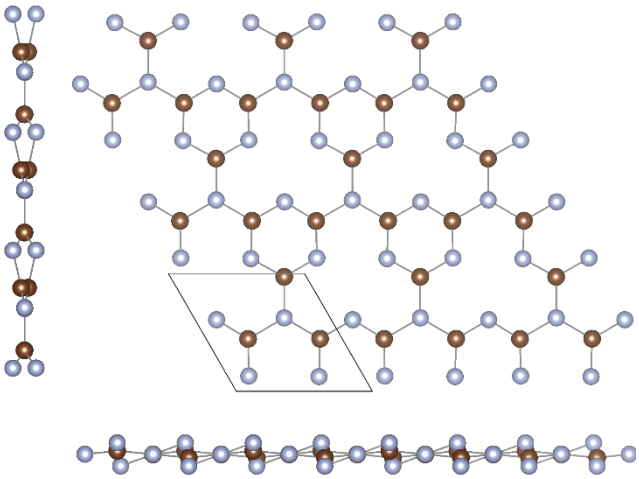
Formula	C_3N_4	**ID**	mp-971683
Measure	58.4	**Symbol**	$P3_1$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	2.337	**Energy-Above-Hull (eV/atom)**	0.108
Formation Energy (eV/atom)	0.108	**Band Gap (eV)**	2.194

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of C_3N_4 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	2.35795000	-4.08408000	0.00000000
a_2	2.35795000	4.08408000	0.00000000
a_3	0.00000000	0.00000000	10.18896000

	x (Å)	*y* (Å)	*z* (Å)
C	4.26450000	0.55180000	3.27920000
C	1.77420000	0.55690000	3.39270000
C	3.02770000	-1.59840000	3.51540000
C	2.22840000	-0.66280000	6.91180000
C	2.10580000	3.41720000	6.67550000
C	3.34650000	1.25800000	6.78900000
C	1.95320000	2.26920000	10.18530000
C	1.81780000	-1.82280000	0.11910000
C	0.70360000	0.11500000	10.07190000
N	2.10930000	-3.44490000	6.38810000
N	2.22810000	0.64520000	7.18890000
N	3.34570000	-1.34920000	6.79670000
N	1.85360000	-0.51200000	0.00400000
N	4.28660000	-0.53490000	9.78440000
N	3.04310000	1.60700000	0.39630000
N	1.80260000	1.83190000	3.79260000
N	1.87460000	-2.22280000	3.40040000
N	0.67790000	-0.10430000	2.99180000
N	3.02850000	-0.16730000	3.40110000
N	0.98860000	-1.37770000	6.79740000
N	3.05670000	-2.53910000	0.00480000



Orthographic projections: views of C_3N_4 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

22. LiC_{12} (P6/mmm)

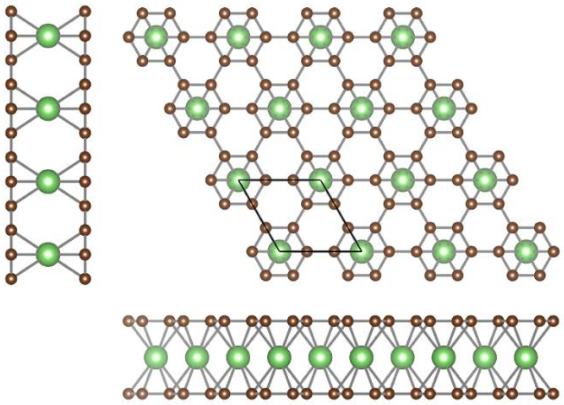
Formula	LiC_{12}	**ID**	mp-1021323
Measure	58.1	**Symbol**	P6/mmm
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	2.019	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.006	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of LiC_{12} in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	2.14896000	-3.72210000	0.00000000
a_2	2.14896000	3.72210000	0.00000000
a_3	0.00000000	0.00000000	7.76503000

	x (Å)	*y* (Å)	*z* (Å)
Li	0.00000000	0.00000000	0.00000000
C	1.43260000	-2.48130000	5.87220000
C	1.43260000	2.48130000	5.87220000
C	1.43280000	0.00000000	5.87220000
C	0.71640000	-1.24080000	5.87220000
C	0.71640000	1.24080000	5.87220000
C	2.86520000	0.00000000	5.87220000
C	0.71640000	-1.24080000	1.89290000
C	0.71640000	1.24080000	1.89290000
C	2.86520000	0.00000000	1.89290000
C	1.43260000	-2.48130000	1.89290000
C	1.43260000	2.48130000	1.89290000
C	1.43280000	0.00000000	1.89290000



Orthographic projections: views of LiC_{12} as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

23. SmBrO (P4/nmm)

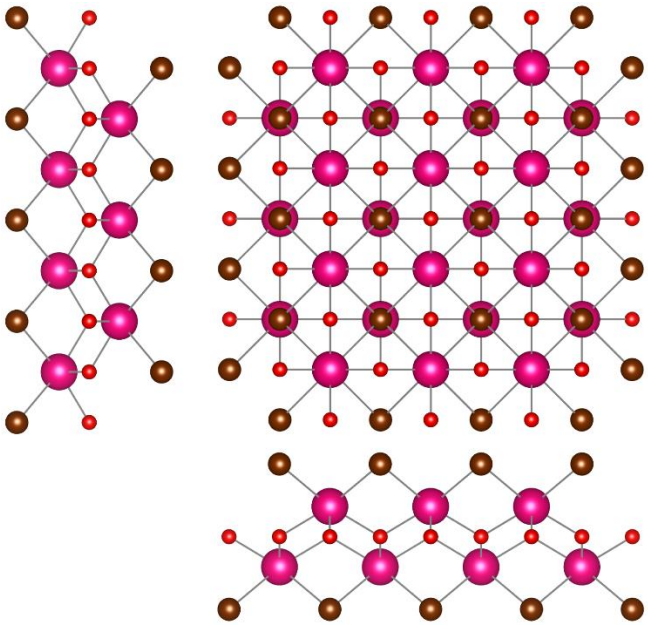
Formula	SmBrO	**ID**	mp-29327
Measure	56.9	**Symbol**	P4/nmm
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	6.013	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-3.138	**Band Gap (eV)**	4.524

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of SmBrO in Cartesian coordinates.

	x (Å)	y (Å)	z (Å)
a_1	3.95297000	0.00000000	0.00000000
a_2	0.00000000	3.95297000	0.00000000
a_3	0.00000000	0.00000000	8.70466000

	x (Å)	y (Å)	z (Å)
Sm	1.97650000	0.00000000	7.52310000
Sm	0.00000000	1.97650000	1.18150000
Br	0.00000000	1.97650000	5.86610000
Br	1.97650000	0.00000000	2.83850000
O	0.00000000	0.00000000	0.00000000
O	1.97650000	1.97650000	0.00000000



Orthographic projections: views of SmBrO as seen from the x axis (left), the y axis (bottom) and the z axis (center). The primitive cell is also shown.

24. $TiNbS_4$ (C2/m)

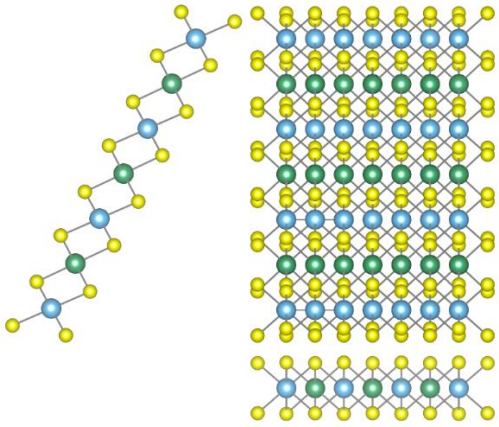
Formula	$TiNbS_4$	**ID**	mp-34289
Measure	56.6	**Symbol**	C2/m
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	3.656	**Energy-Above-Hull (eV/atom)**	0.019
Formation Energy (eV/atom)	-1.567	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $TiNbS_4$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	0.00000000	13.58651000	0.00000000
a_2	3.38541000	0.00000000	0.00000000
a_3	0.00000000	-2.52407000	-5.31296000

	x (Å)	*y* (Å)	*z* (Å)
Ti	0.00000000	0.00000000	0.00000000
Ti	1.69270000	6.79330000	0.00000000
Nb	1.69270000	-1.26200000	-2.65650000
Nb	0.00000000	5.53120000	-2.65650000
S	1.69270000	4.60580000	-1.08770000
S	1.69270000	0.91880000	-1.49720000
S	0.00000000	3.35030000	-3.81580000
S	0.00000000	-0.33660000	-4.22530000
S	0.00000000	11.39900000	-1.08770000
S	0.00000000	7.71210000	-1.49720000
S	1.69270000	10.14360000	-3.81580000
S	1.69270000	6.45660000	-4.22530000



Orthographic projections: views of $TiNbS_4$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

25. $MoSe_2$ (R3m)

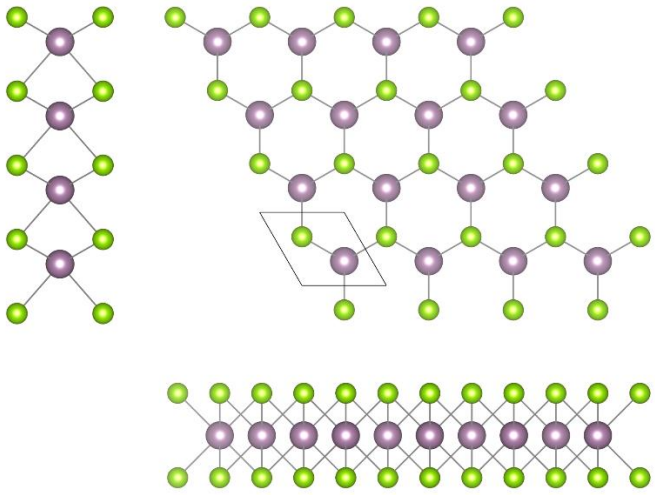
Formula	$MoSe_2$	**ID**	mp-7581
Measure	55.1	**Symbol**	R3m
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	5.970	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.673	**Band Gap (eV)**	1.481

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $MoSe_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.66389000	-2.88195000	0.00000000
a_2	1.66389000	2.88195000	0.00000000
a_3	0.00000000	0.00000000	22.08799000

	x (Å)	*y* (Å)	*z* (Å)
Mo	1.66390000	-0.96060000	0.00240000
Mo	1.66390000	0.96060000	7.36510000
Mo	0.00000000	0.00000000	14.72770000
Se	1.66390000	0.96060000	1.67530000
Se	0.00000000	0.00000000	5.69230000
Se	0.00000000	0.00000000	9.03800000
Se	1.66390000	-0.96060000	13.05500000
Se	1.66390000	-0.96060000	16.40060000
Se	1.66390000	0.96060000	20.41760000



Orthographic projections: views of $MoSe_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

26. PtS_2 ($P\bar{3}m1$)

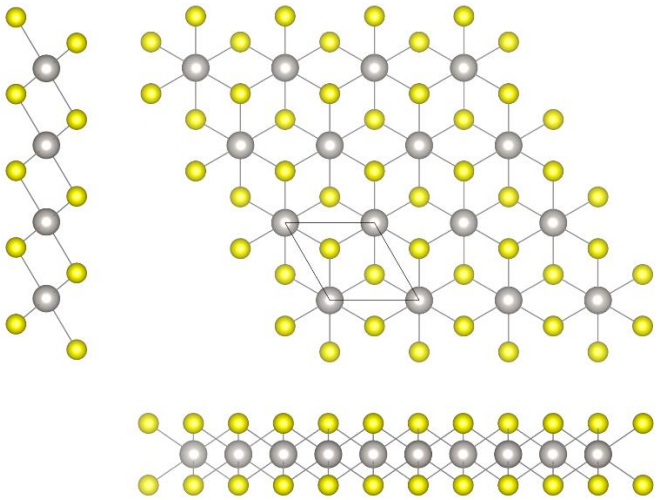
Formula	PtS_2	**ID**	mp-762
Measure	55.1	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	6.204	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.792	**Band Gap (eV)**	1.444

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of PtS_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.79004000	-3.10044000	0.00000000
a_2	1.79004000	3.10044000	0.00000000
a_3	0.00000000	0.00000000	6.25087000

	x (Å)	*y* (Å)	*z* (Å)
Pt	0.00000000	0.00000000	0.00000000
S	1.79000000	-1.03350000	5.02240000
S	1.79000000	1.03350000	1.22840000



Orthographic projections: views of PtS_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

27. NbS_2 (I4/mmm)

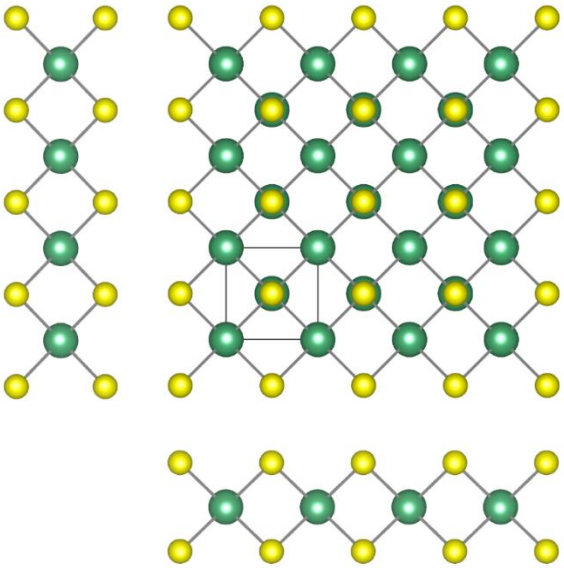
Formula	NbS_2	**ID**	mp-1008860
Measure	54.3	**Symbol**	I4/mmm
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.003
Density (g/cm^3)	4.146	**Energy-Above-Hull (eV/atom)**	0.269
Formation Energy (eV/atom)	-1.187	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of NbS_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.06569000	0.00000000	0.00000000
a_2	0.00000000	3.06569000	0.00000000
a_3	0.00000000	0.00000000	13.38580000

	x (Å)	*y* (Å)	*z* (Å)
Nb	0.00000000	0.00000000	0.00000000
Nb	1.53280000	1.53280000	6.69290000
S	1.53280000	1.53280000	1.48040000
S	0.00000000	0.00000000	5.21250000
S	0.00000000	0.00000000	8.17330000
S	1.53280000	1.53280000	11.90540000



Orthographic projections: views of NbS_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

28. SnS_2 ($P\bar{3}m1$)

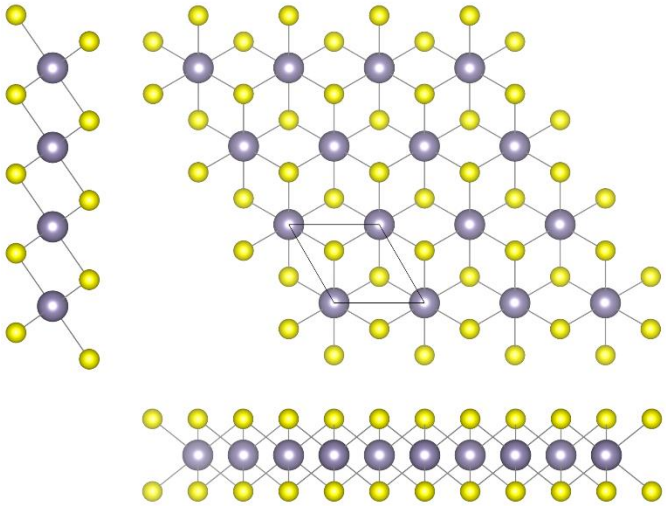
Formula	SnS_2	**ID**	mp-1170
Measure	52.2	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	3.670	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.823	**Band Gap (eV)**	1.562

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of SnS_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.84996000	-3.20422000	0.00000000
a_2	1.84996000	3.20422000	0.00000000
a_3	0.00000000	0.00000000	6.97796000

	x (Å)	*y* (Å)	*z* (Å)
Sn	0.00000000	0.00000000	0.00000000
S	1.85000000	1.06810000	1.47780000
S	1.85000000	-1.06810000	5.50010000



Orthographic projections: views of SnS_2as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

29. $TeMoWSeS_2$ (P3m1)

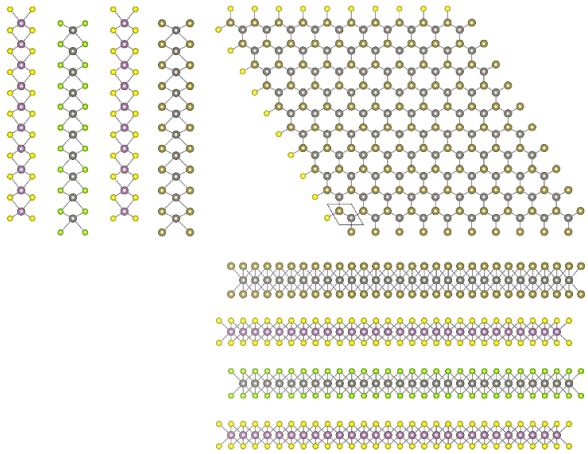
Formula	$TeMoWSeS_2$	**ID**	mp-1027164
Measure	50.1	**Symbol**	P3m1
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.001
Density (g/cm^3)	5.115	**Energy-Above-Hull (eV/atom)**	0.130
Formation Energy (eV/atom)	-0.760	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $TeMoWSeS_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.65558000	-2.86755000	0.00000000
a_2	1.65558000	2.86755000	0.00000000
a_3	0.00000000	0.00000000	37.64060000

	x (Å)	*y* (Å)	*z* (Å)
Te	1.65560000	0.95580000	26.67310000
Te	1.65560000	0.95580000	22.82760000
Mo	1.65560000	0.95580000	3.53510000
Mo	1.65560000	0.95580000	17.67800000
W	1.65560000	-0.95580000	10.60700000
W	1.65560000	-0.95580000	24.75110000
Se	1.65560000	0.95580000	12.29510000
Se	1.65560000	0.95580000	8.91840000
S	1.65560000	-0.95580000	2.00760000
S	1.65560000	-0.95580000	16.15060000
S	1.65560000	-0.95580000	5.06290000
S	1.65560000	-0.95580000	19.20540000



Orthographic projections: views of $TeMoWSeS_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

30. SnGe (P3m1)

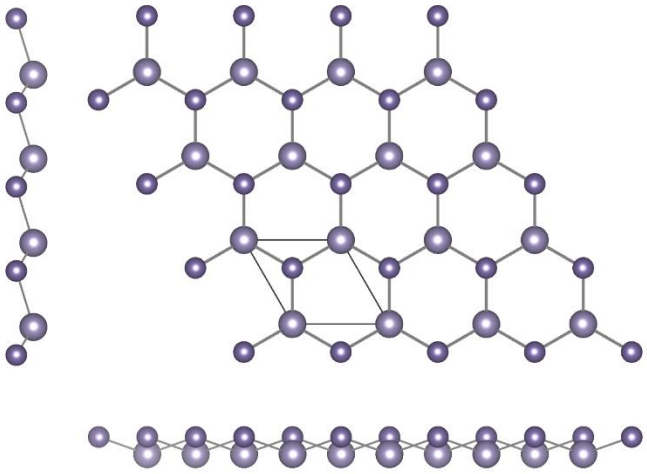
Formula	SnGe	**ID**	mp-995181
Measure	48.1	**Symbol**	P3m1
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	1.531	**Energy-Above-Hull (eV/atom)**	0.481
Formation Energy (eV/atom)	0.481	**Band Gap (eV)**	0.609

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of SnGe in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	2.18181000	-3.77901000	0.00000000
a_2	2.18181000	3.77901000	0.00000000
a_3	0.00000000	0.00000000	12.58620000

	x (Å)	*y* (Å)	*z* (Å)
Sn	0.00000000	0.00000000	6.06560000
Ge	2.18180000	1.25970000	6.83530000



Orthographic projections: views of SnGe as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

31. $AlCl_3$ (C2/m)

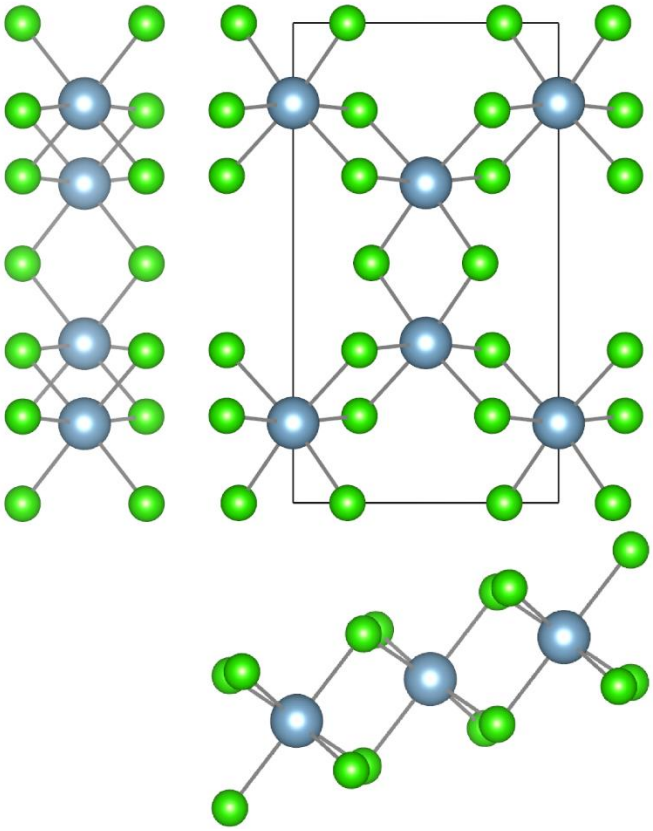
Formula	$AlCl_3$	**ID**	mp-25469
Measure	44.7	**Symbol**	C2/m
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	2.215	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.951	**Band Gap (eV)**	5.311

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $AlCl_3$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	0.00000000	6.02688000	0.00000000
a_2	10.43260000	0.00000000	0.00000000
a_3	0.00000000	-1.95790000	-6.35863000

	x (Å)	*y* (Å)	*z* (Å)
Al	6.95460000	3.01340000	0.00000000
Al	3.47810000	3.01340000	0.00000000
Al	1.73820000	0.00000000	0.00000000
Al	8.69440000	0.00000000	0.00000000
Cl	0.00000000	3.25000000	-5.01530000
Cl	0.00000000	0.81900000	-1.34340000
Cl	1.89450000	4.10770000	-1.33770000
Cl	1.89450000	-0.03880000	-5.02100000
Cl	8.53810000	-0.03880000	-5.02100000
Cl	8.53810000	4.10770000	-1.33770000
Cl	5.21630000	0.23650000	-5.01530000
Cl	5.21630000	3.83250000	-1.34340000
Cl	7.11080000	1.09430000	-1.33770000
Cl	7.11080000	2.97470000	-5.02100000
Cl	3.32180000	2.97470000	-5.02100000
Cl	3.32180000	1.09430000	-1.33770000



Orthographic projections: views of $AlCl_3$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

32. Nb_2CS_2 ($P\bar{3}m1$)

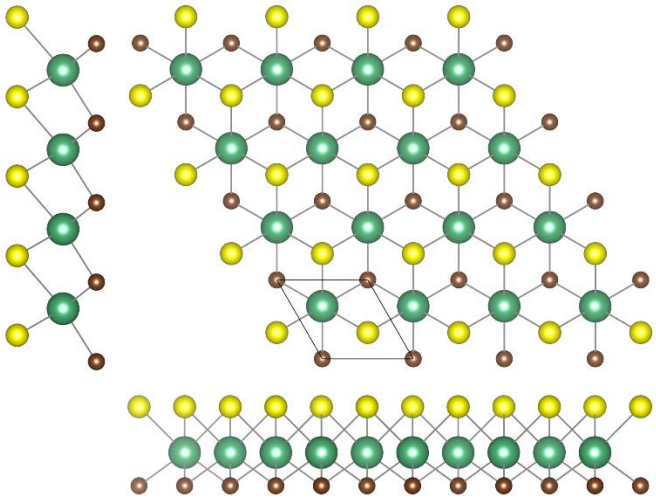
Formula	Nb_2CS_2	**ID**	mp-5745
Measure	44.6	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	4.974	**Energy-Above-Hull (eV/atom)**	0.022
Formation Energy (eV/atom)	-1.114	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Nb_2CS_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.64498000	-2.84919000	0.00000000
a_2	1.64498000	2.84919000	0.00000000
a_3	0.00000000	0.00000000	9.32907000

	x (Å)	*y* (Å)	*z* (Å)
Nb	1.64500000	-0.94970000	8.13120000
Nb	1.64500000	0.94970000	1.19790000
C	0.00000000	0.00000000	0.00000000
S	1.64500000	-0.94970000	2.84600000
S	1.64500000	0.94970000	6.48300000



Orthographic projections: views of Nb_2CS_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

33. SnO_2 ($R\bar{3}m$)

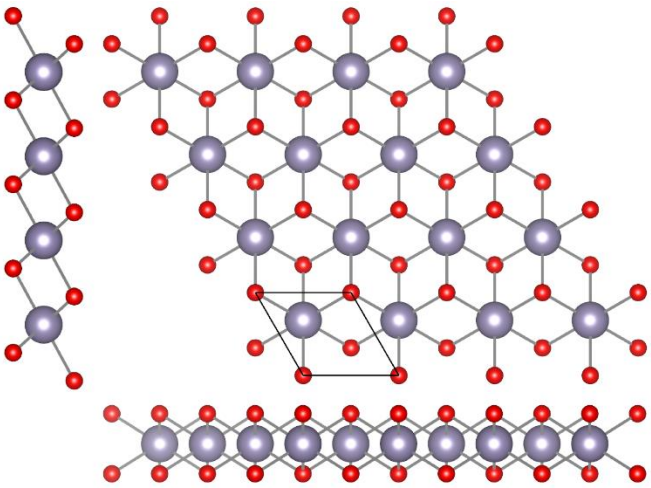
Formula	SnO_2	**ID**	mvc-11686
Measure	42.6	**Symbol**	$R\bar{3}m$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	5.755	**Energy-Above-Hull (eV/atom)**	0.153
Formation Energy (eV/atom)	-1.970	**Band Gap (eV)**	2.005

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of SnO_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.61709000	-2.80089000	0.00000000
a_2	1.61709000	2.80089000	0.00000000
a_3	0.00000000	0.00000000	14.40178000

	x (Å)	*y* (Å)	*z* (Å)
Sn	1.61710000	0.93360000	2.40030000
Sn	3.23420000	0.00000000	7.20090000
Sn	1.61710000	-0.93360000	12.00150000
O	0.00000000	0.00000000	3.41570000
O	1.61710000	-0.93360000	1.38490000
O	1.61710000	-0.93360000	8.21630000
O	1.61710000	0.93360000	6.18550000
O	1.61710000	0.93360000	13.01690000
O	0.00000000	0.00000000	10.98610000



Orthographic projections: views of SnO_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

34. AlClO (Pmmn)

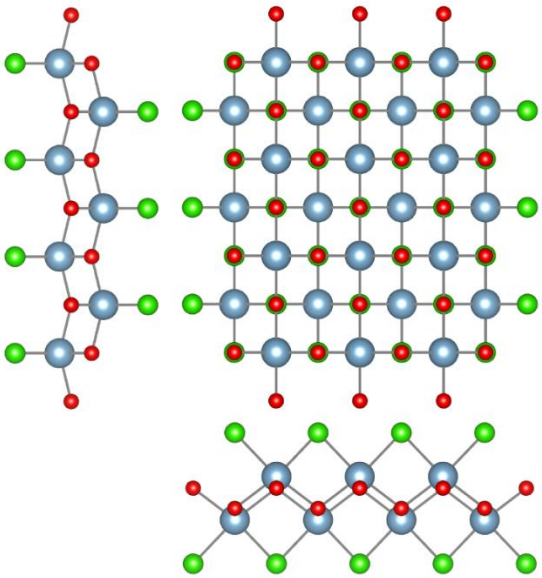
Formula	AlClO	**ID**	mp-27863
Measure	42.3	**Symbol**	Pmmn
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	2.642	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-2.784	**Band Gap (eV)**	5.597

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of AlClO in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.16990000	0.00000000	0.00000000
a_2	0.00000000	3.66076000	0.00000000
a_3	0.00000000	0.00000000	8.49549000

	x (Å)	*y* (Å)	*z* (Å)
Al	1.58490000	0.00000000	7.66350000
Al	0.00000000	1.83040000	0.83200000
Cl	0.00000000	0.00000000	5.97810000
Cl	1.58500000	1.83040000	2.51740000
O	1.58500000	1.83040000	8.10740000
O	0.00000000	0.00000000	0.38810000



Orthographic projections: views of AlClO as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

35. $SrMg_6Ga$ (Amm2)

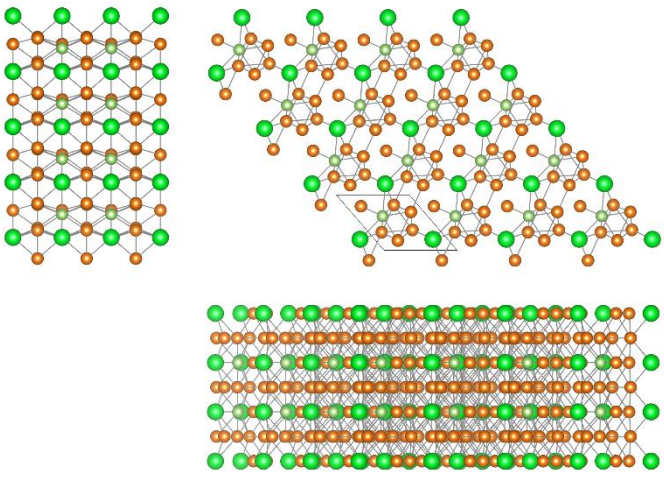
Formula	$SrMg_6Ga$	**ID**	mp-1016442
Measure	41.4	**Symbol**	Amm2
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.030
Density (g/cm^3)	2.428	**Energy-Above-Hull (eV/atom)**	0.116
Formation Energy (eV/atom)	-0.013	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $SrMg_6Ga$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	6.16994	0.000000	0.00000
a_2	0.00000	13.48872	0.00000
a_3	0.00000	0.000000	4.98269

	x (Å)	*y* (Å)	*z* (Å)
Sr	0.0000	2.69260	2.4913
Sr	3.0850	9.43700	2.4913
Mg	1.5917	5.87380	2.4913
Mg	4.5782	5.87380	2.4913
Mg	4.6010	0.98850	0.0000
Mg	1.5689	0.98850	0.0000
Mg	0.0000	4.97750	0.0000
Mg	3.0850	3.99500	0.0000
Mg	4.6767	12.6182	2.4913
Mg	1.4932	12.6182	2.4913
Mg	1.5160	7.73290	0.0000
Mg	4.6539	7.73290	0.0000
Mg	3.0850	11.7219	0.0000
Mg	0.0000	10.7394	0.0000
Ga	3.0850	1.58760	2.4913
Ga	0.0000	8.33200	2.4913



Orthographic projections: views of $SrMg_6Ga$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

36. WSe_2 ($P\bar{3}m1$)

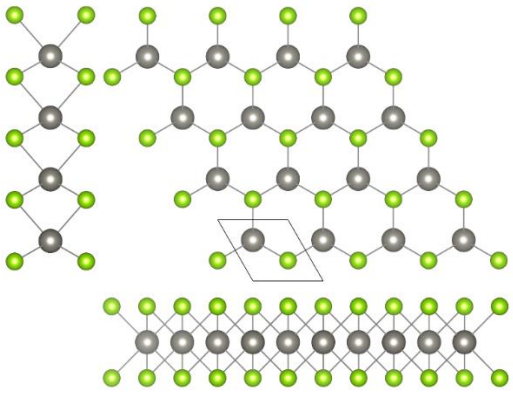
Formula	WSe_2	**ID**	mp-1028698
Measure	39.7	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	5.900	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.557	**Band Gap (eV)**	1.677

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of WSe_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.66353000	-2.88133000	0.00000000
a_2	1.66353000	2.88133000	0.00000000
a_3	0.00000000	0.00000000	40.13790000

	x (Å)	*y* (Å)	*z* (Å)
W	1.66350000	-0.96040000	36.37060000
W	1.66350000	-0.96040000	11.30170000
W	1.66350000	0.96040000	28.83620000
W	1.66350000	0.96040000	3.76730000
Se	1.66350000	0.96040000	38.05190000
Se	1.66350000	0.96040000	12.98290000
Se	1.66350000	-0.96040000	30.51740000
Se	1.66350000	-0.96040000	5.44850000
Se	1.66350000	0.96040000	34.68940000
Se	1.66350000	0.96040000	9.62050000
Se	1.66350000	-0.96040000	27.15500000
Se	1.66350000	-0.96040000	2.08600000



Orthographic projections: views of WSe_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

37. ZrNCl ($R\bar{3}m$)

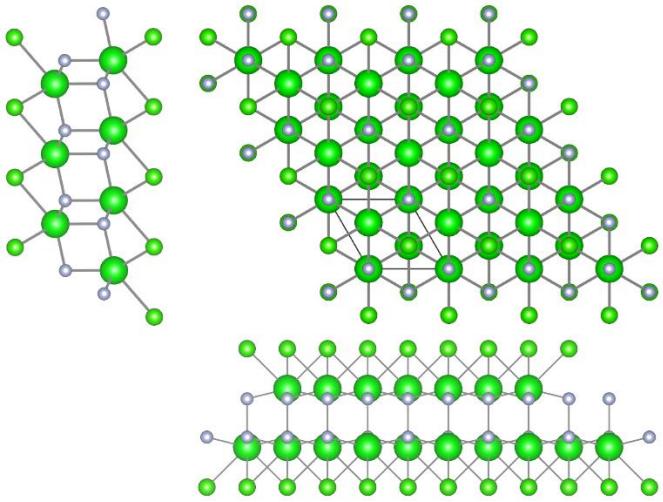
Formula	ZrNCl	**ID**	mp-568592
Measure	39.5	**Symbol**	$R\bar{3}m$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	4.199	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-2.092	**Band Gap (eV)**	1.756

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of ZrNCl in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.82292000	-3.15738000	0.00000000
a_2	1.82292000	3.15738000	0.00000000
a_3	0.00000000	0.00000000	28.99855000

	x (Å)	*y* (Å)	*z* (Å)
Zr	0.00000000	0.00000000	6.15150000
Zr	1.82290000	-1.05250000	3.51470000
Zr	1.82290000	-1.05250000	15.81760000
Zr	1.82290000	1.05250000	13.18090000
Zr	1.82290000	1.05250000	25.48380000
Zr	0.00000000	0.00000000	22.84710000
N	0.00000000	0.00000000	3.96550000
N	1.82290000	-1.05250000	5.70070000
N	1.82290000	-1.05250000	13.63170000
N	1.82290000	1.05250000	15.36680000
N	1.82290000	1.05250000	23.29790000
N	0.00000000	0.00000000	25.03300000
Cl	1.82290000	1.05250000	7.96720000
Cl	1.82290000	1.05250000	1.69900000
Cl	0.00000000	0.00000000	17.63340000
Cl	0.00000000	0.00000000	11.36520000
Cl	1.82290000	-1.05250000	27.29960000
Cl	1.82290000	-1.05250000	21.03140000



Orthographic projections: views of ZrNCl as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

38. YBr_3 (C2/m)

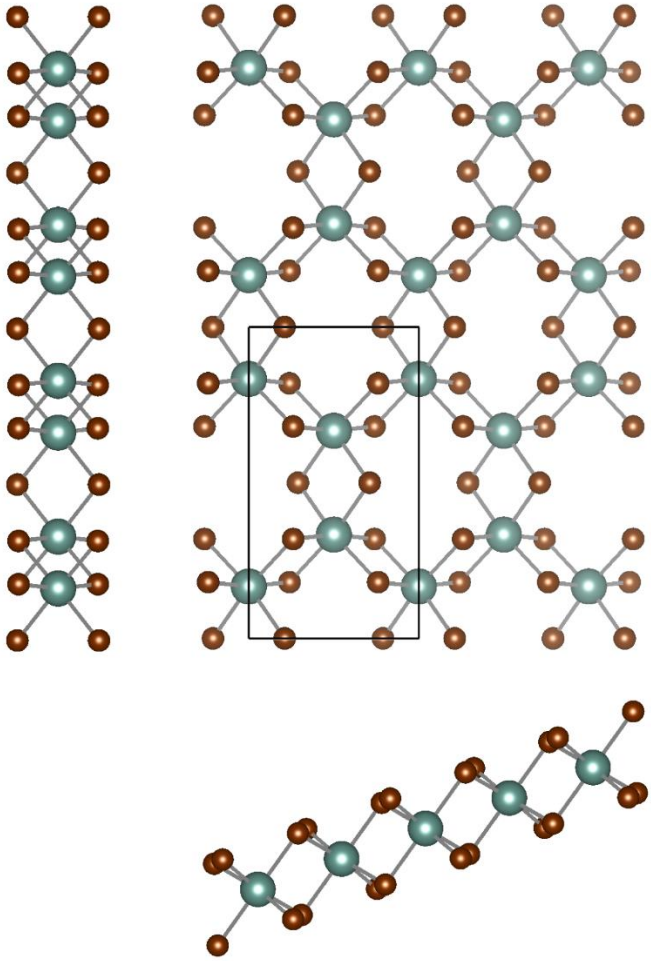
Formula	YBr_3	**ID**	mp-754815
Measure	39.0	**Symbol**	C2/m
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	3.482	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.916	**Band Gap (eV)**	4.052

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of YBr_3 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	0.00000000	7.28199000	0.00000000
a_2	12.55225000	0.00000000	0.00000000
a_3	0.00000000	-2.49705000	-6.85881000

	x (Å)	*y* (Å)	*z* (Å)
Y	8.36960000	3.64100000	0.00000000
Y	4.18260000	3.64100000	0.00000000
Y	2.09350000	0.00000000	0.00000000
Y	10.45880000	0.00000000	0.00000000
Br	10.28400000	-0.17420000	-5.26510000
Br	2.26820000	-0.17420000	-5.26510000
Br	0.00000000	0.93700000	-1.64090000
Br	0.00000000	3.84790000	-5.21790000
Br	10.28400000	4.95910000	-1.59370000
Br	2.26820000	4.95910000	-1.59370000
Br	4.00790000	3.46680000	-5.26510000
Br	8.54440000	3.46680000	-5.26510000
Br	6.27610000	4.57800000	-1.64090000
Br	6.27610000	0.20690000	-5.21790000
Br	4.00790000	1.31810000	-1.59370000
Br	8.54440000	1.31810000	-1.59370000



Orthographic projections: views of YBr_3 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

39. $Te_2Mo_3W(Se_2S)_2$ (P3m1)

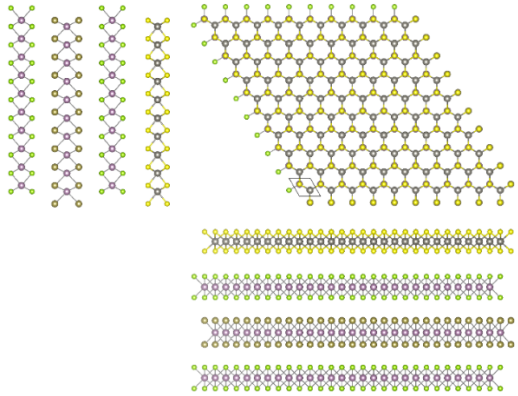
Formula	$Te_2Mo_3W(Se_2S)_2$	**ID**	mp-1030827
Measure	37.6	**Symbol**	P3m1
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.001
Density (g/cm^3)	4.977	**Energy-Above-Hull (eV/atom)**	0.087
Formation Energy (eV/atom)	-0.679	**Band Gap (eV)**	0.397

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $Te_2Mo_3W(Se_2S)_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.67096000	-2.89419000	0.00000000
a_2	1.67096000	2.89419000	0.00000000
a_3	0.00000000	0.00000000	38.18365000

	x (Å)	*y* (Å)	*z* (Å)
Te	1.67100000	-0.96470000	12.65650000
Te	1.67100000	-0.96470000	8.86350000
Mo	1.67100000	-0.96470000	3.58240000
Mo	1.67100000	-0.96470000	17.93680000
Mo	0.00000000	0.00000000	10.75980000
W	0.00000000	0.00000000	25.10720000
Se	0.00000000	0.00000000	1.91550000
Se	0.00000000	0.00000000	16.26830000
Se	0.00000000	0.00000000	5.25080000
Se	0.00000000	0.00000000	19.60520000
S	1.67100000	-0.96470000	26.63020000
S	1.67100000	-0.96470000	23.58410000



Orthographic projections: views of $Te_2Mo_3W(Se_2S)_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

40. ZrIN (Pmmn)

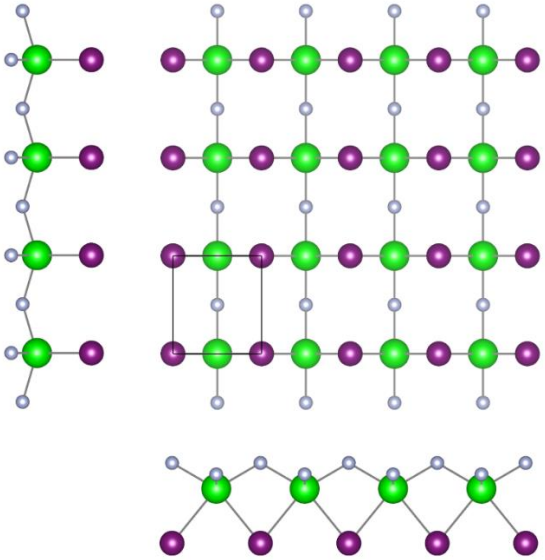
Formula	ZrIN	**ID**	mp-23052
Measure	37.5	**Symbol**	Pmmn
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	4.968	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.502	**Band Gap (eV)**	1.217

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of ZrIN in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.77230000	0.00000000	0.00000000
a_2	0.00000000	4.16290000	0.00000000
a_3	0.00000000	0.00000000	9.88208000

	x (Å)	*y* (Å)	*z* (Å)
Zr	0.00000000	2.08140000	9.02710000
Zr	1.88610000	0.00000000	0.85490000
I	1.88610000	2.08140000	6.70510000
I	0.00000000	0.00000000	3.17700000
N	0.00000000	0.00000000	9.64000000
N	1.88610000	2.08140000	0.24200000



Orthographic projections: views of ZrIN as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

41. TmBrO (P4/nmm)

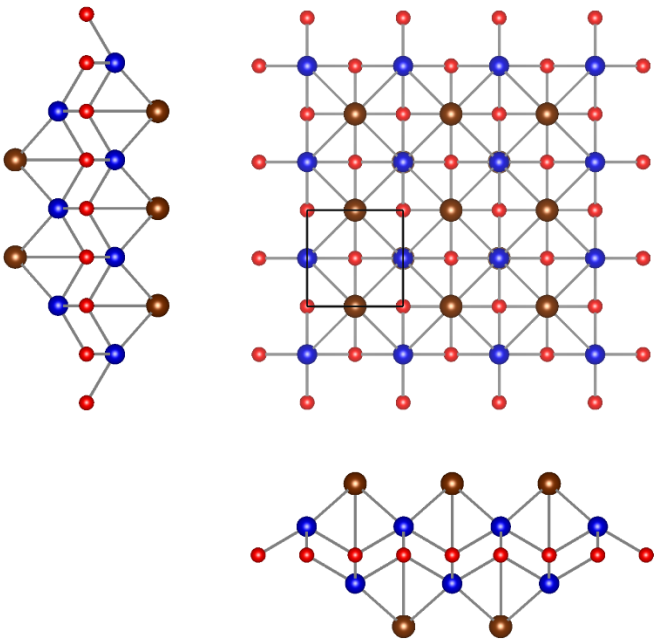
Formula	TmBrO	**ID**	mp-754969
Measure	37.2	**Symbol**	P4/nmm
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	7.072	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-3.191	**Band Gap (eV)**	4.377

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of TmBrO in Cartesian coordinates.

	x (Å)	y (Å)	z (Å)
a_1	3.80095000	0.00000000	0.00000000
a_2	0.00000000	3.80095000	0.00000000
a_3	0.00000000	0.00000000	8.60892000

	x (Å)	y (Å)	z (Å)
Tm	0.00000000	1.90050000	1.11270000
Tm	1.90050000	0.00000000	7.49630000
Br	0.00000000	1.90050000	5.81660000
Br	1.90050000	0.00000000	2.79230000
O	0.00000000	0.00000000	0.00000000
O	1.90050000	1.90050000	0.00000000



Orthographic projections: views of TmBrO as seen from the x axis (left), the y axis (bottom) and the z axis (center). The primitive cell is also shown.

42. PtO_2 ($P6_3mc$)

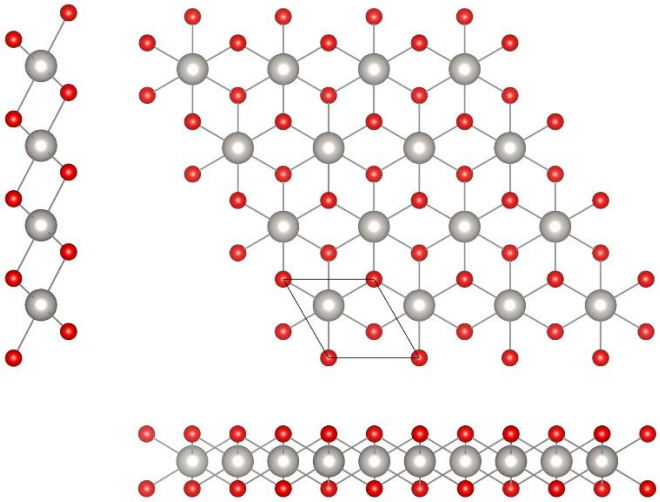
Formula	PtO_2	**ID**	mp-7868
Measure	34.9	**Symbol**	$P6_3mc$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.001
Density (g/cm^3)	9.219	**Energy-Above-Hull (eV/atom)**	0.005
Formation Energy (eV/atom)	-0.932	**Band Gap (eV)**	1.542

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of PtO_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.58203000	-2.74016000	0.00000000
a_2	1.58203000	2.74016000	0.00000000
a_3	0.00000000	0.00000000	9.43584000

	x (Å)	*y* (Å)	*z* (Å)
Pt	1.58200000	0.91340000	0.00000000
Pt	1.58200000	-0.91340000	4.71790000
O	0.00000000	0.00000000	5.66590000
O	0.00000000	0.00000000	0.94790000
O	1.58200000	-0.91340000	8.48790000
O	1.58200000	0.91340000	3.77000000



Orthographic projections: views of PtO_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

43.TiIN (Pmmn)

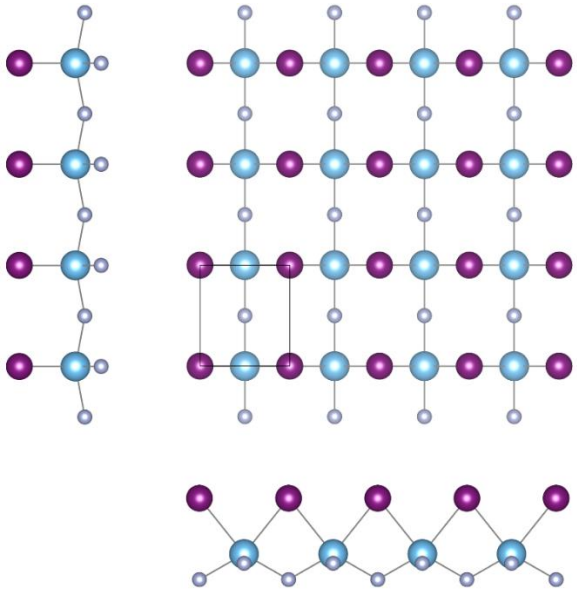
Formula	TiIN	**ID**	mp-27848
Measure	33.9	**Symbol**	Pmmn
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	4.638	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.279	**Band Gap (eV)**	0.015

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of TiIN in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.54132000	0.00000000	0.00000000
a_2	0.00000000	3.97658000	0.00000000
a_3	0.00000000	0.00000000	9.60004000

	x (Å)	*y* (Å)	*z* (Å)
Ti	0.00000000	1.98830000	8.90920000
Ti	1.77070000	0.00000000	0.69090000
I	1.77070000	1.98830000	6.69840000
I	0.00000000	0.00000000	2.90160000
N	0.00000000	0.00000000	9.27820000
N	1.77070000	1.98830000	0.32180000



Orthographic projections: views of TiIN as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

44. $TiMn_2O_6$ (C2/m)

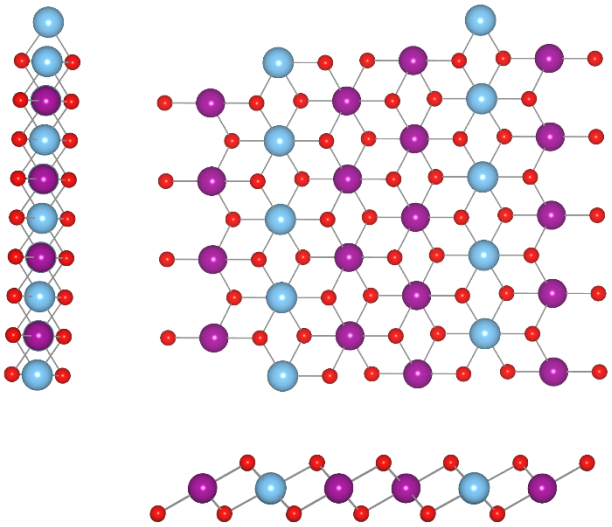
Formula	$TiMn_2O_6$	**ID**	mp-775831
Measure	33.2	**Symbol**	C2/m
Magnetic Ordering	FM	**Tot. Magnetization (μ_B/cell)**	6.000
Density (g/cm^3)	3.931	**Energy-Above-Hull (eV/atom)**	0.085
Formation Energy (eV/atom)	-2.299	**Band Gap (eV)**	1.499

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $TiMn_2O_6$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	0.00000000	12.73030000	0.00000000
a_2	2.95693000	0.00000000	0.00000000
a_3	0.00000000	-1.22784000	-5.69546000

	x (Å)	*y* (Å)	*z* (Å)
Ti	0.00000000	-0.61390000	-2.84770000
Ti	1.47850000	5.75120000	-2.84770000
Mn	1.47850000	10.39690000	-0.93980000
Mn	0.00000000	7.47070000	-4.75560000
Mn	0.00000000	4.03170000	-0.93980000
Mn	1.47850000	1.10560000	-4.75560000
O	0.00000000	10.23460000	-2.19570000
O	1.47850000	8.55690000	-0.32760000
O	1.47850000	7.63300000	-3.49980000
O	0.00000000	5.62360000	-4.14410000
O	1.47850000	12.24400000	-1.55130000
O	0.00000000	9.31070000	-5.36790000
O	1.47850000	3.86940000	-2.19570000
O	0.00000000	2.19180000	-0.32760000
O	0.00000000	1.26790000	-3.49980000
O	1.47850000	-0.74160000	-4.14410000
O	0.00000000	5.87890000	-1.55130000
O	1.47850000	2.94550000	-5.36790000



Orthographic projections: views of $TiMn_2O_6$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

45. NbS_2 ($P\bar{3}m1$)

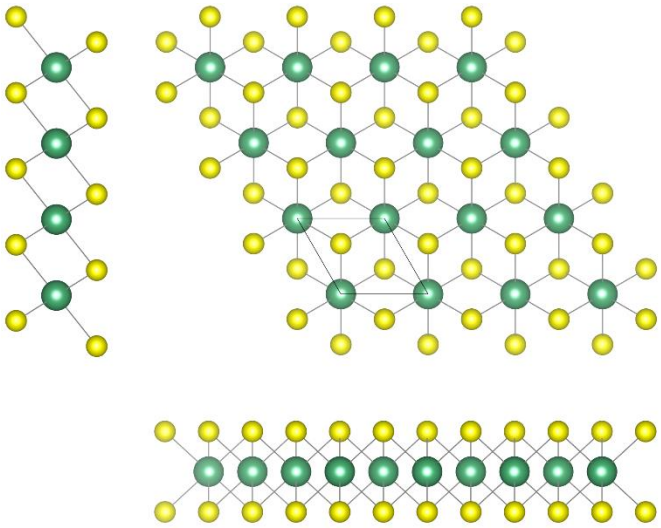
Formula	NbS_2	**ID**	mp-995122
Measure	33.0	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.043
Density (g/cm^3)	4.184	**Energy-Above-Hull (eV/atom)**	0.037
Formation Energy (eV/atom)	-1.419	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of NbS_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.68832000	-2.92426000	0.00000000
a_2	1.68832000	2.92426000	0.00000000
a_3	0.00000000	0.00000000	6.31127000

	x (Å)	*y* (Å)	*z* (Å)
Nb	0.00000000	0.00000000	0.00000000
S	1.68830000	-0.97480000	4.75890000
S	1.68830000	0.97480000	1.55230000



Orthographic projections: views of NbS_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

46. PdS_2 (Pbca)

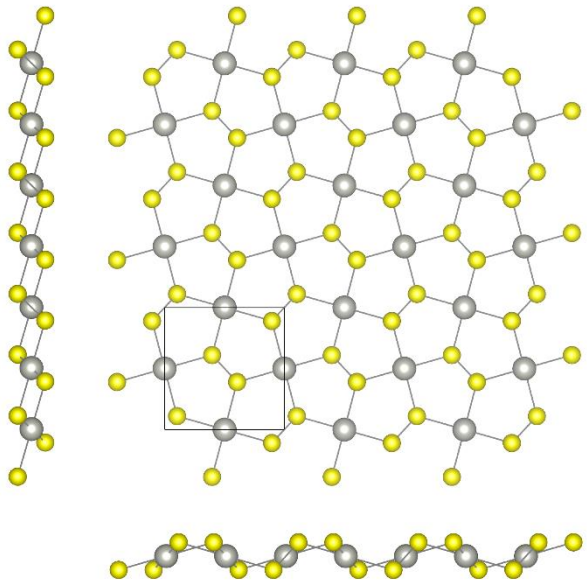
Formula	PdS_2	**ID**	mp-13682
Measure	32.2	**Symbol**	Pbca
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	4.277	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.713	**Band Gap (eV)**	0.654

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of PdS_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	5.50171000	0.00000000	0.00000000
a_2	0.00000000	5.59392000	0.00000000
a_3	0.00000000	0.00000000	8.60709000

	x (Å)	*y* (Å)	*z* (Å)
Pd	2.75090000	0.00000000	4.30350000
Pd	0.00000000	2.79700000	4.30350000
Pd	2.75090000	2.79700000	0.00000000
Pd	0.00000000	0.00000000	0.00000000
S	3.32410000	0.61700000	0.62920000
S	0.57320000	2.18000000	7.97780000
S	2.17760000	3.41390000	3.67430000
S	4.92850000	4.97690000	4.93280000
S	0.57320000	0.61700000	3.67430000
S	3.32410000	2.18000000	4.93280000
S	4.92850000	3.41390000	0.62920000
S	2.17760000	4.97690000	7.97780000



Orthographic projections: views of PdS_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

47. NdI_2 (I4/mmm)

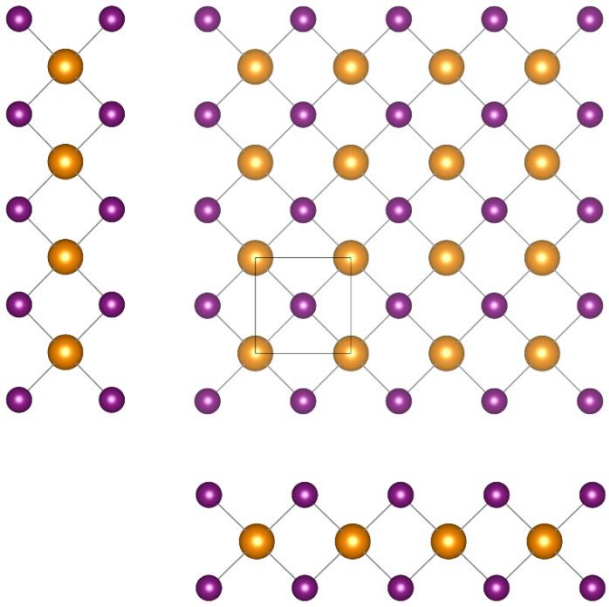
Formula	NdI_2	**ID**	mp-28753
Measure	32.1	**Symbol**	I4/mmm
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.016
Density (g/cm^3)	5.590	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.295	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of NdI_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.88336000	0.00000000	0.00000000
a_2	0.00000000	3.88336000	0.00000000
a_3	0.00000000	0.00000000	15.68178000

	x (Å)	*y* (Å)	*z* (Å)
Nd	0.00000000	0.00000000	0.00000000
Nd	1.94170000	1.94170000	7.84090000
I	1.94170000	1.94170000	1.88790000
I	0.00000000	0.00000000	5.95300000
I	0.00000000	0.00000000	9.72880000
I	1.94170000	1.94170000	13.79390000



Orthographic projections: views of NdI_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

48. $NiCl_2$ ($R\bar{3}m$)

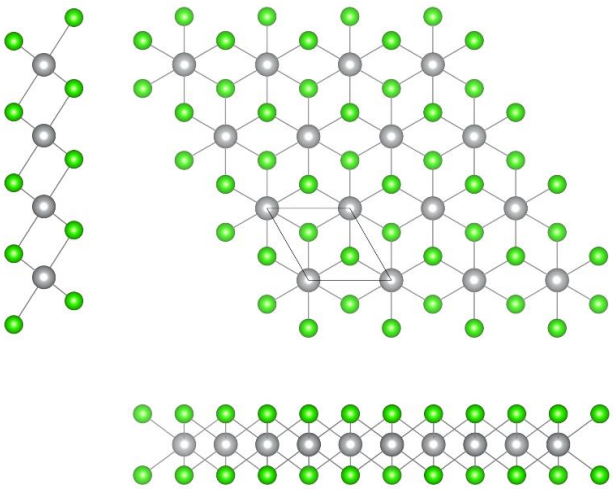
Formula	$NiCl_2$	**ID**	mp-27396
Measure	31.4	**Symbol**	$R\bar{3}m$
Magnetic Ordering	FM	**Tot. Magnetization (μ_B/cell)**	0.140
Density (g/cm^3)	3.221	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.765	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $NiCl_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.73244000	-3.00067000	0.00000000
a_2	1.73244000	3.00067000	0.00000000
a_3	0.00000000	0.00000000	19.27680000

	x (Å)	*y* (Å)	*z* (Å)
Ni	0.00000000	0.00000000	0.00000000
Ni	1.73240000	-1.00020000	6.42560000
Ni	1.73240000	1.00020000	12.85120000
Cl	1.73240000	-1.00020000	1.27570000
Cl	0.00000000	0.00000000	5.14990000
Cl	1.73240000	1.00020000	7.70130000
Cl	1.73240000	-1.00020000	11.57550000
Cl	0.00000000	0.00000000	14.12690000
Cl	1.73240000	1.00020000	18.00110000



Orthographic projections: views of $NiCl_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

49. $ScCl_3$ ($R\bar{3}$)

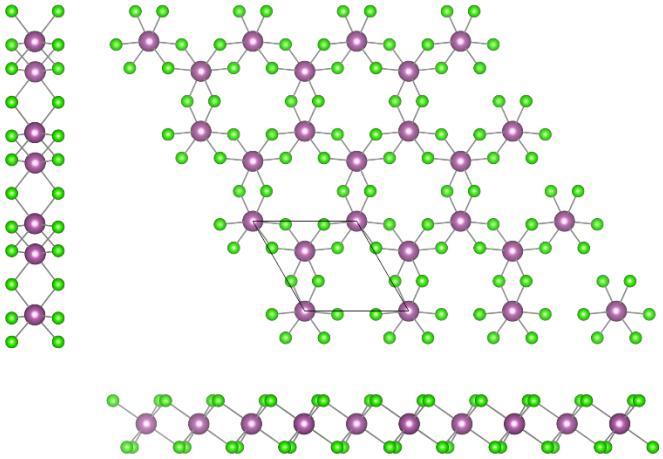
Formula	$ScCl_3$	**ID**	mp-23309
Measure	31.2	**Symbol**	$R\bar{3}$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	2.137	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-2.564	**Band Gap (eV)**	3.879

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $ScCl_3$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.24662000	-5.62331000	0.00000000
a_2	3.24662000	5.62331000	0.00000000
a_3	0.00000000	0.00000000	19.32475000

	x (Å)	*y* (Å)	*z* (Å)
Sc	3.24660000	1.87440000	6.42990000
Sc	3.24660000	1.87440000	0.01160000
Sc	0.00000000	0.00000000	12.87150000
Sc	0.00000000	0.00000000	6.45320000
Sc	3.24660000	-1.87440000	19.31310000
Sc	3.24660000	-1.87440000	12.89480000
Cl	4.44850000	0.20080000	5.00550000
Cl	4.09510000	3.75210000	5.00550000
Cl	2.05030000	-3.54480000	1.43600000
Cl	2.39820000	-0.00320000	1.43600000
Cl	5.29130000	-2.07530000	1.43600000
Cl	1.19630000	1.67040000	5.00550000
Cl	1.20190000	-1.67360000	11.44710000
Cl	4.09510000	-3.74560000	11.44710000
Cl	2.05030000	0.20410000	7.87760000
Cl	2.39820000	3.74560000	7.87760000
Cl	5.29130000	1.67360000	7.87760000
Cl	4.44290000	-0.20410000	11.44710000
Cl	1.20190000	2.07530000	17.88870000
Cl	4.09510000	0.00320000	17.88870000
Cl	5.29690000	-1.67040000	14.31920000
Cl	2.39820000	-3.75210000	14.31920000
Cl	2.04470000	-0.20080000	14.31920000
Cl	4.44290000	3.54480000	17.88870000



Orthographic projections: views of $ScCl_3$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

50. TiS_2 ($P\bar{3}m1$)

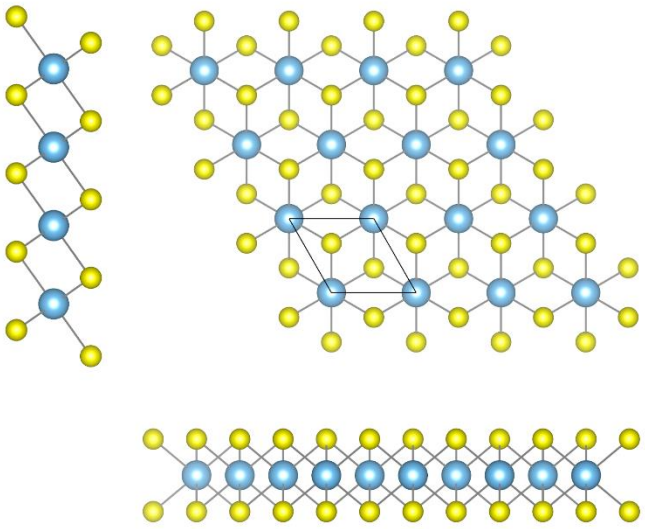
Formula	TiS_2	**ID**	mp-2156
Measure	31.0	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	2.865	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.715	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of TiS_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.70850000	-2.95921000	0.00000000
a_2	1.70850000	2.95921000	0.00000000
a_3	0.00000000	0.00000000	6.41899000

	x (Å)	*y* (Å)	*z* (Å)
Ti	0.00000000	0.00000000	0.00000000
S	1.70850000	0.98640000	1.41840000
S	1.70850000	-0.98640000	5.00060000



Orthographic projections: views of TiS_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

51. Te_2W ($Pmn2_1$)

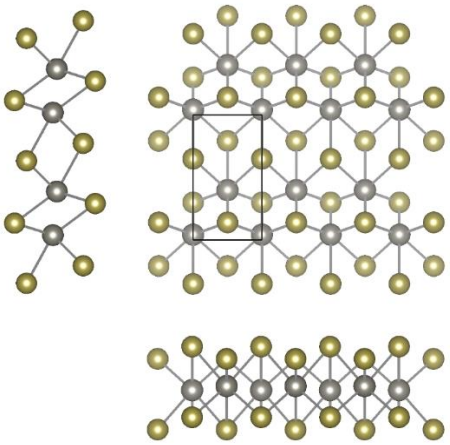
Formula	Te_2W	**ID**	mp-22693
Measure	29.8	**Symbol**	$Pmn2_1$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	8.523	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.106	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Te_2W in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.49794000	0.00000000	0.00000000
a_2	0.00000000	6.33827000	0.00000000
a_3	0.00000000	0.00000000	15.43185000

	x (Å)	*y* (Å)	*z* (Å)
Te	1.74900000	5.02130000	14.07310000
Te	0.00000000	1.31700000	6.35720000
Te	1.74900000	4.43360000	5.73510000
Te	0.00000000	1.90470000	13.45110000
Te	0.00000000	5.44630000	9.92980000
Te	1.74900000	0.89200000	2.21390000
Te	0.00000000	4.11140000	1.59150000
Te	1.74900000	2.22690000	9.30740000
W	1.74900000	6.07030000	7.93480000
W	0.00000000	0.26800000	0.21890000
W	1.74900000	2.52660000	0.01420000
W	0.00000000	3.81170000	7.73010000



Orthographic projections: views of Te_2W as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

52. NiS_2 (P4/nmm)

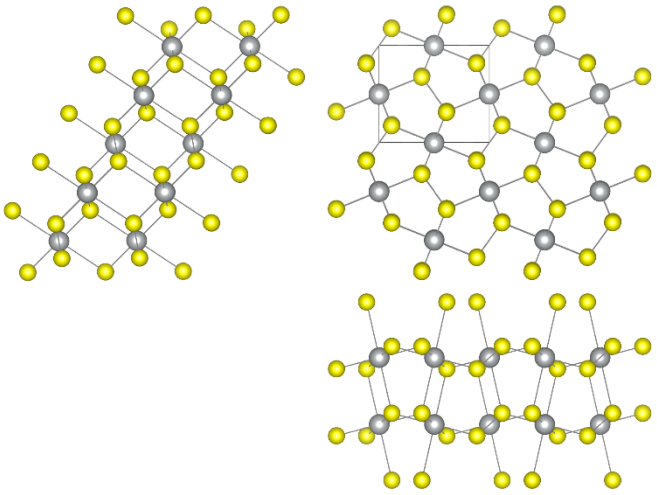
Formula	NiS_2	**ID**	mp-850131
Measure	29.0	**Symbol**	$P2_1/c$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	4.323	**Energy-Above-Hull (eV/atom)**	0.022
Formation Energy (eV/atom)	-0.678	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of NiS_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	0	3.76092	0
a_2	5.35066	0	0
a_3	0	-2.77059	-4.68861

	x (Å)	*y* (Å)	*z* (Å)
Ni	0	0.4952	-2.3443
Ni	2.6753	1.8805	0
S	4.7412	2.0166	-0.8416
S	3.2848	0.6314	-3.1859
S	0.6095	-1.0263	-3.847
S	2.0658	0.359	-1.5027



Orthographic projections: views of NiS_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

53. BiBrO (P4/nmm)

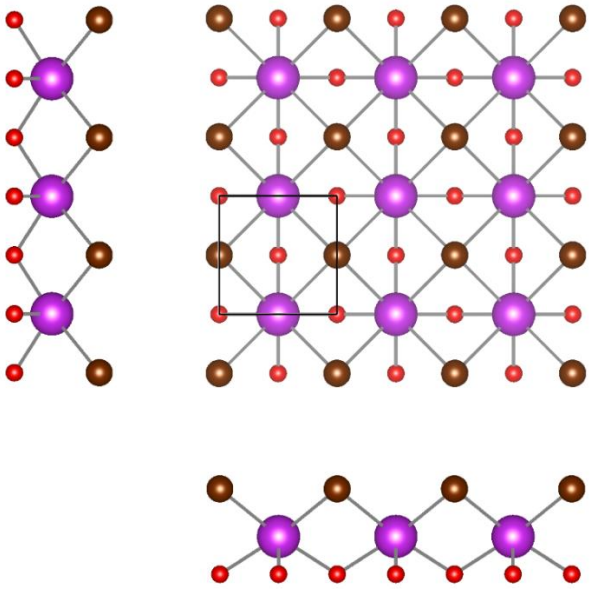
Formula	BiBrO	**ID**	mp-23072
Measure	28.4	**Symbol**	P4/nmm
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	7.294	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.384	**Band Gap (eV)**	2.308

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of BiBrO in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.95291000	0.00000000	0.00000000
a_2	0.00000000	3.95291000	0.00000000
a_3	0.00000000	0.00000000	8.88375000

	x (Å)	*y* (Å)	*z* (Å)
Bi	0.00000000	1.97650000	7.61890000
Bi	1.97650000	0.00000000	1.26480000
Br	1.97650000	0.00000000	6.01800000
Br	0.00000000	1.97650000	2.86570000
O	0.00000000	0.00000000	0.00000000
O	1.97650000	1.97650000	0.00000000



Orthographic projections: views of BiBrO as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

54. SnS (Aem2)

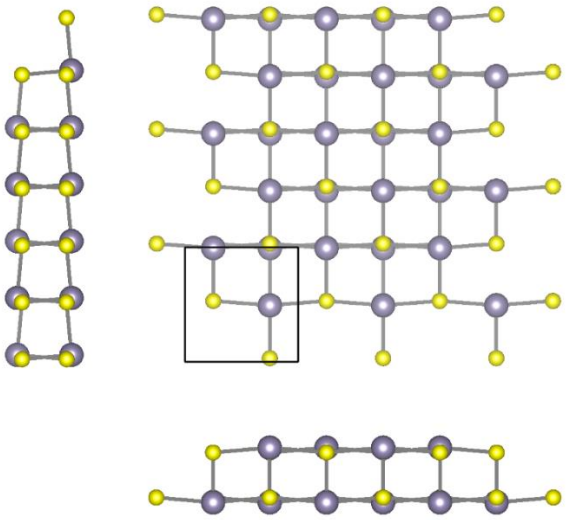
Formula	SnS	**ID**	mp-8781
Measure	27.5	**Symbol**	Aem2
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	2.572	**Energy-Above-Hull (eV/atom)**	0.046
Formation Energy (eV/atom)	-0.732	**Band Gap (eV)**	1.532

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of SnS in Cartesian coordinates.

	x (Å)	y (Å)	z (Å)
a_1	5.85129000	0.00000000	0.00000000
a_2	0.00000000	5.92309000	0.00000000
a_3	0.00000000	0.00000000	11.23619000

	x (Å)	y (Å)	z (Å)
Sn	1.46280000	5.87950000	1.41110000
Sn	4.38850000	5.87950000	9.82510000
Sn	4.38850000	2.91800000	1.41110000
Sn	1.46280000	2.91800000	9.82510000
S	4.38850000	0.18570000	1.16120000
S	1.46280000	0.18570000	10.07500000
S	1.46280000	3.14730000	1.16120000
S	4.38850000	3.14730000	10.07500000



Orthographic projections: views of SnS as seen from the x axis (left), the y axis (bottom) and the z axis (center). The primitive cell is also shown.

55. ZrIN ($R\bar{3}m$)

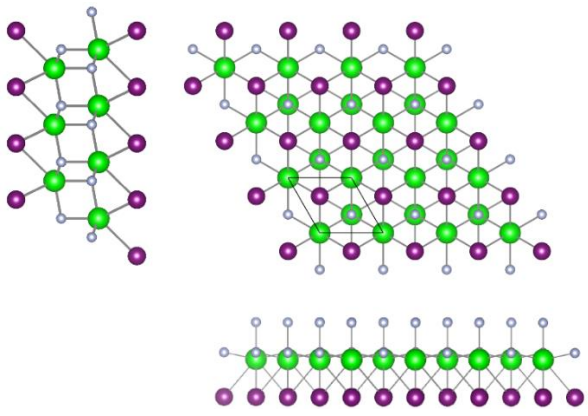
Formula	ZrIN	**ID**	mp-580886
Measure	27.4	**Symbol**	$R\bar{3}m$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	5.816	**Energy-Above-Hull (eV/atom)**	0.030
Formation Energy (eV/atom)	-1.472	**Band Gap (eV)**	1.018

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of ZrIN in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.83797000	-3.18345000	0.00000000
a_2	1.83797000	3.18345000	0.00000000
a_3	0.00000000	0.00000000	19.72199000

	x (Å)	*y* (Å)	*z* (Å)
Zr	0.00000000	0.00000000	0.00000000
Zr	1.83800000	-1.06110000	6.57400000
Zr	1.83800000	1.06110000	13.14800000
Zr	1.83800000	-1.06110000	1.37320000
Zr	0.00000000	0.00000000	5.20080000
Zr	1.83800000	1.06110000	7.94720000
I	1.83800000	-1.06110000	11.77480000
I	0.00000000	0.00000000	14.52120000
I	1.83800000	1.06110000	18.34880000
I	0.00000000	0.00000000	0.00000000
I	1.83800000	-1.06110000	6.57400000
I	1.83800000	1.06110000	13.14800000
N	1.83800000	-1.06110000	1.37320000
N	0.00000000	0.00000000	5.20080000
N	1.83800000	1.06110000	7.94720000
N	1.83800000	-1.06110000	11.77480000
N	0.00000000	0.00000000	14.52120000
N	1.83800000	1.06110000	18.34880000



Orthographic projections: views of ZrIN as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

56. $Na_3(CuO_2)_2$ (C2/m)

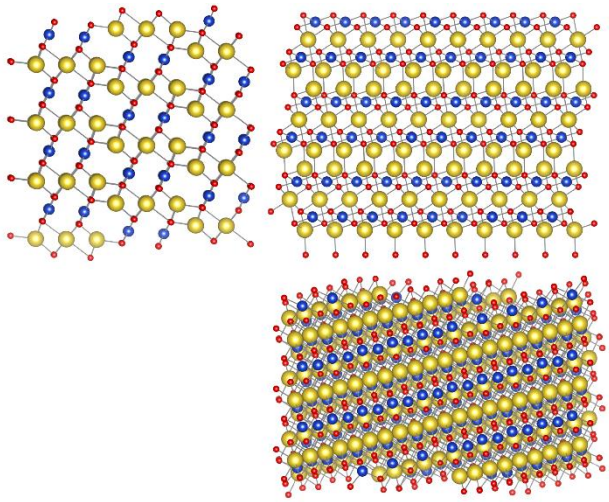
Formula	$Na_3(CuO_2)_2$	**ID**	mp-754483
Measure	27.0	**Symbol**	C2/m
Magnetic Ordering	FM	**Tot. Magnetization (μ_B/cell)**	1.005
Density (g/cm^3)	3.689	**Energy-Above-Hull (eV/atom)**	0.042
Formation Energy (eV/atom)	-1.350	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $Na_3(CuO_2)_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	0	10.87126	0
a_2	2.88966	0	0
a_3	0	-3.3415	-7.45198

	x (Å)	*y* (Å)	*z* (Å)
Na	1.4448	9.1546	-0.8681
Na	0	-1.6707	-3.726
Na	1.4448	-1.6248	-6.5839
Na	0	3.719	-0.8681
Na	1.4448	3.7649	-3.726
Na	0	3.8108	-6.5839
Cu	1.4448	6.3645	-2.082
Cu	1.4448	1.1653	-5.37
Cu	0	0.9288	-2.082
Cu	0	6.6009	-5.37
O	0	0.0529	-5.9888
O	1.4448	7.7602	-4.88
O	1.4448	-0.2304	-2.572
O	0	7.4768	-1.4632
O	1.4448	5.4886	-5.9888
O	0	2.3245	-4.88
O	0	5.2052	-2.572
O	1.4448	2.0412	-1.4632



Orthographic projections: views of $Na_3(CuO_2)_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

57. $MgCl_2$ ($R\bar{3}m$)

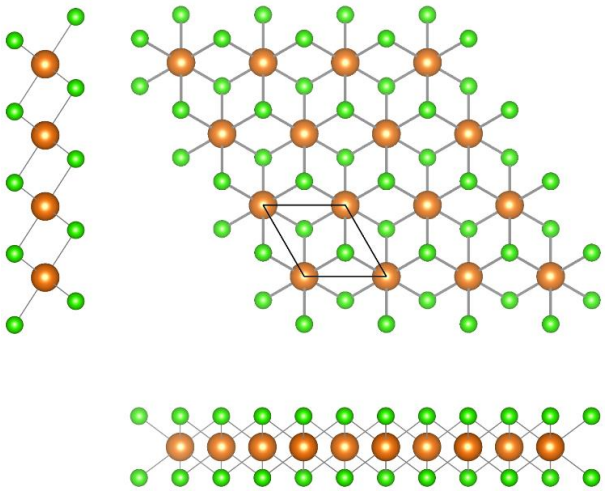
Formula	$MgCl_2$	**ID**	mp-23210
Measure	26.9	**Symbol**	$R\bar{3}m$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	2.055	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-2.254	**Band Gap (eV)**	5.674

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $MgCl_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.83797000	-3.18345000	0.00000000
a_2	1.83797000	3.18345000	0.00000000
a_3	0.00000000	0.00000000	19.72199000

	x (Å)	*y* (Å)	*z* (Å)
Mg	0.00000000	0.00000000	0.00000000
Mg	1.83800000	-1.06110000	6.57400000
Mg	1.83800000	1.06110000	13.14800000
Cl	1.83800000	-1.06110000	1.37320000
Cl	0.00000000	0.00000000	5.20080000
Cl	1.83800000	1.06110000	7.94720000
Cl	1.83800000	-1.06110000	11.77480000
Cl	0.00000000	0.00000000	14.52120000
Cl	1.83800000	1.06110000	18.34880000



Orthographic projections: views of $MgCl_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

58. TaS_2 ($P6_3/mmc$)

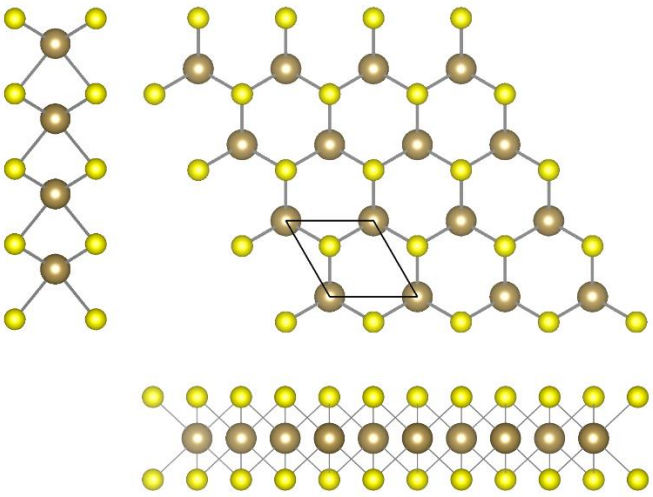
Formula	TaS_2	**ID**	mp-1984
Measure	26.5	**Symbol**	$P6_3/mmc$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.013
Density (g/cm^3)	6.115	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.491	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of TaS_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.67106000	-2.89436000	0.00000000
a_2	1.67106000	2.89436000	0.00000000
a_3	0.00000000	0.00000000	13.76023000

	x (Å)	*y* (Å)	*z* (Å)
Ta	0.00000000	0.00000000	10.32020000
Ta	0.00000000	0.00000000	3.44010000
S	1.67110000	-0.96480000	8.75640000
S	1.67110000	0.96480000	1.87630000
S	1.67110000	0.96480000	5.00380000
S	1.67110000	-0.96480000	11.88390000



Orthographic projections: views of TaS_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

59. $Sr_2Cu(BrO)_2$ (I4/mmm)

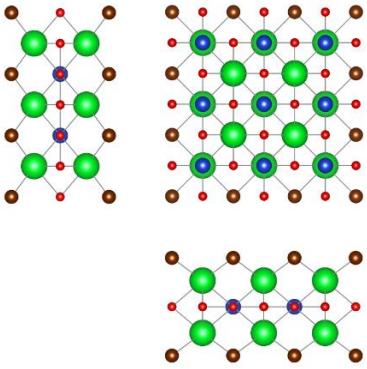
Formula	$Sr_2Cu(BrO)_2$	**ID**	mp-546898
Measure	25.8	**Symbol**	I4/mmm
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.005
Density (g/cm^3)	4.735	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-2.139	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $Sr_2Cu(BrO)_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.99400000	0.00000000	0.00000000
a_2	0.00000000	3.99400000	0.00000000
a_3	0.00000000	0.00000000	18.93217000

	x (Å)	*y* (Å)	*z* (Å)
Sr	1.99700000	1.99700000	1.70220000
Sr	0.00000000	0.00000000	7.76380000
Sr	0.00000000	0.00000000	11.16830000
Sr	1.99700000	1.99700000	17.22990000
Cu	0.00000000	0.00000000	0.00000000
Cu	1.99700000	1.99700000	9.46610000
Br	1.99700000	1.99700000	6.28750000
Br	0.00000000	0.00000000	3.17860000
Br	0.00000000	0.00000000	15.75360000
Br	1.99700000	1.99700000	12.64460000
O	1.99700000	0.00000000	0.00000000
O	0.00000000	1.99700000	0.00000000
O	0.00000000	1.99700000	9.46610000
O	1.99700000	0.00000000	9.46610000



Orthographic projections: views of $Sr_2Cu(BrO)_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

60. LaFeSi (P4/nmm)

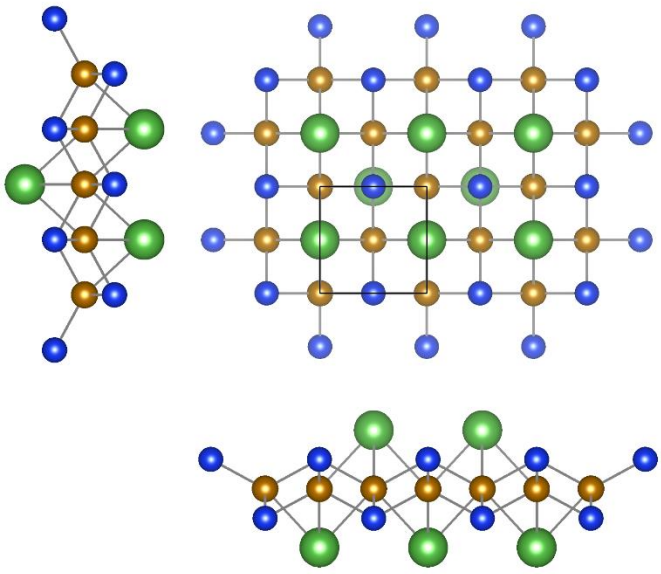
Formula	LaFeSi	**ID**	mp-505332
Measure	25.7	**Symbol**	P4/nmm
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.077
Density (g/cm^3)	6.128	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.583	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of LaFeSi in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	4.10139000	0.00000000	0.00000000
a_2	0.00000000	4.10139000	0.00000000
a_3	0.00000000	0.00000000	7.17982000

	x (Å)	*y* (Å)	*z* (Å)
La	2.05070000	0.00000000	4.96620000
La	0.00000000	2.05070000	2.21360000
Fe	0.00000000	0.00000000	0.00000000
Fe	2.05070000	2.05070000	0.00000000
Si	2.05070000	0.00000000	1.11220000
Si	0.00000000	2.05070000	6.06760000



Orthographic projections: views of LaFeSi as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

61. $MgPSe_3$ ($R\bar{3}$)

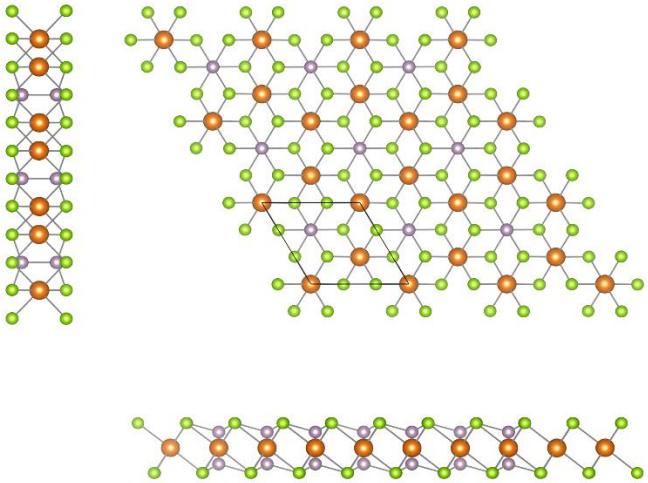
Formula	$MgPSe_3$	**ID**	mp-30943
Measure	25.7	**Symbol**	$R\bar{3}$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	3.593	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.606	**Band Gap (eV)**	2.296

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $MgPSe_3$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.22917000	-5.59309000	0.00000000
a_2	3.22917000	5.59309000	0.00000000
a_3	0.00000000	0.00000000	22.42938000

	x (Å)	*y* (Å)	*z* (Å)
Mg	3.22920000	-1.86440000	3.72370000
Mg	0.00000000	0.00000000	3.75270000
Mg	3.22920000	1.86440000	11.20020000
Mg	3.22920000	-1.86440000	11.22920000
Mg	0.00000000	0.00000000	18.67670000
Mg	3.22920000	1.86440000	18.70560000
P	3.22920000	1.86440000	4.85760000
P	3.22920000	1.86440000	2.61890000
P	0.00000000	0.00000000	12.33400000
P	0.00000000	0.00000000	10.09540000
P	3.22920000	-1.86440000	19.81050000
P	3.22920000	-1.86440000	17.57180000
Se	5.35860000	1.87780000	5.47340000
Se	2.15280000	3.70180000	5.47340000
Se	2.17610000	0.01350000	5.47340000
Se	1.09980000	1.85090000	2.00310000
Se	4.30550000	0.02700000	2.00310000
Se	4.28220000	3.71520000	2.00310000
Se	2.12940000	0.01340000	12.94980000
Se	5.38200000	1.83740000	12.94980000
Se	2.17610000	3.74220000	12.94980000
Se	4.32890000	-0.01340000	9.47950000
Se	1.07640000	-1.83740000	9.47950000
Se	4.28220000	-3.74220000	9.47950000
Se	5.35860000	-1.85090000	20.42630000
Se	2.15280000	-0.02700000	20.42630000
Se	2.17610000	-3.71520000	20.42630000
Se	1.09980000	-1.87780000	16.95600000
Se	4.30550000	-3.70180000	16.95600000
Se	4.28220000	-0.01350000	16.95600000



Orthographic projections: views of $MgPSe_3$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

62. $CrSiTe_3$ ($R\bar{3}$)

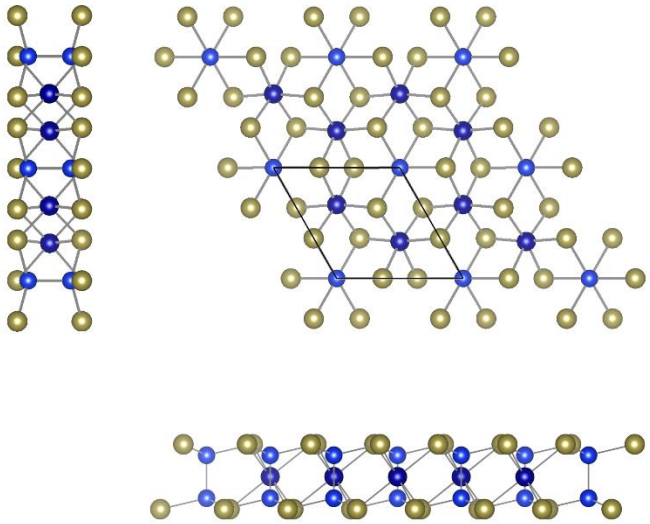
Formula	$CrSiTe_3$	**ID**	mp-3779
Measure	25.3	**Symbol**	$R\bar{3}$
Magnetic Ordering	FM	**Tot. Magnetization (μ_B/cell)**	0.491
Density (g/cm^3)	4.995	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.177	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $CrSiTe_3$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.41899000	-5.92187000	0.00000000
a_2	3.41899000	5.92187000	0.00000000
a_3	0.00000000	0.00000000	22.80152000

	x (Å)	*y* (Å)	*z* (Å)
Cr	3.41900000	1.97400000	7.59210000
Cr	3.41900000	1.97400000	0.00840000
Cr	0.00000000	0.00000000	15.19260000
Cr	0.00000000	0.00000000	7.60890000
Cr	3.41900000	-1.97400000	22.79310000
Cr	3.41900000	-1.97400000	15.20940000
Si	0.00000000	0.00000000	1.14230000
Si	3.41900000	-1.97400000	6.45820000
Si	3.41900000	-1.97400000	8.74280000
Si	3.41900000	1.97400000	14.05870000
Si	3.41900000	1.97400000	16.34330000
Si	0.00000000	0.00000000	21.65920000
Te	1.24450000	-2.14670000	1.72290000
Te	4.65580000	-3.77080000	1.72290000
Te	4.35670000	-0.00450000	1.72290000
Te	2.48130000	3.95240000	5.87760000
Te	5.60120000	1.79680000	5.87760000
Te	2.17450000	0.17270000	5.87760000
Te	1.24450000	1.80130000	9.32340000
Te	4.65580000	0.17720000	9.32340000
Te	4.35670000	3.94340000	9.32340000
Te	2.48130000	-3.94340000	13.47810000
Te	2.18220000	-0.17720000	13.47810000
Te	5.59350000	-1.80130000	13.47810000
Te	4.66350000	-0.17270000	16.92390000
Te	1.23680000	-1.79680000	16.92390000
Te	4.35670000	-3.95240000	16.92390000
Te	2.48130000	0.00450000	21.07860000
Te	2.18220000	3.77080000	21.07860000
Te	5.59350000	2.14670000	21.07860000



Orthographic projections: views of $CrSiTe_3$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

63. $CrBr_3$ ($R\bar{3}$)

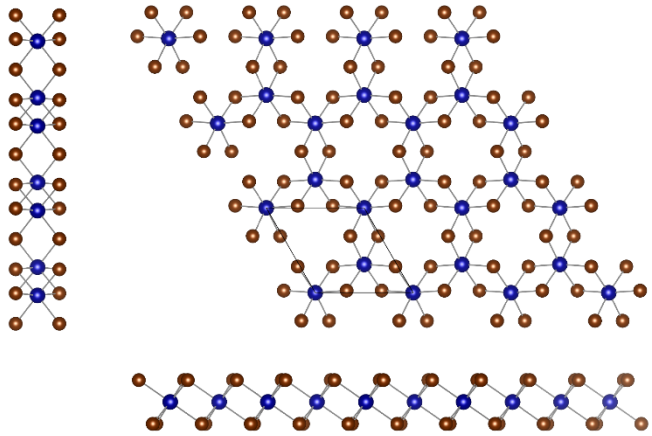
Formula	$CrBr_3$	**ID**	mp-27734
Measure	25.2	**Symbol**	$R\bar{3}$
Magnetic Ordering	FM	**Tot. Magnetization (μ_B/cell)**	2.992
Density (g/cm^3)	3.943	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.817	**Band Gap (eV)**	1.291

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $CrBr_3$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.22303000	-5.58245000	0.00000000
a_2	3.22303000	5.58245000	0.00000000
a_3	0.00000000	0.00000000	20.48524000

	x (Å)	*y* (Å)	*z* (Å)
Cr	3.22300000	1.86080000	6.82650000
Cr	3.22300000	1.86080000	0.00190000
Cr	0.00000000	0.00000000	13.65490000
Cr	0.00000000	0.00000000	6.83040000
Cr	3.22300000	-1.86080000	20.48330000
Cr	3.22300000	-1.86080000	13.65880000
Br	2.06660000	0.13970000	5.39200000
Br	2.31070000	3.72290000	5.39200000
Br	5.29180000	1.71990000	5.39200000
Br	4.13540000	-0.00130000	1.43640000
Br	4.37730000	-3.58070000	1.43640000
Br	1.15650000	-2.00050000	1.43640000
Br	5.28960000	-1.72110000	12.22040000
Br	2.31070000	-3.72030000	12.22040000
Br	2.06880000	-0.14100000	12.22040000
Br	4.13540000	3.72030000	8.26480000
Br	4.37730000	0.14100000	8.26480000
Br	1.15650000	1.72110000	8.26480000
Br	5.28960000	2.00050000	19.04880000
Br	2.31070000	0.00130000	19.04880000
Br	2.06880000	3.58070000	19.04880000
Br	4.13540000	-3.72290000	15.09320000
Br	1.15420000	-1.71990000	15.09320000
Br	4.37950000	-0.13970000	15.09320000



Orthographic projections: views of $CrBr_3$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

64. H_3ClO (R3m)

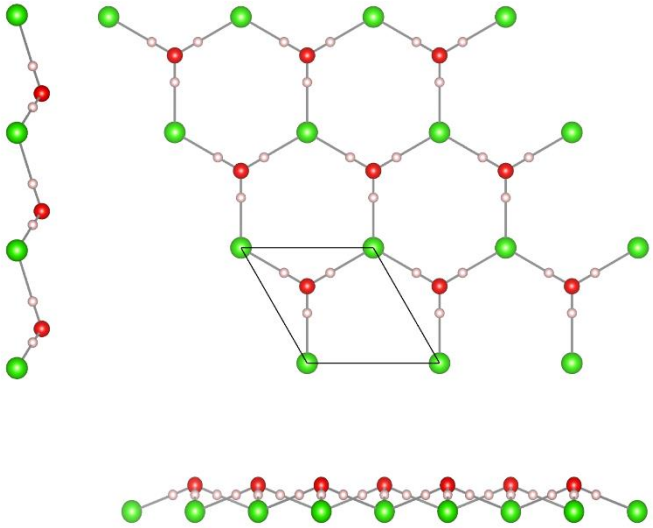
Formula	H_3ClO	**ID**	mp-34078
Measure	24.9	**Symbol**	R3m
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	1.419	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.234	**Band Gap (eV)**	5.390

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of H_3ClO in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	2.42382000	-4.19818000	0.00000000
a_2	2.42382000	4.19818000	0.00000000
a_3	0.00000000	0.00000000	9.39467000

	x (Å)	*y* (Å)	*z* (Å)
H	3.27010000	0.91080000	0.74530000
H	2.42380000	2.37660000	0.74530000
H	1.57750000	0.91080000	0.74530000
H	0.84630000	-0.48860000	3.87690000
H	2.42380000	-3.22100000	3.87690000
H	4.00140000	-0.48860000	3.87690000
H	3.27010000	-1.88800000	7.00840000
H	2.42380000	-0.42220000	7.00840000
H	1.57750000	-1.88800000	7.00840000
H	2.42380000	1.39940000	6.43640000
H	0.00000000	0.00000000	0.17330000
H	2.42380000	-1.39940000	3.30490000
Cl	2.42380000	1.39940000	1.07300000
Cl	0.00000000	0.00000000	4.20460000
Cl	2.42380000	-1.39940000	7.33620000
O	3.27010000	0.91080000	0.74530000
O	2.42380000	2.37660000	0.74530000
O	1.57750000	0.91080000	0.74530000



Orthographic projections: views of H_3ClO as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

65. GaS ($R\bar{3}m$)

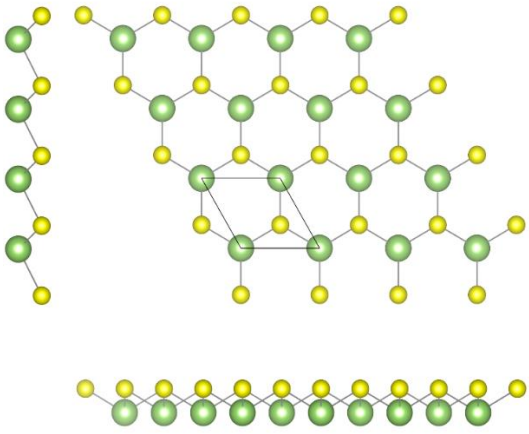
Formula	GaS	**ID**	mp-9889
Measure	24.0	**Symbol**	$R\bar{3}m$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	3.392	**Energy-Above-Hull (eV/atom)**	0.006
Formation Energy (eV/atom)	-0.977	**Band Gap (eV)**	1.948

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of GaS in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.81850000	-3.14973000	0.00000000
a_2	1.81850000	3.14973000	0.00000000
a_3	0.00000000	0.00000000	26.09888000

	x (Å)	*y* (Å)	*z* (Å)
Ga	0.00000000	0.00000000	1.23300000
Ga	1.81850000	-1.04990000	7.46660000
Ga	1.81850000	-1.04990000	9.93260000
Ga	1.81850000	1.04990000	16.16620000
Ga	1.81850000	1.04990000	18.63230000
Ga	0.00000000	0.00000000	24.86590000
S	1.81850000	-1.04990000	2.31160000
S	0.00000000	0.00000000	6.38810000
S	1.81850000	1.04990000	11.01120000
S	1.81850000	-1.04990000	15.08770000
S	0.00000000	0.00000000	19.71080000
S	1.81850000	1.04990000	23.78730000



Orthographic projections: views of GaS as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

66. $TiGeO_3$ ($R\bar{3}$)

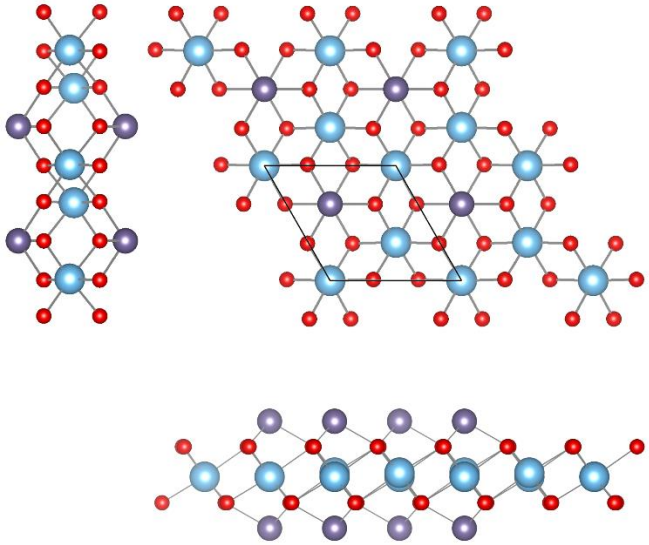
Formula	$TiGeO_3$	**ID**	mp-780260
Measure	23.8	**Symbol**	$R\bar{3}$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	3.933	**Energy-Above-Hull (eV/atom)**	0.040
Formation Energy (eV/atom)	-2.693	**Band Gap (eV)**	1.123

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $TiGeO_3$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	2.52251000	-4.36911000	0.00000000
a_2	2.52251000	4.36911000	0.00000000
a_3	0.00000000	0.00000000	19.36563000

	x (Å)	*y* (Å)	*z* (Å)
Ti	2.52250000	-1.45640000	3.30770000
Ti	0.00000000	0.00000000	3.14750000
Ti	2.52250000	1.45640000	9.76290000
Ti	2.52250000	-1.45640000	9.60270000
Ti	0.00000000	0.00000000	16.21810000
Ti	2.52250000	1.45640000	16.05790000
Ge	2.52250000	1.45640000	5.28840000
Ge	2.52250000	1.45640000	1.16680000
Ge	0.00000000	0.00000000	11.74360000
Ge	0.00000000	0.00000000	7.62200000
Ge	2.52250000	-1.45640000	18.19880000
Ge	2.52250000	-1.45640000	14.07720000
O	0.86620000	-1.41580000	4.30630000
O	3.31560000	-2.91110000	4.30630000
O	3.38580000	-0.04220000	4.30630000
O	4.18180000	-1.41420000	2.14890000
O	1.72940000	-2.91440000	2.14890000
O	1.65630000	-0.04050000	2.14890000
O	0.86620000	1.49690000	10.76150000
O	3.31560000	0.00170000	10.76150000
O	3.38580000	2.87050000	10.76150000
O	1.65920000	-2.87050000	8.60410000
O	1.72940000	-0.00170000	8.60410000
O	4.17880000	-1.49690000	8.60410000
O	3.38870000	0.04050000	17.21670000
O	3.31560000	2.91440000	17.21670000
O	0.86330000	1.41420000	17.21670000
O	1.65920000	0.04220000	15.05930000
O	1.72940000	2.91110000	15.05930000
O	4.17880000	1.41580000	15.05930000



Orthographic projections: views of $TiGeO_3$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

67. CrP_2S_7 (C2)

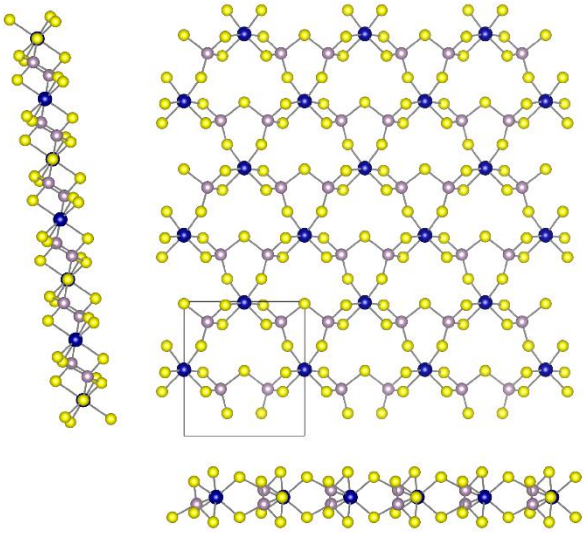
Formula	CrP_2S_7	**ID**	mp-768680
Measure	23.5	**Symbol**	C2
Magnetic Ordering	FM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	2.131	**Energy-Above-Hull (eV/atom)**	0.056
Formation Energy (eV/atom)	-0.689	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CrP_2S_7 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	0.00000000	8.57605000	0.00000000
a_2	9.48287000	0.00000000	0.00000000
a_3	0.00000000	-0.82250000	-6.48341000

	x (Å)	*y* (Å)	*z* (Å)
Cr	9.41750000	4.28800000	0.00000000
Cr	4.67610000	0.00000000	0.00000000
P	8.05280000	1.61490000	-0.49690000
P	8.05280000	6.13860000	-5.98650000
P	3.31140000	5.90290000	-0.49690000
P	3.31140000	1.85060000	-5.98650000
S	7.86710000	2.04840000	-5.38080000
S	1.60480000	2.42570000	-5.06420000
S	9.22630000	2.71590000	-1.76000000
S	4.59390000	4.28800000	0.00000000
S	9.22630000	5.03760000	-4.72340000
S	1.60480000	5.32780000	-1.41920000
S	7.86710000	5.70520000	-1.10260000
S	3.12560000	6.33640000	-5.38080000
S	6.34620000	6.71380000	-5.06420000
S	4.48480000	7.00390000	-1.76000000
S	9.33540000	0.00000000	0.00000000
S	4.48480000	0.74960000	-4.72340000
S	6.34620000	1.03980000	-1.41920000
S	3.12560000	1.41710000	-1.10260000



Orthographic projections: views of CrP_2S_7 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

68. VCl_2 ($P\bar{3}m1$)

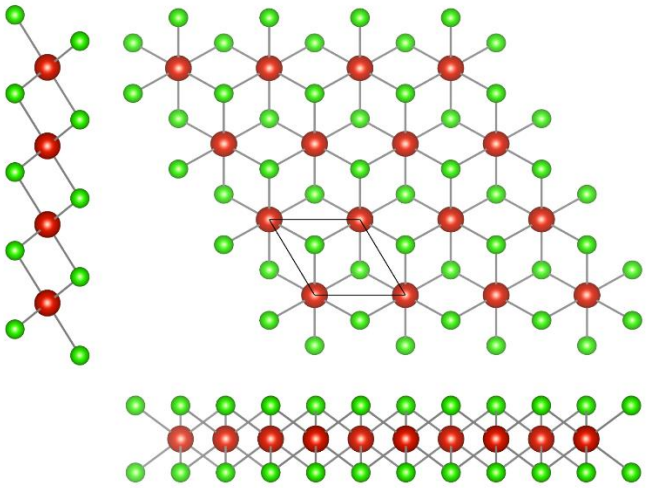
Formula	VCl_2	**ID**	mp-22877
Measure	23.4	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	FM	**Tot. Magnetization (μ_B/cell)**	3.001
Density (g/cm^3)	2.873	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.551	**Band Gap (eV)**	1.260

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of VCl_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.82766000	-3.16561000	0.00000000
a_2	1.82766000	3.16561000	0.00000000
a_3	0.00000000	0.00000000	6.08597000

	x (Å)	*y* (Å)	*z* (Å)
V	0.00000000	0.00000000	0.00000000
Cl	1.82770000	-1.05520000	4.75320000
Cl	1.82770000	1.05520000	1.33280000



Orthographic projections: views of VCl_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

69. $SmBr_3$ (Cmcm)

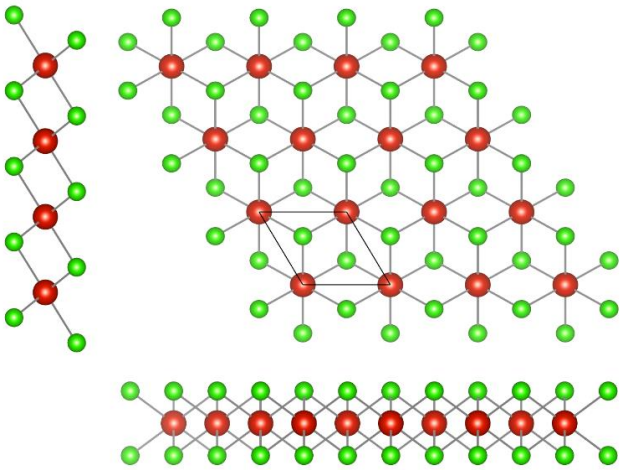
Formula	$SmBr_3$	**ID**	mp-27976
Measure	22.8	**Symbol**	Cmcm
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	4.833	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.895	**Band Gap (eV)**	2.929

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $SmBr_3$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	4.05208000	0.00000000	0.00000000
a_2	0.00000000	14.31397000	0.00000000
a_3	0.00000000	0.00000000	9.24236000

	x (Å)	*y* (Å)	*z* (Å)
Sm	2.02600000	3.45490000	6.93180000
Sm	0.00000000	3.70210000	2.31060000
Sm	0.00000000	10.61190000	6.93180000
Sm	2.02600000	10.85910000	2.31060000
Br	0.00000000	4.91130000	8.61320000
Br	2.02600000	2.24570000	0.62920000
Br	2.02600000	5.75270000	2.31060000
Br	0.00000000	1.40430000	6.93180000
Br	0.00000000	4.91130000	5.25030000
Br	2.02600000	2.24570000	3.99200000
Br	2.02600000	12.06820000	8.61320000
Br	0.00000000	9.40270000	0.62920000
Br	0.00000000	12.90970000	2.31060000
Br	2.02600000	8.56130000	6.93180000
Br	2.02600000	12.06820000	5.25030000
Br	0.00000000	9.40270000	3.99200000



Orthographic projections: views of $SmBr_3$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

70. $Mg_2Al_2Se_5$ ($P\bar{3}m1$)

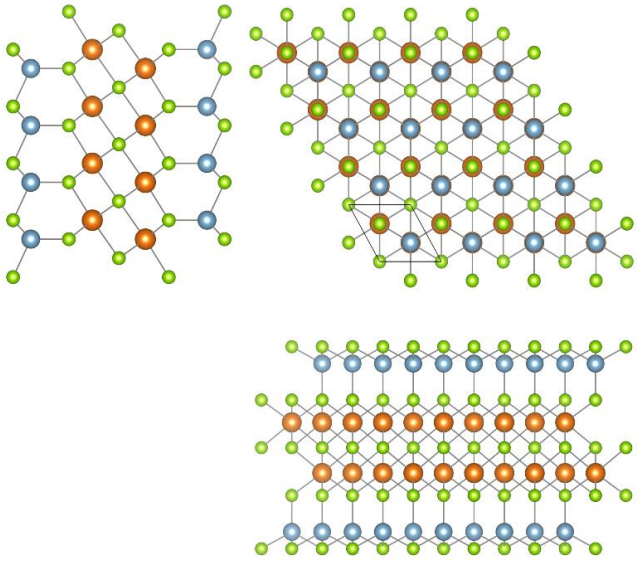
Formula	$Mg_2Al_2Se_5$	**ID**	mp-29624
Measure	22.4	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.012
Density (g/cm^3)	3.776	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.049	**Band Gap (eV)**	1.985

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $Mg_2Al_2Se_5$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.95886000	-3.39285000	0.00000000
a_2	1.95886000	3.39285000	0.00000000
a_3	0.00000000	0.00000000	16.50005000

	x (Å)	*y* (Å)	*z* (Å)
Mg	1.95890000	1.13090000	9.85870000
Mg	1.95890000	-1.13090000	6.64130000
Al	1.95890000	1.13090000	2.91040000
Al	1.95890000	-1.13090000	13.58970000
Se	1.95890000	-1.13090000	1.83920000
Se	1.95890000	1.13090000	14.66080000
Se	1.95890000	-1.13090000	11.27820000
Se	1.95890000	1.13090000	5.22190000
Se	0.00000000	0.00000000	8.25000000



Orthographic projections: views of $Mg_2Al_2Se_5$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

71. LaI_2 (I4/mmm)

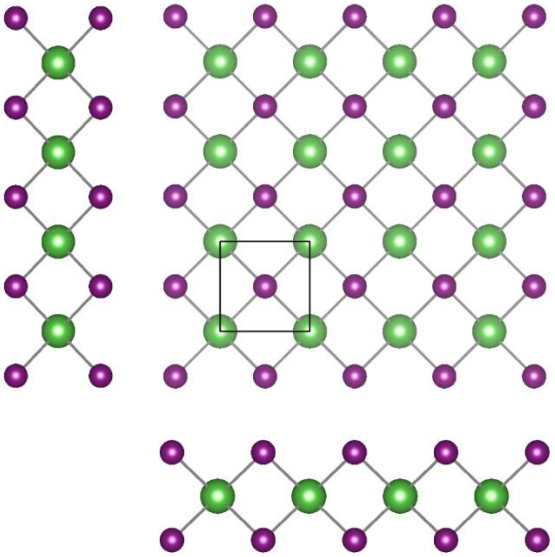
Formula	LaI_2	**ID**	mp-23194
Measure	22.4	**Symbol**	I4/mmm
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.010
Density (g/cm^3)	5.584	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.420	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of LaI_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.95231000	0.00000000	0.00000000
a_2	0.00000000	3.95231000	0.00000000
a_3	0.00000000	0.00000000	14.95242000

	x (Å)	*y* (Å)	*z* (Å)
La	0.00000000	0.00000000	0.00000000
La	1.97620000	1.97620000	7.47620000
I	0.00000000	0.00000000	5.58460000
I	1.97620000	1.97620000	1.89160000
I	1.97620000	1.97620000	13.06090000
I	0.00000000	0.00000000	9.36780000



Orthographic projections: views of LaI_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

72. NdBrO (P4/nmm)

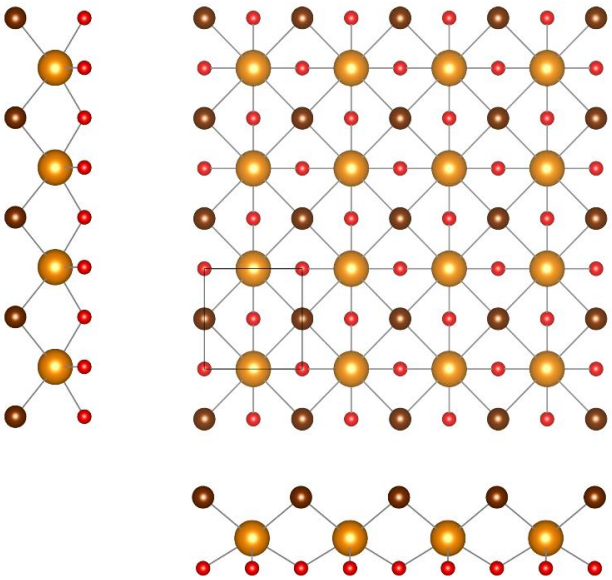
Formula	NdBrO	**ID**	mp-23068
Measure	22.3	**Symbol**	P4/nmm
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	5.810	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-3.111	**Band Gap (eV)**	4.483

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of NdBrO in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	4.01894000	0.00000000	0.00000000
a_2	0.00000000	4.01894000	0.00000000
a_3	0.00000000	0.00000000	8.49946000

	x (Å)	*y* (Å)	*z* (Å)
Nd	0.00000000	2.00950000	7.29470000
Nd	2.00950000	0.00000000	1.20480000
Br	2.00950000	0.00000000	5.65230000
Br	0.00000000	2.00950000	2.84710000
O	0.00000000	0.00000000	0.00000000
O	2.00950000	2.00950000	0.00000000



Orthographic projections: views of NdBrO as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

73. Ta_2CS_2 ($P\bar{3}m1$)

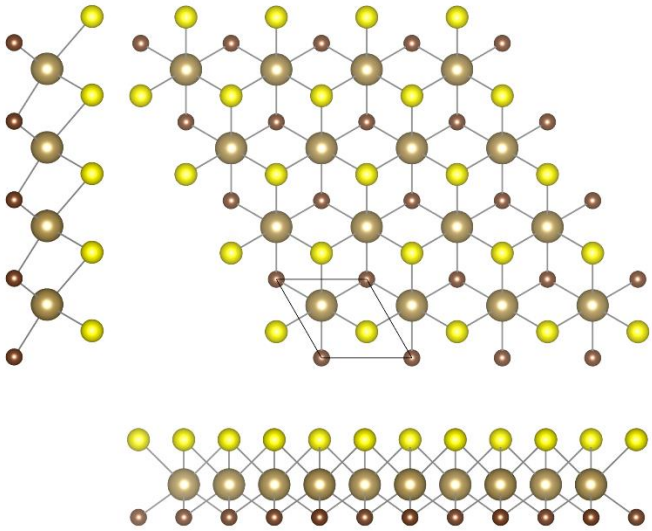
Formula	Ta_2CS_2	**ID**	mp-559976
Measure	22.1	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	8.684	**Energy-Above-Hull (eV/atom)**	0.007
Formation Energy (eV/atom)	-1.193	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Ta_2CS_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.64494000	-2.84912000	0.00000000
a_2	1.64494000	2.84912000	0.00000000
a_3	0.00000000	0.00000000	8.93615000

	x (Å)	*y* (Å)	*z* (Å)
Ta	1.64490000	-0.94970000	7.75130000
Ta	1.64490000	0.94970000	1.18480000
C	0.00000000	0.00000000	0.00000000
S	1.64490000	0.94970000	6.12770000
S	1.64490000	-0.94970000	2.80840000



Orthographic projections: views of Ta_2CS_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

74. Nb_3SBr_7 (P3m1)

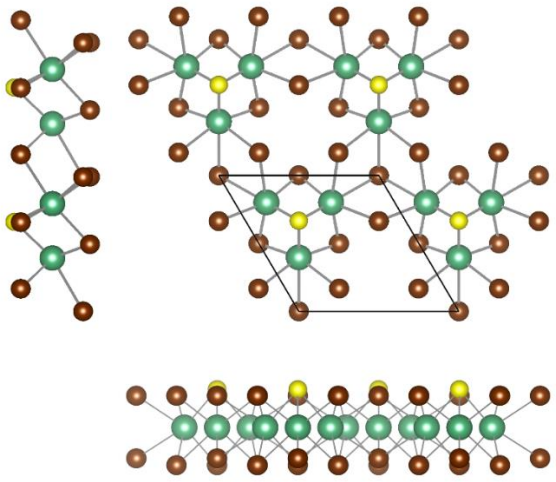
Formula	Nb_3SBr_7	**ID**	mp-29057
Measure	22.1	**Symbol**	P3m1
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	4.636	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.060	**Band Gap (eV)**	0.744

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Nb_3SBr_7 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.60191000	-6.23868000	0.00000000
a_2	3.60191000	6.23868000	0.00000000
a_3	0.00000000	0.00000000	6.93488000

	x (Å)	*y* (Å)	*z* (Å)
Nb	5.05930000	1.23810000	1.54810000
Nb	2.14450000	1.23810000	1.54810000
Nb	3.60190000	3.76240000	1.54810000
S	3.60190000	2.07960000	3.27840000
Br	5.39290000	-3.11360000	6.76990000
Br	1.81090000	-3.11360000	6.76990000
Br	0.00000000	0.00000000	0.14450000
Br	1.81590000	-1.04840000	2.98900000
Br	3.60190000	-4.14190000	2.98900000
Br	5.38790000	-1.04840000	2.98900000
Br	3.60190000	-0.01150000	6.76990000



Orthographic projections: views of Nb_3SBr_7 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

75. ZrS_2 ($P\bar{3}m1$)

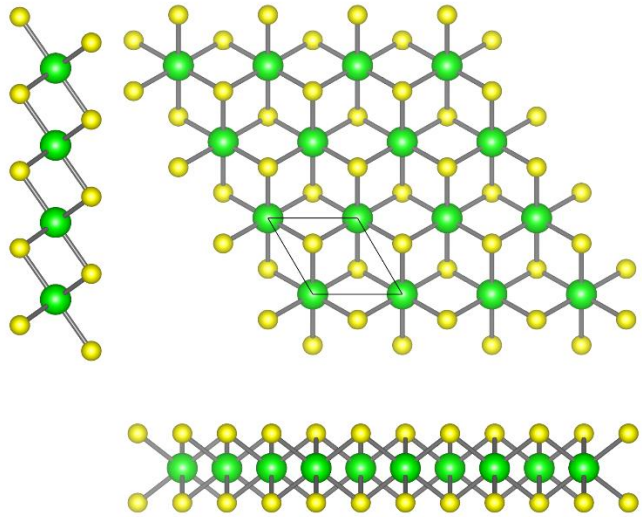
Formula	ZrS_2	**ID**	mp-1186
Measure	21.6	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.002
Density (g/cm^3)	3.307	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.956	**Band Gap (eV)**	1.042

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of ZrS_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.84546000	-3.19643000	0.00000000
a_2	1.84546000	3.19643000	0.00000000
a_3	0.00000000	0.00000000	6.61113000

	x (Å)	*y* (Å)	*z* (Å)
Zr	0.00000000	0.00000000	0.00000000
S	1.84550000	-1.06550000	5.15410000
S	1.84550000	1.06550000	1.45700000



Orthographic projections: views of ZrS_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

76. Sc_2NCl_2 ($P\bar{3}m1$)

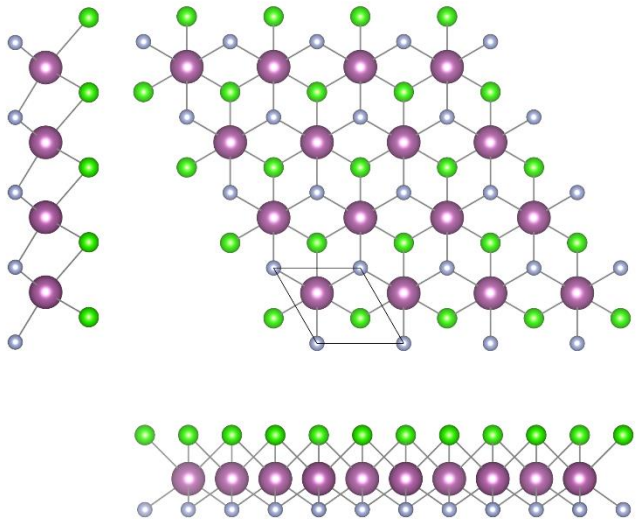
Formula	Sc_2NCl_2	**ID**	mp-28480
Measure	21.5	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.015
Density (g/cm^3)	3.086	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-2.298	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Sc_2NCl_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.68483000	-2.91821000	0.00000000
a_2	1.68483000	2.91821000	0.00000000
a_3	0.00000000	0.00000000	9.56577000

	x (Å)	*y* (Å)	*z* (Å)
Sc	1.68480000	-0.97270000	5.97120000
Sc	1.68480000	0.97270000	3.59460000
N	0.00000000	0.00000000	4.78290000
Cl	1.68480000	-0.97270000	1.90650000
Cl	1.68480000	0.97270000	7.65930000



Orthographic projections: views of Sc_2NCl_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

77. VSe_2 ($P\bar{3}m1$)

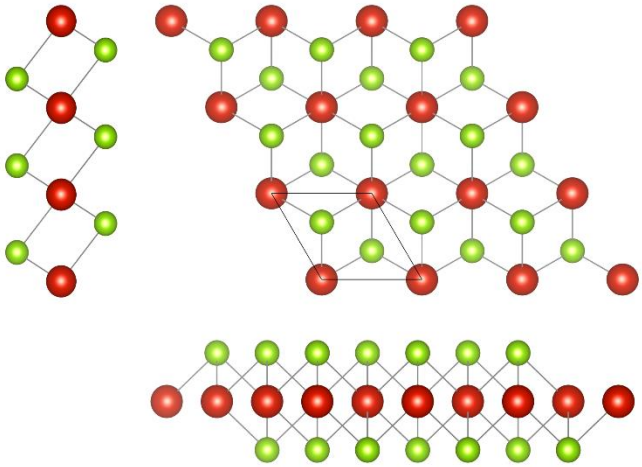
Formula	VSe_2	**ID**	mp-694
Measure	21.4	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	FM	**Tot. Magnetization (μ_B/cell)**	0.731
Density (g/cm^3)	5.086	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.692	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of VSe_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.67690000	-2.90448000	0.00000000
a_2	1.67690000	2.90448000	0.00000000
a_3	0.00000000	0.00000000	7.00043000

	x (Å)	*y* (Å)	*z* (Å)
V	0.00000000	0.00000000	0.00000000
Se	1.67690000	-0.96820000	5.42490000
Se	1.67690000	0.96820000	1.57560000



Orthographic projections: views of VSe_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

78. MgI_2 ($P\bar{3}m1$)

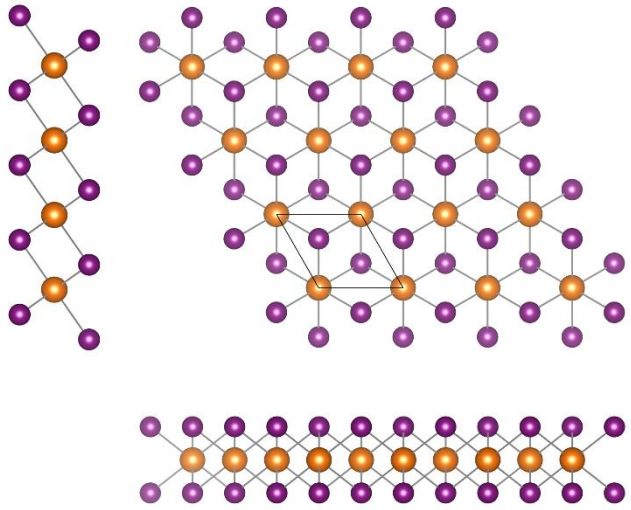
Formula	MgI_2	**ID**	mp-23205
Measure	21.3	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	3.893	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.031	**Band Gap (eV)**	3.677

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of MgI_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	2.10475000	-3.64553000	0.00000000
a_2	2.10475000	3.64553000	0.00000000
a_3	0.00000000	0.00000000	7.73128000

	x (Å)	*y* (Å)	*z* (Å)
Mg	0.00000000	0.00000000	0.00000000
I	2.10470000	1.21520000	1.67350000
I	2.10470000	-1.21520000	6.05780000



Orthographic projections: views of MgI_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

79. TiNCl (Pmmn)

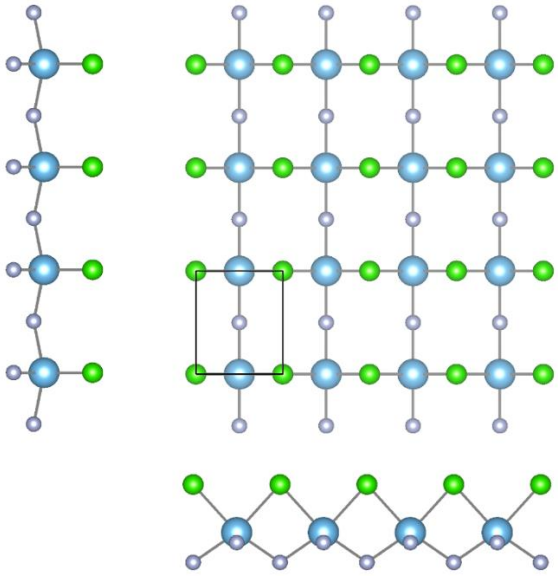
Formula	TiNCl	**ID**	mp-27850
Measure	20.8	**Symbol**	Pmmn
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	2.961	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.861	**Band Gap (eV)**	0.561

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of TiNCl in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.27536000	0.00000000	0.00000000
a_2	0.00000000	3.96669000	0.00000000
a_3	0.00000000	0.00000000	8.40249000

	x (Å)	*y* (Å)	*z* (Å)
Ti	1.63770000	0.00000000	0.77090000
Ti	0.00000000	1.98330000	7.63160000
N	0.00000000	0.00000000	8.02110000
N	1.63770000	1.98330000	0.38140000
Cl	1.63770000	1.98330000	5.79020000
Cl	0.00000000	0.00000000	2.61230000



Orthographic projections: views of TiNCl as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

80. $HfSnO_3$ ($R\bar{3}$)

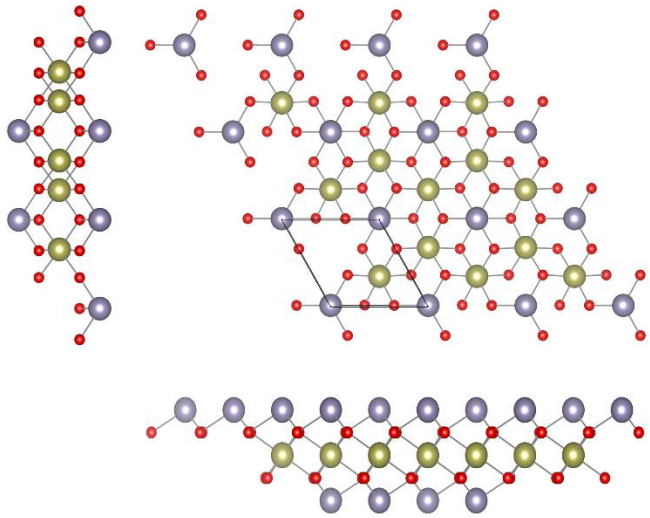
Formula	$HfSnO_3$	**ID**	mp-776083
Measure	20.6	**Symbol**	$R\bar{3}$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.001
Density (g/cm^3)	6.593	**Energy-Above-Hull (eV/atom)**	0.069
Formation Energy (eV/atom)	-3.008	**Band Gap (eV)**	2.378

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $HfSnO_3$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	2.72506000	-4.71995000	0.00000000
a_2	2.72506000	4.71995000	0.00000000
a_3	0.00000000	0.00000000	20.28004000

	x (Å)	*y* (Å)	*z* (Å)
Hf	2.72510000	-1.57330000	0.00580000
Hf	0.00000000	0.00000000	6.75420000
Hf	2.72510000	1.57330000	6.76580000
Hf	2.72510000	-1.57330000	13.51420000
Hf	0.00000000	0.00000000	13.52580000
Hf	2.72510000	1.57330000	20.27430000
Sn	2.72510000	-1.57330000	4.54990000
Sn	0.00000000	0.00000000	2.21010000
Sn	2.72510000	1.57330000	11.30990000
Sn	2.72510000	-1.57330000	8.97020000
Sn	0.00000000	0.00000000	18.06990000
Sn	2.72510000	1.57330000	15.73020000
O	0.95330000	1.50210000	5.64800000
O	3.67270000	0.07450000	5.64800000
O	1.90090000	0.00330000	1.11200000
O	3.54920000	3.14330000	5.64800000
O	1.77750000	3.07210000	1.11200000
O	4.49680000	1.64460000	1.11200000
O	3.67840000	-0.07130000	12.40800000
O	0.94760000	-1.49880000	12.40800000
O	1.90090000	3.14990000	7.87200000
O	3.54920000	-3.14990000	12.40800000
O	4.50250000	1.49880000	7.87200000
O	1.77180000	0.07130000	7.87200000
O	0.95330000	-1.64460000	19.16800000
O	3.67270000	-3.07210000	19.16800000
O	1.90090000	-3.14330000	14.63200000
O	3.54920000	-0.00330000	19.16800000



Orthographic projections: views of $HfSnO_3$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

81. LaI_3 (Cmcm)

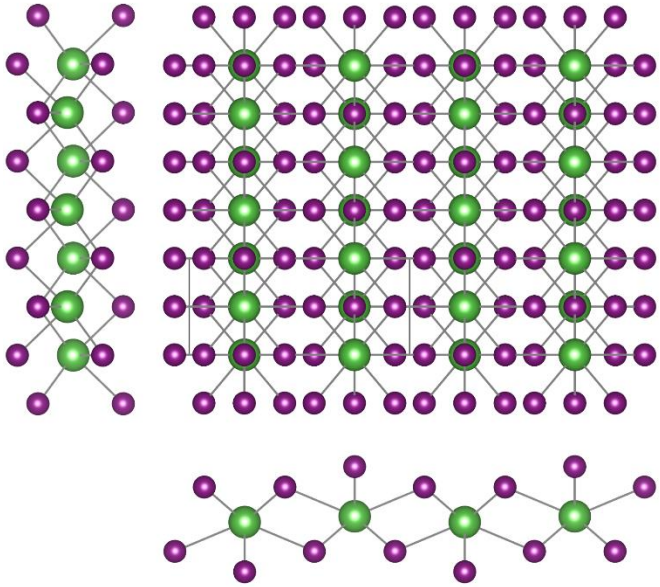
Formula	LaI_3	**ID**	mp-27979
Measure	20.4	**Symbol**	Cmcm
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	4.888	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.547	**Band Gap (eV)**	2.071

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of LaI_3 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	4.44718000	0.00000000	0.00000000
a_2	0.00000000	15.62178000	0.00000000
a_3	0.00000000	0.00000000	10.16318000

	x (Å)	*y* (Å)	*z* (Å)
La	2.22360000	3.77090000	7.62240000
La	0.00000000	4.04000000	2.54080000
La	0.00000000	11.58180000	7.62240000
La	2.22360000	11.85090000	2.54080000
I	0.00000000	5.38920000	9.48480000
I	2.22360000	2.42170000	0.67840000
I	2.22360000	6.33300000	2.54080000
I	0.00000000	1.47790000	7.62240000
I	0.00000000	5.38920000	5.76000000
I	2.22360000	2.42170000	4.40320000
I	2.22360000	13.20000000	9.48480000
I	0.00000000	10.23260000	0.67840000
I	0.00000000	14.14390000	2.54080000
I	2.22360000	9.28880000	7.62240000
I	2.22360000	13.20000000	5.76000000
I	0.00000000	10.23260000	4.40320000



Orthographic projections: views of LaI_3 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

82. Nb_3TeCl_7 ($P\bar{3}m1$)

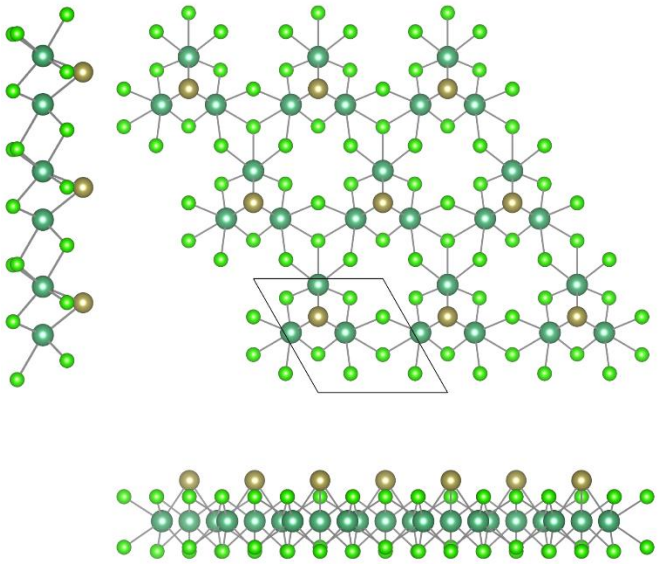
Formula	Nb_3TeCl_7	**ID**	mp-28938
Measure	19.9	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	3.729	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.579	**Band Gap (eV)**	0.703

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Nb_3TeCl_7 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.49285000	-6.04980000	0.00000000
a_2	3.49285000	6.04980000	0.00000000
a_3	0.00000000	0.00000000	13.79209000

	x (Å)	*y* (Å)	*z* (Å)
Nb	3.49290000	-0.32560000	10.46320000
Nb	2.02840000	-2.86210000	10.46320000
Nb	3.49290000	0.32560000	3.32890000
Nb	4.95730000	2.86210000	3.32890000
Nb	2.02840000	2.86210000	3.32890000
Nb	4.95730000	-2.86210000	10.46320000
Te	3.49290000	-2.01660000	8.32210000
Te	3.49290000	2.01660000	5.47000000
Cl	3.49290000	-4.02280000	4.61430000
Cl	5.23030000	-1.01350000	4.61430000
Cl	1.75550000	-1.01350000	4.61430000
Cl	5.23030000	1.01350000	9.17780000
Cl	1.75550000	1.01350000	9.17780000
Cl	3.49290000	4.02280000	9.17780000
Cl	3.49290000	4.00100000	1.74260000
Cl	1.77430000	1.02440000	1.74260000
Cl	3.49290000	2.01660000	11.83690000
Cl	3.49290000	-2.01660000	1.95520000
Cl	3.49290000	-4.00100000	12.04950000
Cl	5.21140000	-1.02440000	12.04950000
Cl	1.77430000	-1.02440000	12.04950000
Cl	5.21140000	1.02440000	1.74260000



Orthographic projections: views of Nb_3TeCl_7 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

83. $TePdI_2$ ($P\bar{1}$)

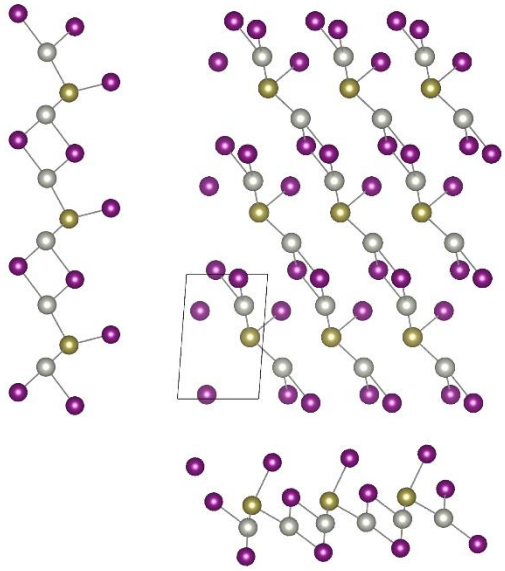
Formula	$TePdI_2$	**ID**	mp-573321
Measure	19.9	**Symbol**	$P\bar{1}$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	5.924	**Energy-Above-Hull (eV/atom)**	0.016
Formation Energy (eV/atom)	-0.245	**Band Gap (eV)**	0.546

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $TePdI_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	4.43913000	0.00000000	0.00000000
a_2	0.91369000	7.19448000	0.00000000
a_3	1.49170000	3.26943000	8.56361000

	x (Å)	*y* (Å)	*z* (Å)
Te	1.40400000	4.12190000	1.28270000
Te	5.44050000	6.34200000	7.28090000
Pd	1.40750000	1.82250000	0.03430000
Pd	5.43700000	8.64140000	8.52930000
I	2.82430000	2.89300000	6.94950000
I	2.38290000	6.94610000	4.89870000
I	4.02020000	7.57090000	1.61410000
I	4.46160000	3.51780000	3.66490000



Orthographic projections: views of $TePdI_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

84. Nb_3Cl_8 ($P\bar{3}m1$)

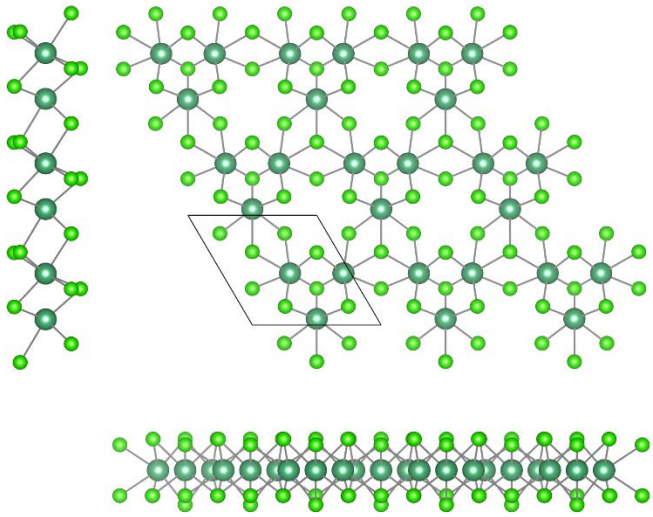
Formula	Nb_3Cl_8	**ID**	mp-29950
Measure	19.9	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	FM	**Tot. Magnetization (μ_B/cell)**	0.991
Density (g/cm^3)	3.361	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.702	**Band Gap (eV)**	0.151

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Nb_3Cl_8 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.41570000	-5.91617000	0.00000000
a_2	3.41570000	5.91617000	0.00000000
a_3	0.00000000	0.00000000	13.74890000

	x (Å)	*y* (Å)	*z* (Å)
Nb	1.99890000	2.79000000	10.35770000
Nb	3.41570000	0.33610000	10.35770000
Nb	4.83250000	2.79000000	10.35770000
Nb	3.41570000	-0.33610000	3.39120000
Nb	4.83250000	-2.79000000	3.39120000
Nb	1.99890000	-2.79000000	3.39120000
Cl	1.73840000	1.00370000	8.70340000
Cl	5.09300000	1.00370000	8.70340000
Cl	3.41570000	3.90880000	8.70340000
Cl	5.09300000	-1.00370000	5.04550000
Cl	3.41570000	-3.90880000	5.04550000
Cl	1.73840000	-1.00370000	5.04550000
Cl	3.41570000	-1.97210000	1.55100000
Cl	3.41570000	1.97210000	12.19790000
Cl	3.41570000	1.97210000	4.73800000
Cl	3.41570000	-1.97210000	9.01090000
Cl	5.13200000	0.98110000	2.03670000
Cl	3.41570000	3.95390000	2.03670000
Cl	1.69940000	0.98110000	2.03670000
Cl	3.41570000	-3.95390000	11.71220000
Cl	1.69940000	-0.98110000	11.71220000
Cl	5.13200000	-0.98110000	11.71220000



Orthographic projections: views of Nb_3Cl_8 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

85. $ZrCl_2$ (R3m)

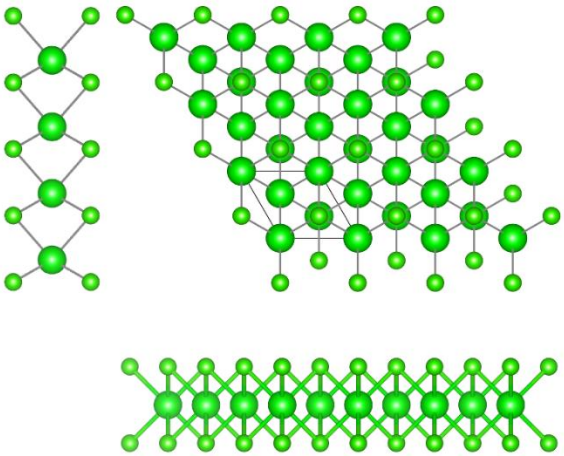
Formula	$ZrCl_2$	**ID**	mp-23162
Measure	19.6	**Symbol**	R3m
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	3.856	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-2.041	**Band Gap (eV)**	0.861

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $ZrCl_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.70839000	-2.95902000	0.00000000
a_2	1.70839000	2.95902000	0.00000000
a_3	0.00000000	0.00000000	20.71732000

	x (Å)	*y* (Å)	*z* (Å)
Zr	1.70840000	-0.98630000	6.90420000
Zr	1.70840000	0.98630000	13.80990000
Zr	0.00000000	0.00000000	20.71570000
Cl	1.70840000	0.98630000	5.18370000
Cl	1.70840000	-0.98630000	1.71880000
Cl	0.00000000	0.00000000	12.08950000
Cl	1.70840000	0.98630000	8.62460000
Cl	1.70840000	-0.98630000	18.99520000
Cl	0.00000000	0.00000000	15.53040000



Orthographic projections: views of $ZrCl_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

86. $TaSe_3$ ($P2_1/m$)

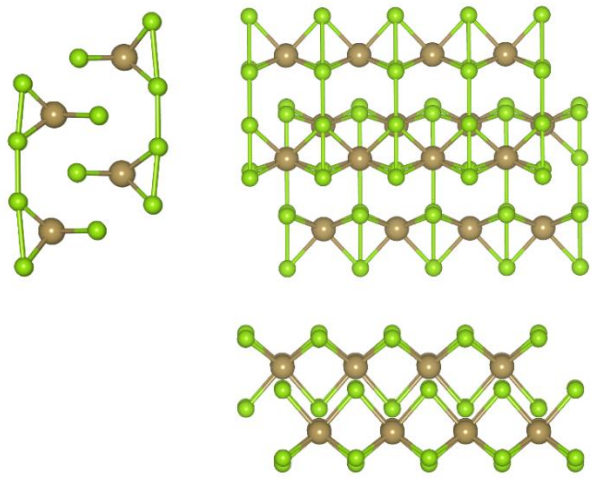
Formula	$TaSe_3$	**ID**	mp-29652
Measure	19.2	**Symbol**	$P2_1/m$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	7.392	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.653	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $TaSe_3$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	0.00000000	10.37457000	0.00000000
a_2	3.51916000	0.00000000	0.00000000
a_3	0.00000000	-3.60334000	-10.28351000

	x (Å)	*y* (Å)	*z* (Å)
Ta	2.63940000	5.83470000	-1.95640000
Ta	0.87980000	0.93650000	-8.32710000
Ta	2.63940000	7.53580000	-6.85900000
Ta	0.87980000	-0.76460000	-3.42450000
Se	2.63940000	2.59670000	-9.45360000
Se	0.87980000	4.17450000	-0.82990000
Se	2.63940000	-1.00350000	-8.92140000
Se	0.87980000	7.77470000	-1.36220000
Se	2.63940000	0.11960000	-1.67950000
Se	0.87980000	6.65160000	-8.60400000
Se	2.63940000	1.94740000	-6.62440000
Se	0.87980000	4.82390000	-3.65910000
Se	2.63940000	1.13980000	-4.05620000
Se	0.87980000	5.63140000	-6.22730000
Se	2.63940000	7.71450000	-4.08870000
Se	0.87980000	-0.94320000	-6.19480000



Orthographic projections: views of $TaSe_3$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

87. $Ni(PS_3)_2$ (C2)

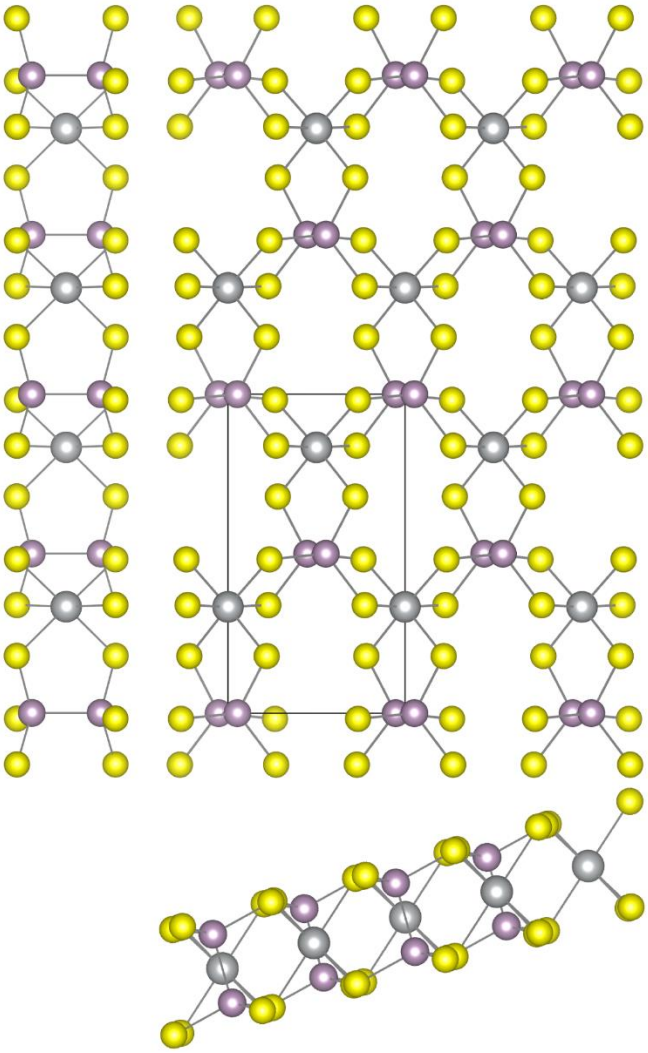
Formula	$Ni(PS_3)_2$	**ID**	mp-769218
Measure	19.0	**Symbol**	C2
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	2.635	**Energy-Above-Hull (eV/atom)**	0.093
Formation Energy (eV/atom)	-0.568	**Band Gap (eV)**	0.325

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $Ni(PS_3)_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	0.00000000	5.82425000	0.00000000
a_2	10.08576000	0.00000000	0.00000000
a_3	0.00000000	-1.87731000	-6.71589000

	x (Å)	*y* (Å)	*z* (Å)
Ni	8.40420000	2.91210000	0.00000000
Ni	3.36130000	0.00000000	0.00000000
P	10.08570000	0.00310000	-1.09120000
P	10.08570000	3.94380000	-5.62460000
P	5.04290000	2.91530000	-1.09120000
P	5.04290000	1.03170000	-5.62460000
S	8.45890000	1.14740000	-1.56160000
S	9.90610000	0.10440000	-5.15570000
S	8.45890000	2.79960000	-5.15430000
S	1.80620000	0.83450000	-1.56760000
S	1.80620000	3.11240000	-5.14830000
S	9.90610000	3.84260000	-1.56020000
S	3.41600000	4.05950000	-1.56160000
S	4.86320000	3.01650000	-5.15570000
S	3.41600000	-0.11260000	-5.15430000
S	6.84910000	3.74660000	-1.56760000
S	6.84910000	0.20030000	-5.14830000
S	4.86320000	0.93050000	-1.56020000



Orthographic projections: views of $Ni(PS_3)_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

88. GaSe ($P6_3/mmc$)

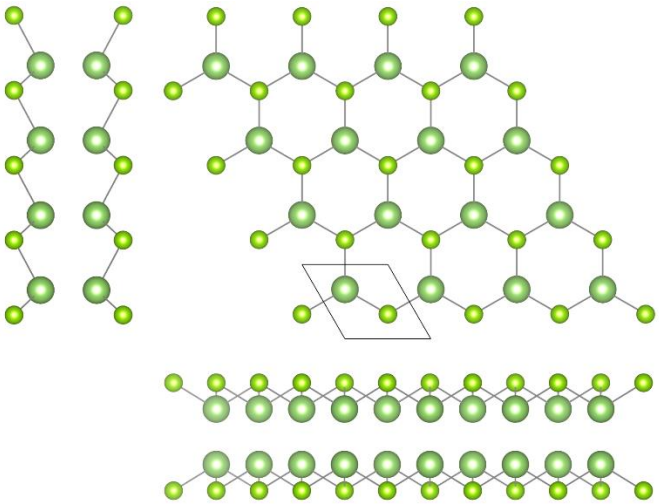
Formula	GaSe	**ID**	mp-1943
Measure	18.5	**Symbol**	$P6_3/mmc$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	4.408	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.591	**Band Gap (eV)**	1.248

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of GaSe in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.90880000	-3.30614000	0.00000000
a_2	1.90880000	3.30614000	0.00000000
a_3	0.00000000	0.00000000	17.75045000

	x (Å)	*y* (Å)	*z* (Å)
Ga	1.90880000	-1.10200000	12.07760000
Ga	1.90880000	1.10200000	3.20240000
Ga	1.90880000	1.10200000	5.67280000
Ga	1.90880000	-1.10200000	14.54800000
Se	1.90880000	-1.10200000	2.02880000
Se	1.90880000	1.10200000	10.90410000
Se	1.90880000	1.10200000	15.72160000
Se	1.90880000	-1.10200000	6.84640000



Orthographic projections: views of GaSe as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

89. $NdBr_3$ (Cmcm)

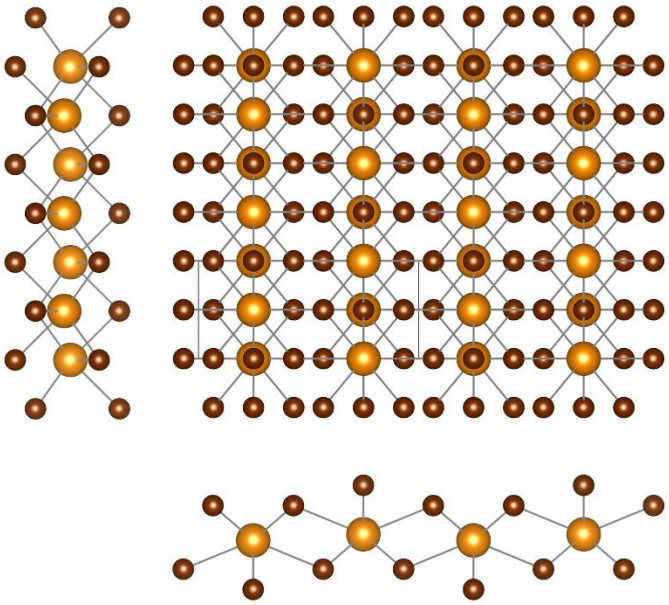
Formula	$NdBr_3$	**ID**	mp-27975
Measure	18.4	**Symbol**	Cmcm
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	4.632	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.910	**Band Gap (eV)**	2.922

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $NdBr_3$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	4.12568000	0.00000000	0.00000000
a_2	0.00000000	14.37956000	0.00000000
a_3	0.00000000	0.00000000	9.28026000

	x (Å)	*y* (Å)	*z* (Å)
Nd	2.06280000	3.46460000	6.96020000
Nd	0.00000000	3.72520000	2.32010000
Nd	0.00000000	10.65440000	6.96020000
Nd	2.06280000	10.91500000	2.32010000
Br	0.00000000	4.93600000	8.65510000
Br	2.06280000	2.25380000	0.62520000
Br	2.06280000	5.78940000	2.32010000
Br	0.00000000	1.40040000	6.96020000
Br	0.00000000	4.93600000	5.26530000
Br	2.06280000	2.25380000	4.01490000
Br	2.06280000	12.12580000	8.65510000
Br	0.00000000	9.44350000	0.62520000
Br	0.00000000	12.97910000	2.32010000
Br	2.06280000	8.59020000	6.96020000
Br	2.06280000	12.12580000	5.26530000
Br	0.00000000	9.44350000	4.01490000



Orthographic projections: views of $NdBr_3$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

90. NbS_3 ($P\bar{1}$)

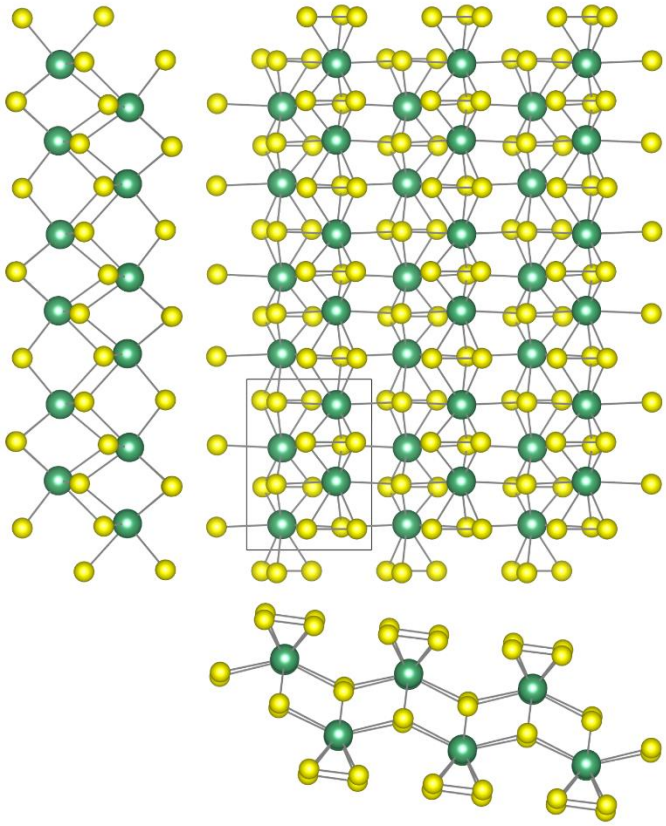
Formula	NbS_3	**ID**	mp-562100
Measure	18.3	**Symbol**	$P\bar{1}$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	3.836	**Energy-Above-Hull (eV/atom)**	0.017
Formation Energy (eV/atom)	-1.253	**Band Gap (eV)**	0.376

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of NbS_3 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	5.03627000	0.00000000	0.00000000
a_2	0.00158000	6.81471000	0.00000000
a_3	1.14211000	0.00652000	9.53936000

	x (Å)	*y* (Å)	*z* (Å)
Nb	4.34970000	5.80150000	6.11410000
Nb	4.34650000	2.74350000	6.19560000
Nb	1.83020000	1.01980000	3.42530000
Nb	1.83340000	4.07770000	3.34380000
S	2.85910000	2.51080000	1.66060000
S	4.34790000	0.91550000	4.37420000
S	4.35120000	4.19180000	4.19520000
S	1.82880000	2.62950000	5.34420000
S	5.33810000	4.30700000	7.91390000
S	1.83210000	5.90570000	5.16520000
S	2.84400000	5.98040000	1.89860000
S	3.33590000	0.84080000	7.64070000
S	3.32090000	4.31050000	7.87880000
S	0.84180000	2.51420000	1.62550000
S	0.82740000	5.97880000	1.89040000
S	5.35260000	0.84240000	7.64900000



Orthographic projections: views of NbS_3 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

91. MnS_2 ($R\bar{3}m$)

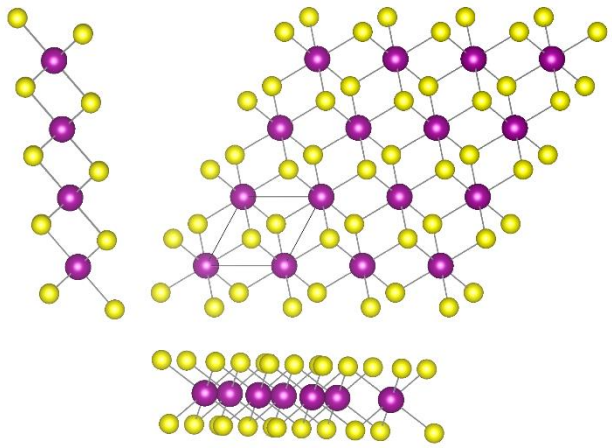
Formula	MnS_2	**ID**	mvc-14047
Measure	18.1	**Symbol**	$R\bar{3}m$
Magnetic Ordering	FM	**Tot. Magnetization (μ_B/cell)**	3.000
Density (g/cm^3)	2.768	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.997	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of MnS_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.67589000	-2.90273000	0.00000000
a_2	1.67589000	2.90273000	0.00000000
a_3	0.00000000	0.00000000	22.02207000

	x (Å)	*y* (Å)	*z* (Å)
Mn	0.00000000	0.00000000	0.00000000
Mn	1.67590000	-0.96760000	7.34070000
Mn	1.67590000	0.96760000	14.68140000
S	1.67590000	0.96760000	1.32070000
S	1.67590000	0.96760000	6.02000000
S	0.00000000	0.00000000	8.66130000
S	0.00000000	0.00000000	13.36070000
S	1.67590000	-0.96760000	16.00200000
S	1.67590000	-0.96760000	20.70140000



Orthographic projections: views of MnS_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

92. $SnSe_2$ ($P\bar{3}m1$)

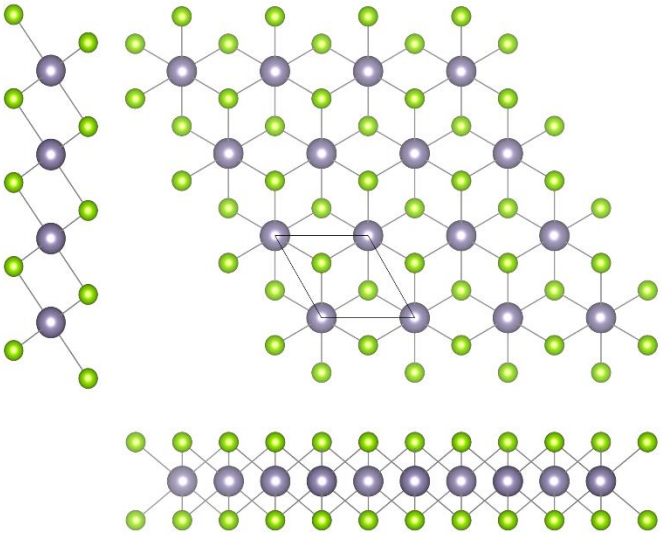
Formula	$SnSe_2$	**ID**	mp-665
Measure	17.8	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	5.121	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.345	**Band Gap (eV)**	0.800

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $SnSe_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.93664000	-3.35436000	0.00000000
a_2	1.93664000	3.35436000	0.00000000
a_3	0.00000000	0.00000000	6.90475000

	x (Å)	*y* (Å)	*z* (Å)
Sn	0.00000000	0.00000000	0.00000000
Se	1.93660000	-1.11810000	5.30830000
Se	1.93660000	1.11810000	1.59640000



Orthographic projections: views of $SnSe_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

93. SiH ($P\bar{3}m1$)

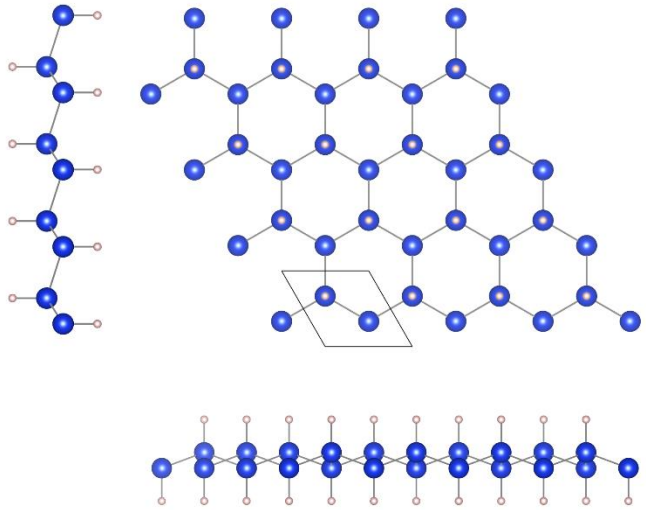
Formula	SiH	**ID**	mp-29803
Measure	17.7	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	1.277	**Energy-Above-Hull (eV/atom)**	0.030
Formation Energy (eV/atom)	-0.042	**Band Gap (eV)**	2.140

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of SiH in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.94459000	-3.36814000	0.00000000
a_2	1.94459000	3.36814000	0.00000000
a_3	0.00000000	0.00000000	5.77584000

	x (Å)	*y* (Å)	*z* (Å)
Si	1.94460000	-1.12270000	5.41610000
Si	1.94460000	1.12270000	0.35970000
H	1.94460000	-1.12270000	3.91480000
H	1.94460000	1.12270000	1.86100000



Orthographic projections: views of SiH as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

94. $DyCl_3$ (Cmcm)

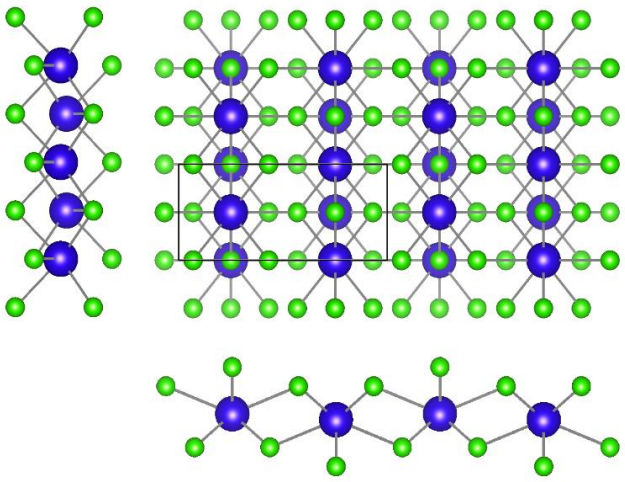
Formula	$DyCl_3$	**ID**	mp-28448
Measure	17.0	**Symbol**	Cmcm
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	3.904	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-2.698	**Band Gap (eV)**	3.900

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $DyCl_3$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.79538000	0.00000000	0.00000000
a_2	0.00000000	14.05850000	0.00000000
a_3	0.00000000	0.00000000	8.57311000

	x (Å)	*y* (Å)	*z* (Å)
Dy	0.00000000	3.39650000	2.14330000
Dy	0.00000000	10.66200000	6.42980000
Dy	1.89770000	10.42580000	2.14330000
Dy	0.00000000	2.30300000	4.87720000
Cl	1.89770000	4.72630000	3.69590000
Cl	1.89770000	1.54140000	2.14330000
Cl	0.00000000	5.48780000	6.42980000
Cl	0.00000000	2.30300000	7.98240000
Cl	1.89770000	4.72630000	0.59070000
Cl	1.89770000	9.33220000	4.87720000
Cl	0.00000000	11.75550000	3.69590000
Cl	0.00000000	8.57070000	2.14330000
Cl	1.89770000	12.51710000	6.42980000
Cl	1.89770000	9.33220000	7.98240000
Cl	0.00000000	11.75550000	0.59070000
Cl	0.00000000	3.39650000	2.14330000



Orthographic projections: views of $DyCl_3$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

95. HfSiTe (P4/nmm)

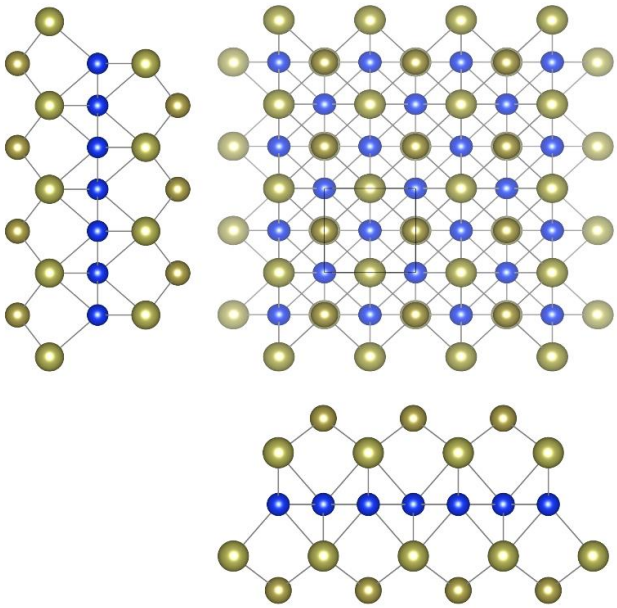
Formula	HfSiTe	**ID**	mp-13963
Measure	16.8	**Symbol**	P4/nmm
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	8.002	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.720	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of HfSiTe in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.66266000	0.00000000	0.00000000
a_2	0.00000000	3.66266000	0.00000000
a_3	0.00000000	0.00000000	10.33823000

	x (Å)	*y* (Å)	*z* (Å)
Hf	0.00000000	1.83130000	8.23440000
Hf	1.83130000	0.00000000	2.10390000
Si	0.00000000	0.00000000	0.00000000
Si	1.83130000	1.83130000	0.00000000
Te	1.83130000	0.00000000	6.83620000
Te	0.00000000	1.83130000	3.50200000



Orthographic projections: views of HfSiTe as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

96. $MnBr_2$ ($P\bar{3}m1$)

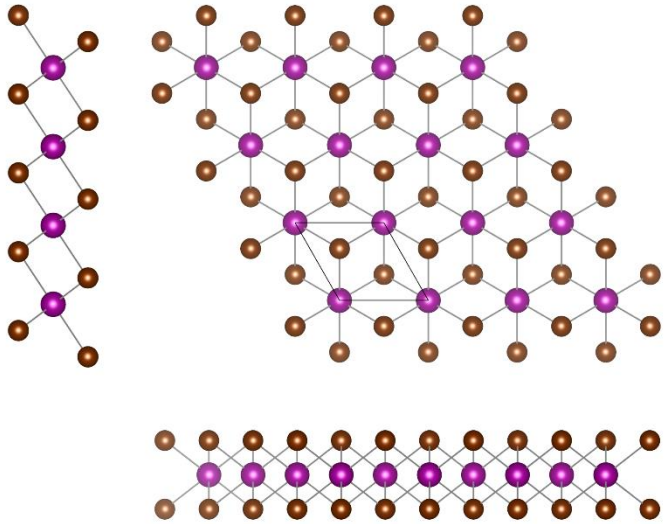
Formula	$MnBr_2$	**ID**	mp-28306
Measure	16.4	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	FM	**Tot. Magnetization (μ_B/cell)**	5.001
Density (g/cm^3)	3.826	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.813	**Band Gap (eV)**	1.611

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $MnBr_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.94898000	-3.37573000	0.00000000
a_2	1.94898000	3.37573000	0.00000000
a_3	0.00000000	0.00000000	7.08352000

	x (Å)	*y* (Å)	*z* (Å)
Mn	0.00000000	0.00000000	0.00000000
Br	1.94900000	1.12520000	1.50200000
Br	1.94900000	-1.12520000	5.58150000



Orthographic projections: views of $MnBr_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

97. Ti_2Te_2P ($R\bar{3}m$)

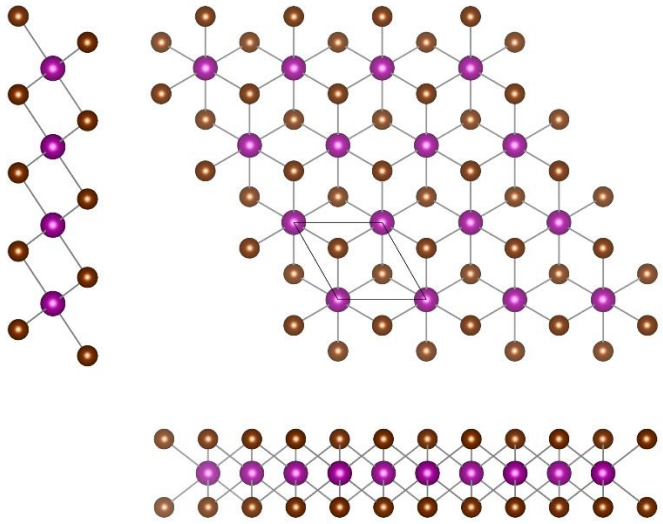
Formula	Ti_2Te_2P	**ID**	mp-12527
Measure	16.0	**Symbol**	$R\bar{3}m$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.025
Density (g/cm^3)	5.513	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.915	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Ti_2Te_2P in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.82815000	-3.16645000	0.00000000
a_2	1.82815000	3.16645000	0.00000000
a_3	0.00000000	0.00000000	29.80666000

	x (Å)	*y* (Å)	*z* (Å)
Ti	1.82810000	1.05550000	1.32360000
Ti	1.82810000	1.05550000	8.61200000
Ti	0.00000000	0.00000000	11.25910000
Ti	0.00000000	0.00000000	18.54750000
Ti	1.82810000	-1.05550000	21.19470000
Ti	1.82810000	-1.05550000	28.48310000
Te	1.82810000	-1.05550000	3.13870000
Te	0.00000000	0.00000000	6.79680000
Te	1.82810000	1.05550000	13.07430000
Te	1.82810000	-1.05550000	16.73240000
Te	0.00000000	0.00000000	23.00990000
Te	1.82810000	1.05550000	26.66790000
P	0.00000000	0.00000000	0.00000000
P	1.82810000	-1.05550000	9.93560000
P	1.82810000	1.05550000	19.87110000



Orthographic projections: views of Ti_2Te_2P as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

98. $TiSe_2$ ($P\bar{3}m1$)

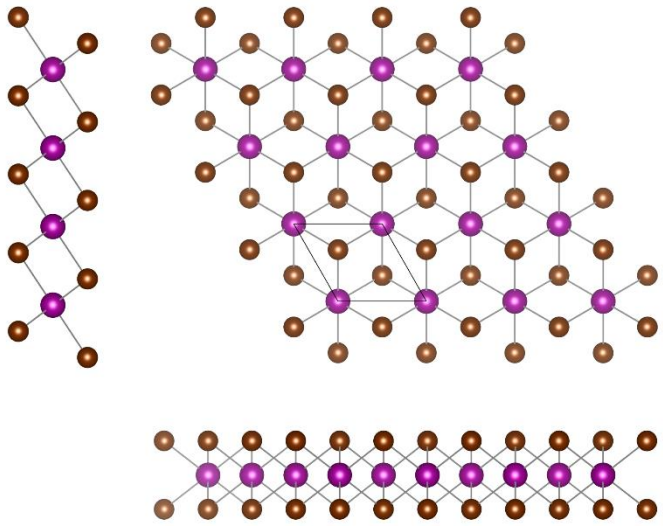
Formula	$TiSe_2$	**ID**	mp-2194
Measure	16.1	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	4.693	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.112	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $TiSe_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.77213000	-3.06942000	0.00000000
a_2	1.77213000	3.06942000	0.00000000
a_3	0.00000000	0.00000000	6.69381000

	x (Å)	*y* (Å)	*z* (Å)
Ti	0.00000000	0.00000000	0.00000000
Se	1.77210000	1.02310000	1.54750000
Se	1.77210000	-1.02310000	5.14630000



Orthographic projections: views of $TiSe_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

99. $CoCl_2$ (C2/m)

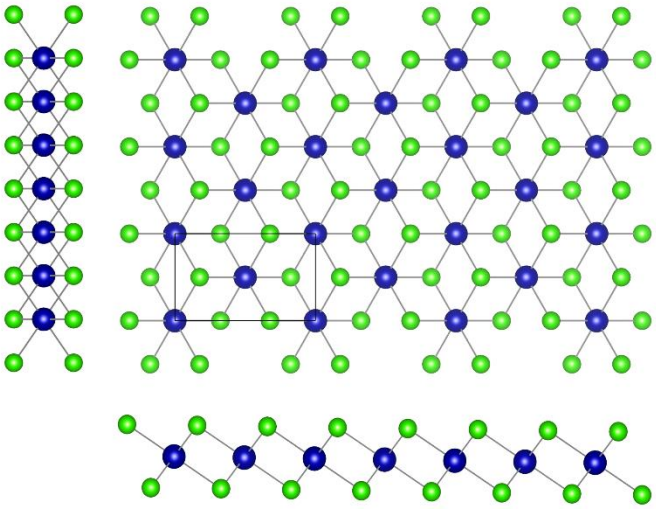
Formula	$CoCl_2$	**ID**	mp-632413
Measure	15.9	**Symbol**	C2/m
Magnetic Ordering	FM	**Tot. Magnetization (μ_B/cell)**	3.000
Density (g/cm^3)	3.488	**Energy-Above-Hull (eV/atom)**	0.024
Formation Energy (eV/atom)	-0.945	**Band Gap (eV)**	0.068

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $CoCl_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	**3.91387000**	0.00000000	0.00000000
a_2	0.00000000	3.91387000	0.00000000
a_3	0.00000000	0.00000000	7.82779000

	x (Å)	*y* (Å)	*z* (Å)
Co	0.00000000	1.95690000	6.55200000
Co	1.95690000	0.00000000	1.27580000
Cl	1.95690000	0.00000000	5.17790000
Cl	0.00000000	1.95690000	2.64990000
Cl	0.00000000	0.00000000	0.00000000
Cl	1.95690000	1.95690000	0.00000000



Orthographic projections: views of $CoCl_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

100. BiClO (P4/nmm)

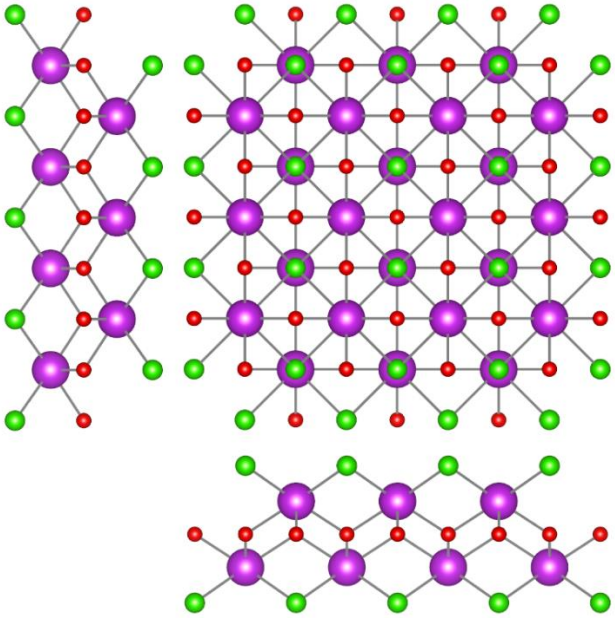
Formula	BiClO	**ID**	mp-22939
Measure	15.9	**Symbol**	P4/nmm
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	7.213	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.696	**Band Gap (eV)**	2.639

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of BiClO in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.91387000	0.00000000	0.00000000
a_2	0.00000000	3.91387000	0.00000000
a_3	0.00000000	0.00000000	7.82779000

	x (Å)	*y* (Å)	*z* (Å)
Bi	0.00000000	1.95690000	6.55200000
Bi	1.95690000	0.00000000	1.27580000
Cl	1.95690000	0.00000000	5.17790000
Cl	0.00000000	1.95690000	2.64990000
O	0.00000000	0.00000000	0.00000000
O	1.95690000	1.95690000	0.00000000



Orthographic projections: views of BiClO as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

101. TiOF (Pmmn)

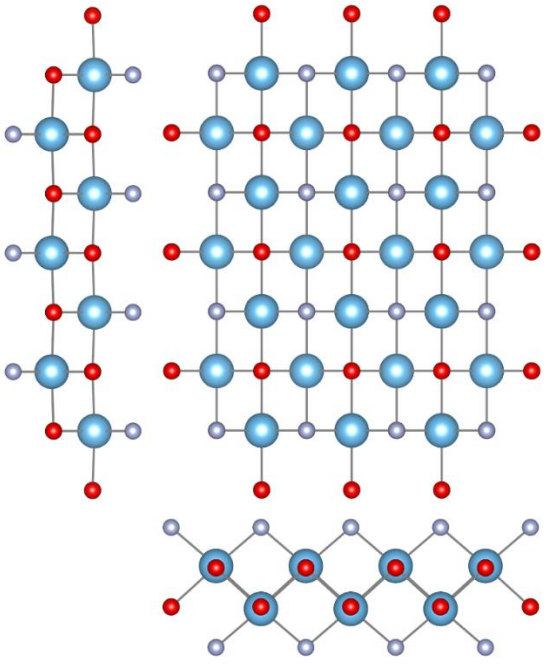
Formula	TiOF	**ID**	mp-753059
Measure	15.4	**Symbol**	Pmmn
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	3.431	**Energy-Above-Hull (eV/atom)**	0.069
Formation Energy (eV/atom)	-3.413	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of TiOF in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.05483000	0.00000000	0.00000000
a_2	0.00000000	4.03532000	0.00000000
a_3	0.00000000	0.00000000	6.50602000

	x (Å)	*y* (Å)	*z* (Å)
Ti	1.52740000	0.00000000	3.98180000
Ti	0.00000000	2.01770000	2.52420000
O	0.00000000	0.00000000	2.59010000
O	1.52740000	2.01770000	3.91590000
F	0.00000000	0.00000000	5.29140000
F	1.52740000	2.01770000	1.21460000



Orthographic projections: views of TiOF as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

102. $CrGeTe_3$ ($R\bar{3}$)

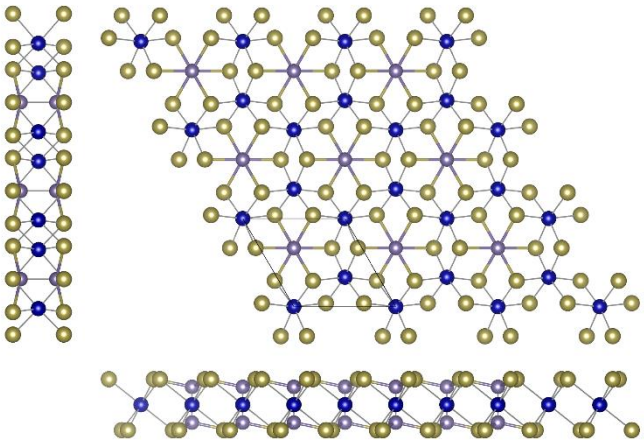
Formula	$CrGeTe_3$	**ID**	mp-541449
Measure	15.3	**Symbol**	$R\bar{3}$
Magnetic Ordering	FM	**Tot. Magnetization (μ_B/cell)**	0.214
Density (g/cm^3)	5.599	**Energy-Above-Hull (eV/atom)**	0.260
Formation Energy (eV/atom)	0.110	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $CrGeTr_3$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.45646000	-5.98676000	0.00000000
a_2	3.45646000	5.98676000	0.00000000
a_3	0.00000000	0.00000000	21.81841000

	x (Å)	*y* (Å)	*z* (Å)
Cr	3.45650000	1.99560000	0.00590000
Cr	3.45650000	1.99560000	7.26690000
Cr	0.00000000	0.00000000	7.27870000
Cr	0.00000000	0.00000000	14.53970000
Cr	3.45650000	-1.99560000	14.55150000
Cr	3.45650000	-1.99560000	21.81250000
Ge	0.00000000	0.00000000	1.20890000
Ge	3.45650000	-1.99560000	6.06390000
Ge	3.45650000	-1.99560000	8.48170000
Ge	3.45650000	1.99560000	13.33670000
Ge	3.45650000	1.99560000	15.75450000
Ge	0.00000000	0.00000000	20.60950000
Te	4.33430000	3.99500000	5.55050000
Te	4.74910000	0.23570000	5.55050000
Te	1.28600000	1.75610000	5.55050000
Te	2.57860000	-0.00380000	1.72230000
Te	5.62030000	-2.23120000	1.72230000
Te	2.17050000	-3.75170000	1.72230000
Te	4.33430000	-3.98730000	12.82330000
Te	1.29270000	-1.75990000	12.82330000
Te	4.74240000	-0.23950000	12.82330000
Te	2.57860000	3.98730000	8.99510000
Te	5.62030000	1.75990000	8.99510000
Te	2.17050000	0.23950000	8.99510000
Te	4.33430000	0.00380000	20.09610000
Te	1.29270000	2.23120000	20.09610000
Te	4.74240000	3.75170000	20.09610000
Te	2.57860000	-3.99500000	16.26790000
Te	2.16380000	-0.23570000	16.26790000
Te	5.62690000	-1.75610000	16.26790000



Orthographic projections: views of $CrGeTr_3$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

103. $CuTeO_4$ (P2/m)

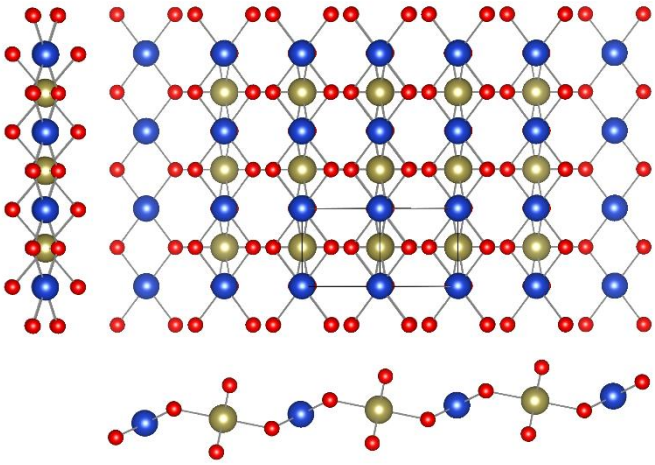
Formula	$CuTeO_4$	**ID**	mp-755455
Measure	15.2	**Symbol**	P2/m
Magnetic Ordering	FM	**Tot. Magnetization (μ_B/cell)**	0.228
Density (g/cm^3)	5.073	**Energy-Above-Hull (eV/atom)**	0.017
Formation Energy (eV/atom)	-1.218	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $CuTeO_4$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	0.00000000	5.35575000	0.00000000
a_2	3.00618000	0.00000000	0.00000000
a_3	0.00000000	-2.20977000	-5.18746000

	x (Å)	*y* (Å)	*z* (Å)
Cu	0.00000000	0.00000000	0.00000000
Te	1.50310000	1.57300000	-2.59370000
O	0.00000000	0.65660000	-3.53610000
O	1.50310000	0.18280000	-1.23960000
O	0.00000000	2.48940000	-1.65140000
O	1.50310000	2.96310000	-3.94780000



Orthographic projections: views of $CuTeO_4$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

104. Rb_2O ($R\bar{3}m$)

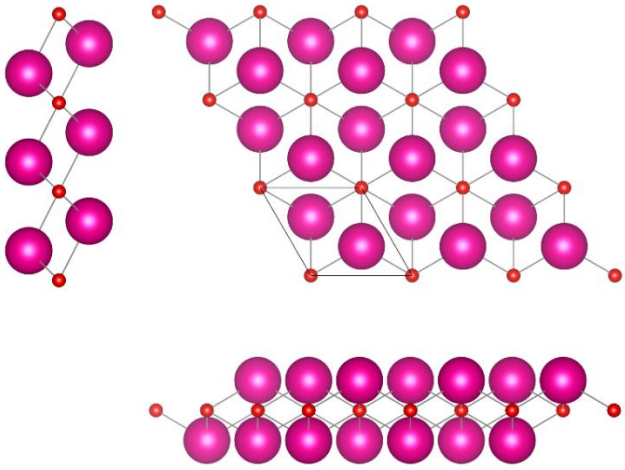
Formula	Rb_2O	**ID**	mp-753746
Measure	15.2	**Symbol**	$R\bar{3}m$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.001
Density (g/cm^3)	3.226	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.138	**Band Gap (eV)**	0.484

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Rb_2O in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	2.16249000	-3.74554000	0.00000000
a_2	2.16249000	3.74554000	0.00000000
a_3	0.00000000	0.00000000	17.81696000

	x (Å)	*y* (Å)	*z* (Å)
Rb	0.00000000	0.00000000	4.66450000
Rb	2.16250000	-1.24850000	1.27450000
Rb	2.16250000	-1.24850000	10.60350000
Rb	2.16250000	1.24850000	7.21350000
Rb	2.16250000	1.24850000	16.54250000
Rb	0.00000000	0.00000000	13.15250000
O	0.00000000	0.00000000	0.00000000
O	2.16250000	-1.24850000	5.93900000
O	2.16250000	1.24850000	11.87800000



Orthographic projections: views of Rb_2O as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

105. $CdCl_2$ ($R\bar{3}m$)

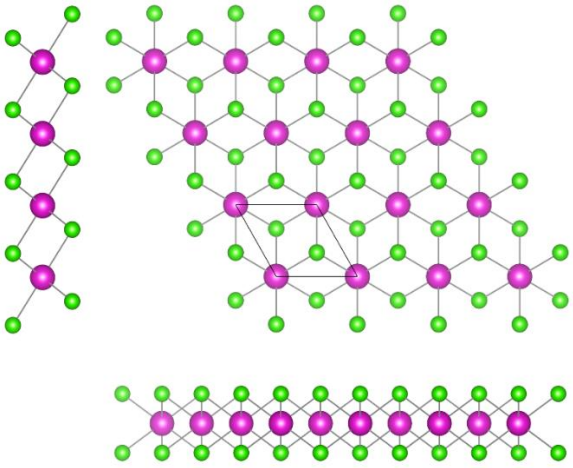
Formula	$CdCl_2$	**ID**	mp-22881
Measure	15.1	**Symbol**	$R\bar{3}m$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	3.611	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.489	**Band Gap (eV)**	3.595

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $CdCl_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.96294000	-3.39990000	0.00000000
a_2	1.96294000	3.39990000	0.00000000
a_3	0.00000000	0.00000000	18.94683000

	x (Å)	*y* (Å)	*z* (Å)
Cd	0.00000000	0.00000000	0.00000000
Cd	1.96290000	-1.13330000	6.31560000
Cd	1.96290000	1.13330000	12.63120000
Cl	0.00000000	0.00000000	4.88300000
Cl	1.96290000	-1.13330000	1.43260000
Cl	1.96290000	-1.13330000	11.19860000
Cl	1.96290000	1.13330000	7.74820000
Cl	1.96290000	1.13330000	17.51420000
Cl	0.00000000	0.00000000	14.06380000



Orthographic projections: views of $CdCl_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

106. InSe (C2/m)

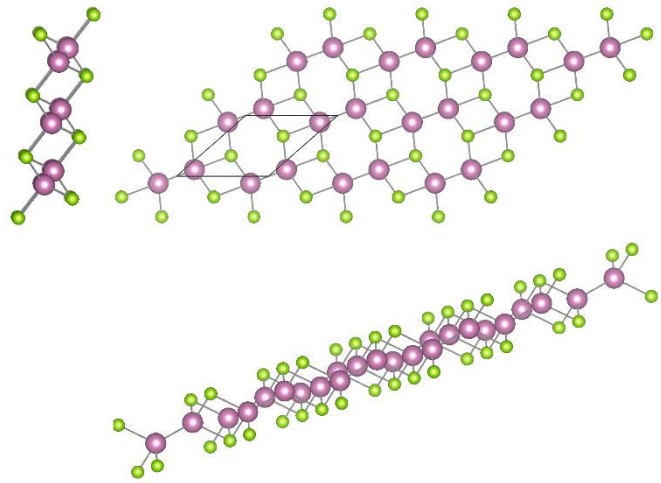
Formula	InSe	**ID**	mp-21405
Measure	14.6	**Symbol**	C2/m
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	5.390	**Energy-Above-Hull (eV/atom)**	0.036
Formation Energy (eV/atom)	-0.474	**Band Gap (eV)**	1.076

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of InSe in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	0.00000000	11.70274000	0.00000000
a_2	4.14491000	0.00000000	0.00000000
a_3	0.00000000	-1.76786000	-4.92278000

	x (Å)	*y* (Å)	*z* (Å)
In	2.07250000	4.45260000	-0.24750000
In	0.00000000	-0.36910000	-4.67520000
In	0.00000000	10.30400000	-0.24750000
In	2.07250000	5.48230000	-4.67520000
Se	2.07250000	0.70430000	-3.30210000
Se	0.00000000	3.37920000	-1.62070000
Se	0.00000000	6.55570000	-3.30210000
Se	2.07250000	9.23060000	-1.62070000



Orthographic projections: views of InSe as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

107. $MnCl_2$ ($R\bar{3}m$)

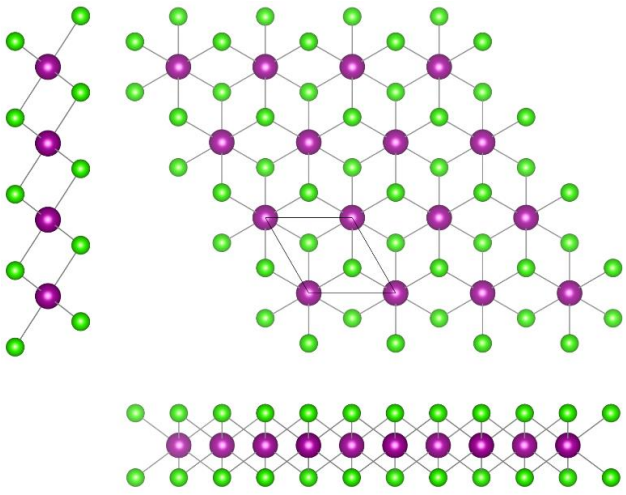
Formula	$MnCl_2$	**ID**	mp-28233
Measure	14.6	**Symbol**	$R\bar{3}m$
Magnetic Ordering	FM	**Tot. Magnetization (μ_B/cell)**	5.000
Density (g/cm^3)	2.673	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.482	**Band Gap (eV)**	1.797

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $MnCl_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.85834000	-3.21874000	0.00000000
a_2	1.85834000	3.21874000	0.00000000
a_3	0.00000000	0.00000000	19.60309000

	x (Å)	*y* (Å)	*z* (Å)
Mn	0.00000000	0.00000000	0.00000000
Mn	1.85830000	-1.07290000	6.53440000
Mn	1.85830000	1.07290000	13.06870000
Cl	1.85830000	-1.07290000	1.38300000
Cl	0.00000000	0.00000000	5.15130000
Cl	1.85830000	1.07290000	7.91740000
Cl	1.85830000	-1.07290000	11.68570000
Cl	0.00000000	0.00000000	14.45180000
Cl	1.85830000	1.07290000	18.22000000



Orthographic projections: views of $MnCl_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

108. $TiSnO_3$ ($R\bar{3}$)

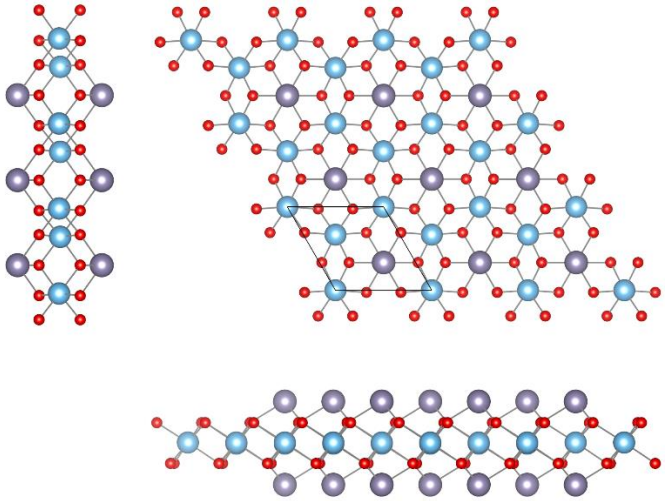
Formula	$TiSnO_3$	**ID**	mp-754246
Measure	14.5	**Symbol**	$R\bar{3}$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	4.572	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-2.767	**Band Gap (eV)**	1.108

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $TiSnO_3$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	2.57090000	-4.45293000	0.00000000
a_2	2.57090000	4.45293000	0.00000000
a_3	0.00000000	0.00000000	20.42161000

	x (Å)	*y* (Å)	*z* (Å)
Ti	2.57090000	1.48430000	6.77870000
Ti	2.57090000	1.48430000	0.02850000
Ti	0.00000000	0.00000000	13.58590000
Ti	0.00000000	0.00000000	6.83570000
Ti	2.57090000	-1.48430000	20.39310000
Ti	2.57090000	-1.48430000	13.64290000
Sn	2.57090000	-1.48430000	4.59970000
Sn	0.00000000	0.00000000	2.20750000
Sn	2.57090000	1.48430000	11.40690000
Sn	2.57090000	-1.48430000	9.01470000
Sn	0.00000000	0.00000000	18.21410000
Sn	2.57090000	1.48430000	15.82190000
O	3.29940000	2.96690000	5.72840000
O	0.92270000	1.37390000	5.72840000
O	1.65120000	2.85650000	1.07880000
O	3.49060000	0.11210000	5.72840000
O	4.21910000	1.59470000	1.07880000
O	1.84240000	0.00170000	1.07880000
O	3.29940000	-2.97030000	12.53560000
O	3.49360000	-0.11040000	12.53560000
O	4.22210000	1.37220000	7.88600000
O	0.91970000	-1.37220000	12.53560000
O	1.64820000	0.11040000	7.88600000
O	1.84240000	2.97030000	7.88600000
O	3.29940000	-0.00170000	19.34280000
O	0.92270000	-1.59470000	19.34280000
O	1.65120000	-0.11210000	14.69320000
O	3.49060000	-2.85650000	19.34280000
O	4.21910000	-1.37390000	14.69320000
O	1.84240000	-2.96690000	14.69320000



Orthographic projections: views of $TiSnO_3$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

109. Nb_3TeI_7 (P3m1)

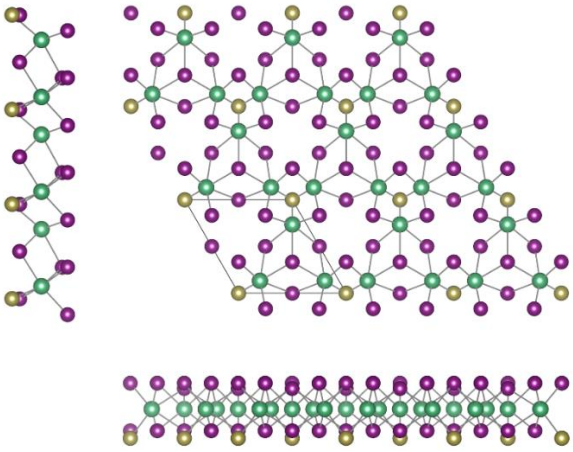
Formula	Nb_3TeI_7	**ID**	mp-567713
Measure	14.4	**Symbol**	P3m1
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	5.728	**Energy-Above-Hull (eV/atom)**	0.002
Formation Energy (eV/atom)	-0.541	**Band Gap (eV)**	0.480

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Nb_3TeI_7 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.86716000	-6.69811000	0.00000000
a_2	3.86716000	6.69811000	0.00000000
a_3	0.00000000	0.00000000	7.24534000

	x (Å)	*y* (Å)	*z* (Å)
Nb	1.53590000	-0.88680000	3.61260000
Nb	3.86720000	-4.92460000	3.61260000
Nb	6.19840000	-0.88680000	3.61260000
Te	0.00000000	0.00000000	1.53030000
I	5.79200000	1.12140000	5.46880000
I	5.79190000	3.34390000	2.06860000
I	3.86720000	4.45530000	5.46880000
I	1.94240000	3.34390000	2.06860000
I	3.86720000	-2.23270000	5.08370000
I	1.94230000	1.12140000	5.46880000
I	3.86720000	0.01020000	2.06860000



Orthographic projections: views of Nb_3TeI_7 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

110. $Mg(AlSe_2)_2$ ($R\bar{3}m$)

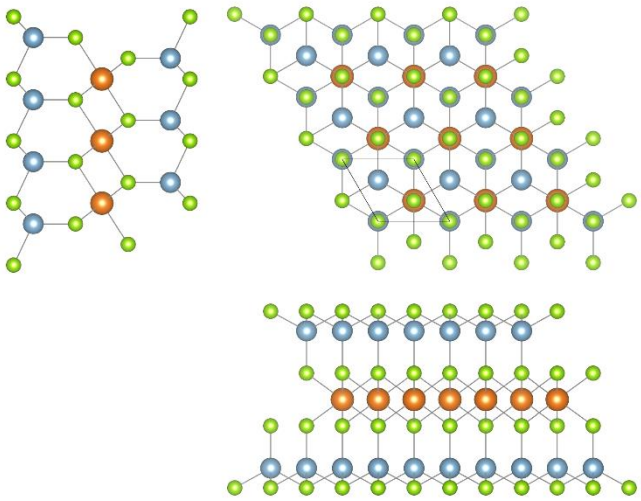
Formula	$Mg(AlSe_2)_2$	**ID**	mp-9479
Measure	14.4	**Symbol**	$R\bar{3}m$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	3.579	**Energy-Above-Hull (eV/atom)**	0.021
Formation Energy (eV/atom)	-0.953	**Band Gap (eV)**	1.072

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $Mg(AlSe_2)_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.96112000	-3.39677000	0.00000000
a_2	1.96112000	3.39677000	0.00000000
a_3	0.00000000	0.00000000	41.17124000

	x (Å)	*y* (Å)	*z* (Å)
Mg	0.00000000	0.00000000	0.00000000
Mg	1.96110000	-1.13230000	13.72370000
Mg	1.96110000	1.13230000	27.44750000
Al	0.00000000	0.00000000	9.97540000
Al	1.96110000	-1.13230000	3.74830000
Al	1.96110000	-1.13230000	23.69920000
Al	1.96110000	1.13230000	17.47210000
Al	1.96110000	1.13230000	37.42290000
Al	0.00000000	0.00000000	31.19580000
Se	1.96110000	-1.13230000	1.43780000
Se	0.00000000	0.00000000	12.28590000
Se	0.00000000	0.00000000	4.82190000
Se	1.96110000	-1.13230000	8.90180000
Se	1.96110000	1.13230000	15.16160000
Se	1.96110000	-1.13230000	26.00970000
Se	1.96110000	-1.13230000	18.54570000
Se	1.96110000	1.13230000	22.62560000
Se	0.00000000	0.00000000	28.88530000
Se	1.96110000	1.13230000	39.73340000
Se	1.96110000	1.13230000	32.26940000
Se	0.00000000	0.00000000	36.34930000



Orthographic projections: views of $Mg(AlSe_2)_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

111. Cu_2WS_4 ($P\bar{4}2m$)

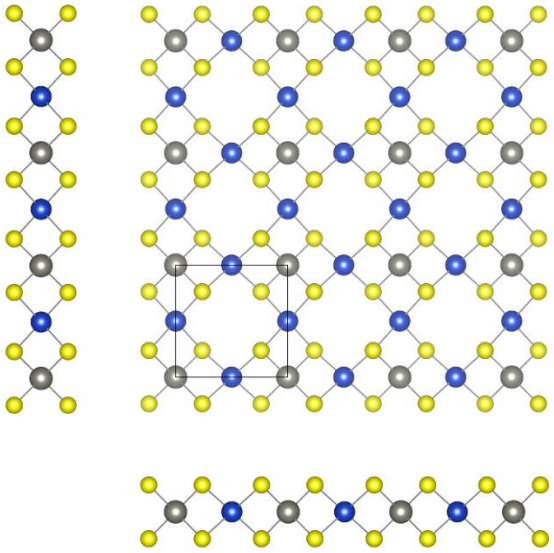
Formula	Cu_2WS_4	**ID**	mp-8976
Measure	14.4	**Symbol**	$P\bar{4}2m$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	4.299	**Energy-Above-Hull (eV/atom)**	0.003
Formation Energy (eV/atom)	-0.838	**Band Gap (eV)**	1.620

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Cu_2WS_4 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	5.45562000	0.00000000	0.00000000
a_2	0.00000000	5.45562000	0.00000000
a_3	0.00000000	0.00000000	5.69899000

	x (Å)	*y* (Å)	*z* (Å)
Cu	0.00000000	2.72780000	0.00000000
Cu	2.72780000	0.00000000	0.00000000
W	0.00000000	0.00000000	0.00000000
S	1.29490000	4.16070000	1.30150000
S	4.16070000	4.16070000	4.39750000
S	1.29490000	1.29490000	4.39750000
S	4.16070000	1.29490000	1.30150000



Orthographic projections: views of Cu_2WS_4 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

112. $TaSe_2$ ($P6_3/mmc$)

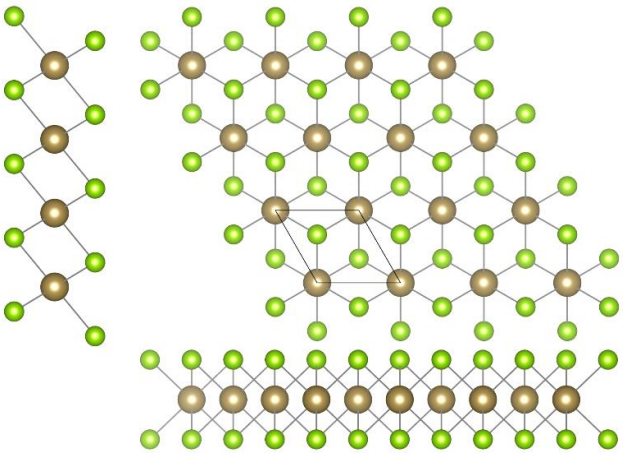
Formula	$TaSe_2$	**ID**	mp-501
Measure	14.1	**Symbol**	$P6_3/mmc$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.003
Density (g/cm^3)	7.840	**Energy-Above-Hull (eV/atom)**	0.013
Formation Energy (eV/atom)	-0.801	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $TaSe_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.74398000	-3.02066000	0.00000000
a_2	1.74398000	3.02066000	0.00000000
a_3	0.00000000	0.00000000	27.24808000

	x (Å)	*y* (Å)	*z* (Å)
Ta	0.00000000	0.00000000	13.62400000
Ta	0.00000000	0.00000000	0.00000000
Ta	0.00000000	0.00000000	20.43610000
Ta	0.00000000	0.00000000	6.81200000
Se	1.74400000	-1.00690000	15.28660000
Se	1.74400000	1.00690000	1.66250000
Se	1.74400000	1.00690000	11.96150000
Se	1.74400000	-1.00690000	25.58560000
Se	1.74400000	-1.00690000	5.14010000
Se	1.74400000	1.00690000	18.76410000
Se	1.74400000	1.00690000	22.10800000
Se	1.74400000	-1.00690000	8.48400000



Orthographic projections: views of $TaSe_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

113. Ga_2NiS_4 ($P\bar{3}m1$)

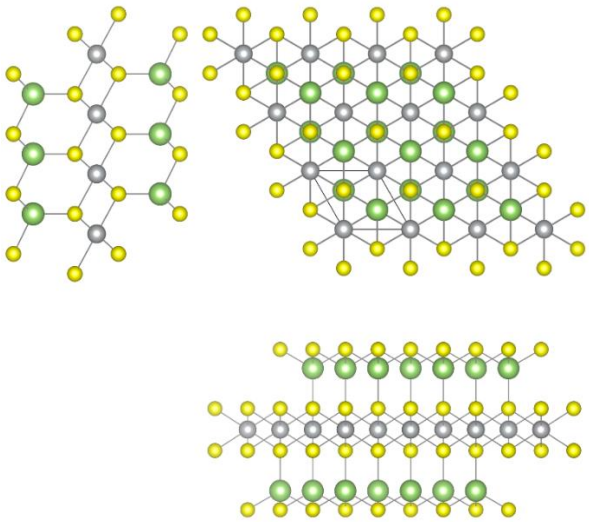
Formula	Ga_2NiS_4	**ID**	mp-6959
Measure	14.1	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.030
Density (g/cm^3)	3.752	**Energy-Above-Hull (eV/atom)**	0.066
Formation Energy (eV/atom)	-0.894	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Ga_2NiS_4 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.82446000	-3.16005000	0.00000000
a_2	1.82446000	3.16005000	0.00000000
a_3	0.00000000	0.00000000	12.52686000

	x (Å)	*y* (Å)	*z* (Å)
Ga	1.82450000	1.05340000	2.87620000
Ga	1.82450000	-1.05340000	9.65060000
Ni	0.00000000	0.00000000	6.26340000
S	1.82450000	-1.05340000	7.42550000
S	1.82450000	1.05340000	5.10130000
S	1.82450000	-1.05340000	1.82910000
S	1.82450000	1.05340000	10.69770000



Orthographic projections: views of Ga_2NiS_4 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

114. Ta_2Se (P4/nmm)

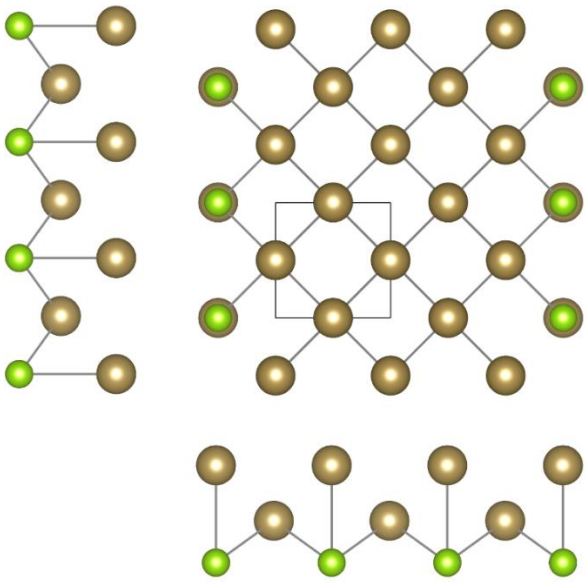
Formula	Ta_2Se	**ID**	mp-8732
Measure	14.0	**Symbol**	P4/nmm
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	12.220	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.445	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Ta_2Se in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.40432000	0.00000000	0.00000000
a_2	0.00000000	3.40432000	0.00000000
a_3	0.00000000	0.00000000	10.33799000

	x (Å)	*y* (Å)	*z* (Å)
Ta	1.70220000	0.00000000	7.95570000
Ta	0.00000000	1.70220000	2.38230000
Ta	0.00000000	1.70220000	9.58190000
Ta	1.70220000	0.00000000	0.75610000
Se	0.00000000	1.70220000	6.72720000
Se	1.70220000	0.00000000	3.61080000



Orthographic projections: views of Ta_2Se as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

115. $ZnBr_2$ ($R\bar{3}m$)

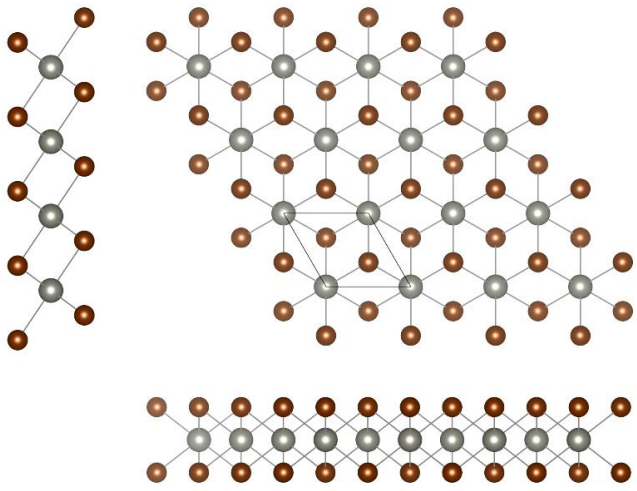
Formula	$ZnBr_2$	**ID**	mp-569960
Measure	14.0	**Symbol**	$R\bar{3}m$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	4.049	**Energy-Above-Hull (eV/atom)**	0.086
Formation Energy (eV/atom)	-0.826	**Band Gap (eV)**	3.308

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $ZnBr_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.90429000	-3.29833000	0.00000000
a_2	1.90429000	3.29833000	0.00000000
a_3	0.00000000	0.00000000	22.05614000

	x (Å)	*y* (Å)	*z* (Å)
Zn	0.00000000	0.00000000	0.00000000
Zn	1.90430000	-1.09940000	7.35200000
Zn	1.90430000	1.09940000	14.70410000
Br	0.00000000	0.00000000	5.87400000
Br	1.90430000	-1.09940000	1.47800000
Br	1.90430000	-1.09940000	13.22610000
Br	1.90430000	1.09940000	8.83010000
Br	1.90430000	1.09940000	20.57810000
Br	0.00000000	0.00000000	16.18210000



Orthographic projections: views of $ZnBr_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

116. BiIO (P4/nmm)

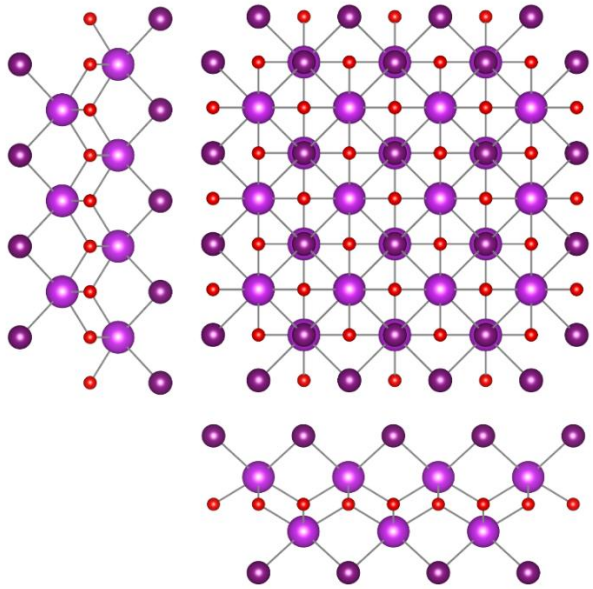
Formula	BiIO	**ID**	mp-22987
Measure	13.4	**Symbol**	P4/nmm
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	7.379	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.215	**Band Gap (eV)**	1.484

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of BiIO in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	4.02830000	0.00000000	0.00000000
a_2	0.00000000	4.02830000	0.00000000
a_3	0.00000000	0.00000000	9.75928000

	x (Å)	*y* (Å)	*z* (Å)
Bi	0.00000000	2.01420000	8.52200000
Bi	2.01420000	0.00000000	1.23730000
I	2.01420000	0.00000000	6.64830000
I	0.00000000	2.01420000	3.11100000
O	0.00000000	0.00000000	0.00000000
O	2.01420000	2.01420000	0.00000000



Orthographic projections: views of BiIO as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

117. NiI_2 ($R\bar{3}m$)

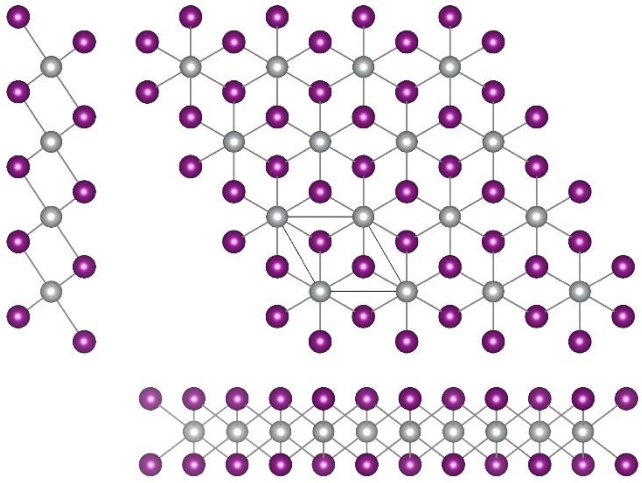
Formula	NiI_2	**ID**	mp-27638
Measure	13.2	**Symbol**	$R\bar{3}m$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.026
Density (g/cm^3)	5.585	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.023	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of NiI_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.97499000	-3.42078000	0.00000000
a_2	1.97499000	3.42078000	0.00000000
a_3	0.00000000	0.00000000	20.62945000

	x (Å)	*y* (Å)	*z* (Å)
Ni	0.00000000	0.00000000	0.00000000
Ni	1.97500000	-1.14030000	6.87650000
Ni	1.97500000	1.14030000	13.75300000
I	0.00000000	0.00000000	5.37260000
I	1.97500000	-1.14030000	1.50390000
I	1.97500000	-1.14030000	12.24910000
I	1.97500000	1.14030000	8.38030000
I	1.97500000	1.14030000	19.12560000
I	0.00000000	0.00000000	15.25680000



Orthographic projections: views of NiI_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

118. TiClO (Pmmn)

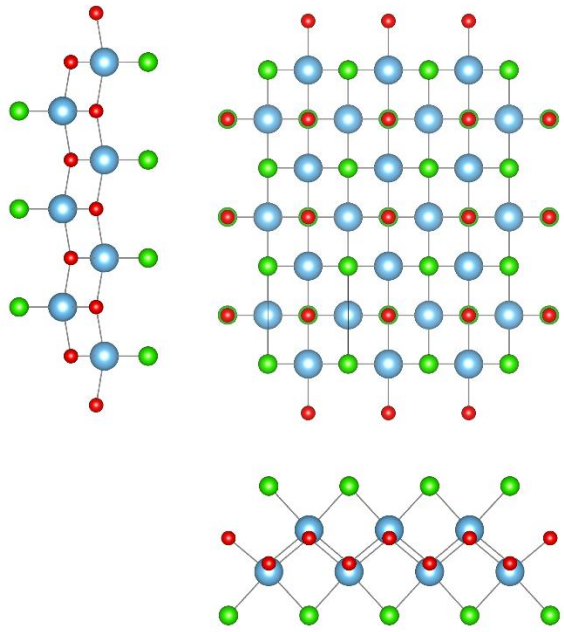
Formula	TiClO	**ID**	mp-22992
Measure	13.0	**Symbol**	Pmmn
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.006
Density (g/cm^3)	3.092	**Energy-Above-Hull (eV/atom)**	0.038
Formation Energy (eV/atom)	-2.716	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of TiClO in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.26893000	0.00000000	0.00000000
a_2	0.00000000	3.97448000	0.00000000
a_3	0.00000000	0.00000000	8.20957000

	x (Å)	*y* (Å)	*z* (Å)
Ti	1.63450000	0.00000000	0.84450000
Ti	0.00000000	1.98720000	7.36510000
Cl	1.63450000	1.98720000	5.59130000
Cl	0.00000000	0.00000000	2.61830000
O	0.00000000	0.00000000	7.69850000
O	1.63450000	1.98720000	0.51100000



Orthographic projections: views of TiClO as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

119. CdI_2 (P3m1)

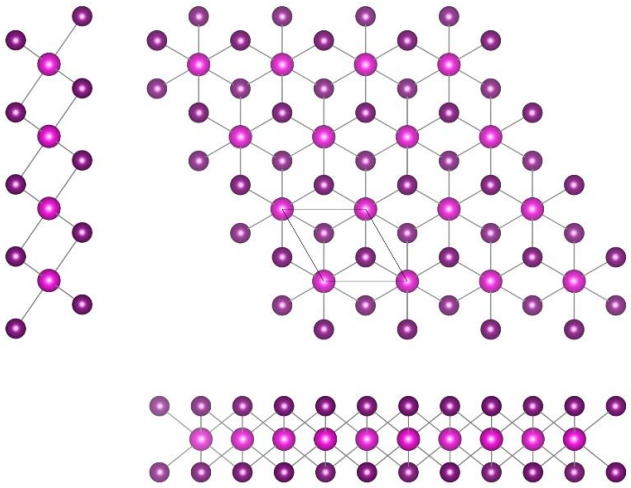
Formula	CdI_2	**ID**	mp-570437
Measure	13.0	**Symbol**	P3m1
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.002
Density (g/cm^3)	5.057	**Energy-Above-Hull (eV/atom)**	0.001
Formation Energy (eV/atom)	-0.591	**Band Gap (eV)**	2.405

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CdI_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	2.16540000	-3.75058000	0.00000000
a_2	2.16540000	3.75058000	0.00000000
a_3	0.00000000	0.00000000	22.20993000

	x (Å)	*y* (Å)	*z* (Å)
Cd	0.00000000	0.00000000	1.85120000
Cd	2.16540000	1.25020000	9.25440000
Cd	2.16540000	1.25020000	16.65670000
I	0.00000000	0.00000000	14.92800000
I	2.16540000	-1.25020000	18.38530000
I	2.16540000	-1.25020000	3.57930000
I	0.00000000	0.00000000	7.52590000
I	2.16540000	1.25020000	0.12370000
I	2.16540000	-1.25020000	10.98290000



Orthographic projections: views of CdI_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

120. TiBrO (Pmmn)

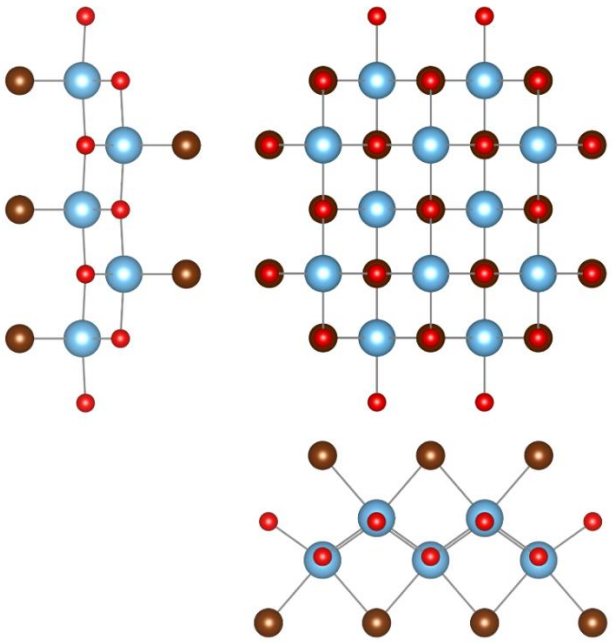
Formula	TiBrO	**ID**	mp-23002
Measure	12.9	**Symbol**	Pmmn
Magnetic Ordering	FM	**Tot. Magnetization (μ_B/cell)**	0.321
Density (g/cm^3)	4.142	**Energy-Above-Hull (eV/atom)**	0.019
Formation Energy (eV/atom)	-2.365	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of TiBrO in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.38711000	0.00000000	0.00000000
a_2	0.00000000	4.04789000	0.00000000
a_3	0.00000000	0.00000000	8.40861000

	x (Å)	*y* (Å)	*z* (Å)
Ti	0.00000000	2.02390000	7.75350000
Ti	1.69360000	0.00000000	0.65510000
Br	1.69360000	2.02390000	5.78940000
Br	0.00000000	0.00000000	2.61920000
O	0.00000000	0.00000000	7.85920000
O	1.69360000	2.02390000	0.54940000



Orthographic projections: views of TiBrO as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

121. InSe ($P6_3/mmc$)

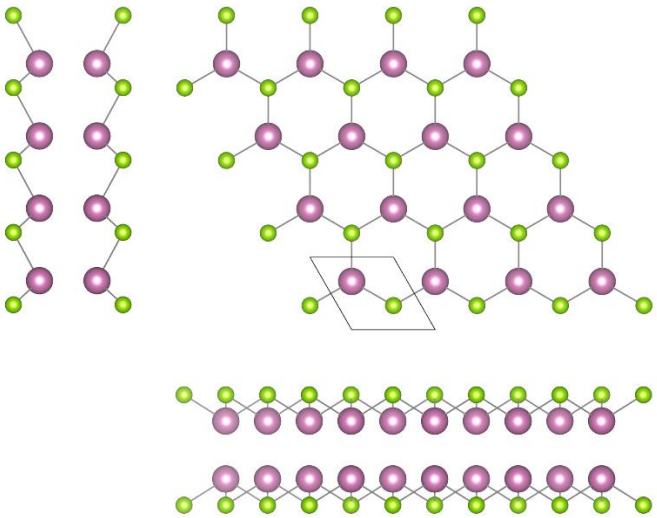
Formula	InSe	**ID**	mp-20485
Measure	12.9	**Symbol**	$P6_3/mmc$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	5.078	**Energy-Above-Hull (eV/atom)**	0.003
Formation Energy (eV/atom)	-0.507	**Band Gap (eV)**	0.459

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of InSe in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	2.04181000	-3.53652000	0.00000000
a_2	2.04181000	3.53652000	0.00000000
a_3	0.00000000	0.00000000	17.55041000

	x (Å)	*y* (Å)	*z* (Å)
In	2.04180000	-1.17880000	14.57370000
In	2.04180000	1.17880000	5.79850000
In	2.04180000	1.17880000	2.97670000
In	2.04180000	-1.17880000	11.75190000
Se	2.04180000	-1.17880000	1.69880000
Se	2.04180000	1.17880000	10.47410000
Se	2.04180000	1.17880000	15.85160000
Se	2.04180000	-1.17880000	7.07640000



Orthographic projections: views of InSe as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

122. $Mg(AlS_2)_2$ ($R\bar{3}m$)

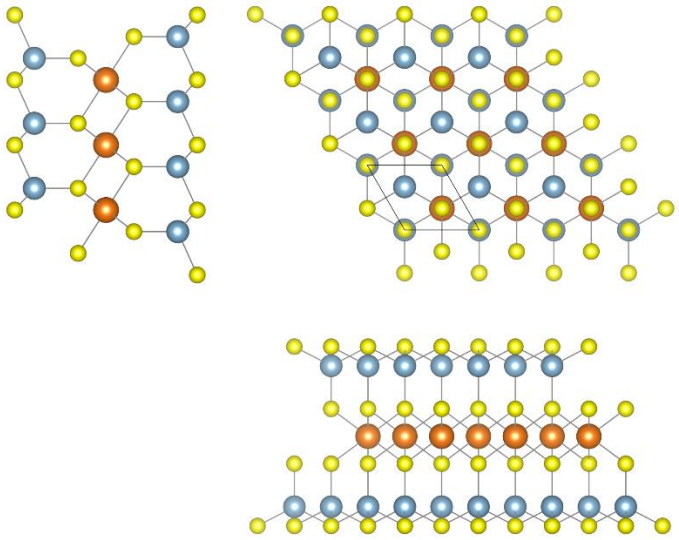
Formula	$Mg(AlS_2)_2$	**ID**	mp-16755
Measure	12.8	**Symbol**	$R\bar{3}m$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	2.214	**Energy-Above-Hull (eV/atom)**	0.030
Formation Energy (eV/atom)	-1.540	**Band Gap (eV)**	2.017

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $Mg(AlS_2)_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.85762000	-3.21749000	0.00000000
a_2	1.85762000	3.21749000	0.00000000
a_3	0.00000000	0.00000000	38.88342000

	x (Å)	*y* (Å)	*z* (Å)
Mg	0.00000000	0.00000000	0.00000000
Mg	1.85760000	-1.07250000	12.96110000
Mg	1.85760000	1.07250000	25.92230000
Al	0.00000000	0.00000000	9.40960000
Al	1.85760000	-1.07250000	3.55150000
Al	1.85760000	-1.07250000	22.37080000
Al	1.85760000	1.07250000	16.51260000
Al	1.85760000	1.07250000	35.33190000
Al	0.00000000	0.00000000	29.47380000
S	0.00000000	0.00000000	4.51920000
S	1.85760000	-1.07250000	8.44200000
S	0.00000000	0.00000000	11.58000000
S	1.85760000	-1.07250000	1.38120000
S	1.85760000	-1.07250000	17.48030000
S	1.85760000	1.07250000	21.40310000
S	1.85760000	-1.07250000	24.54110000
S	1.85760000	1.07250000	14.34230000
S	1.85760000	1.07250000	30.44150000
S	0.00000000	0.00000000	34.36420000
S	1.85760000	1.07250000	37.50230000
S	0.00000000	0.00000000	27.30340000



Orthographic projections: views of $Mg(AlS_2)_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

123. HfS_3 ($P2_1/m$)

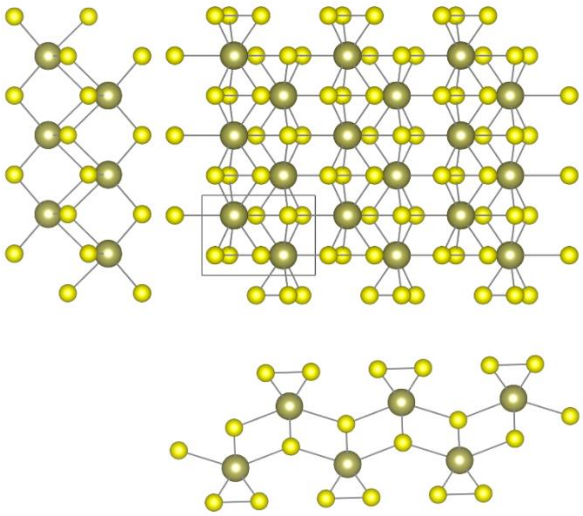
Formula	HfS_3	**ID**	mp-9922
Measure	12.8	**Symbol**	$P2_1/m$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	5.092	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.694	**Band Gap (eV)**	1.136

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of HfS_3 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	0.00000000	5.14921000	0.00000000
a_2	3.61157000	0.00000000	0.00000000
a_3	0.00000000	-1.18089000	-9.63392000

	x (Å)	*y* (Å)	*z* (Å)
Hf	0.90290000	3.27020000	-3.43650000
Hf	2.70870000	0.69810000	-6.19740000
S	0.90290000	-0.35000000	-7.74910000
S	2.70870000	4.31840000	-1.88480000
S	2.70870000	3.27130000	-5.29540000
S	0.90290000	0.69700000	-4.33850000
S	2.70870000	2.23290000	-1.87120000
S	0.90290000	1.73540000	-7.76280000



Orthographic projections: views of HfS_3 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

124. BiO_2 (C2/c)

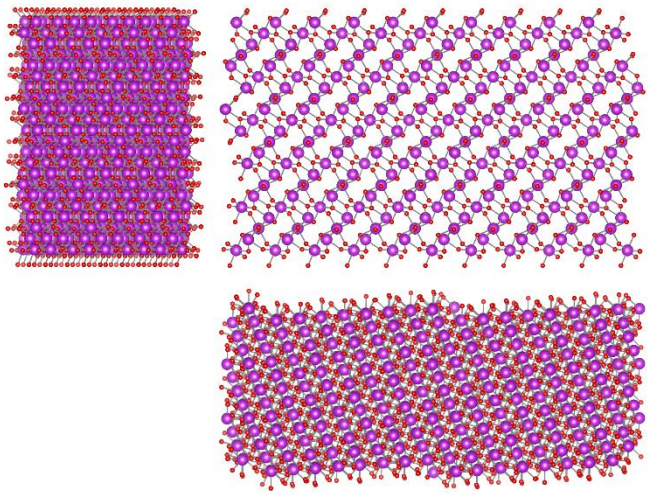
Formula	BiO_2	**ID**	mp-557993
Measure	12.8	**Symbol**	C2/c
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	8.946	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.471	**Band Gap (eV)**	1.083

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of BiO_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	0	12.55203	0
a_2	5.28162	0	0
a_3	0	-1.75962	-5.39765

	x (Å)	*y* (Å)	*z* (Å)
Bi	3.8509	-0.4399	-1.3494
Bi	1.4308	-1.3197	-4.0482
Bi	3.9612	3.138	0
Bi	1.3204	2.2582	-2.6988
Bi	1.2101	5.8361	-1.3494
Bi	4.0716	4.9563	-4.0482
Bi	1.3204	9.414	0
Bi	3.9612	8.5342	-2.6988
O	4.8274	5.0746	-0.117
O	4.9607	1.0609	-3.5091
O	2.9617	3.4555	-1.8885
O	2.3199	2.5757	-4.5873
O	0.3209	1.9407	-0.8103
O	0.4542	4.1947	-2.8159
O	2.1866	0.3216	-2.5818
O	3.095	-0.5582	-5.2806
O	2.1866	11.3506	-0.117
O	2.3199	7.3369	-3.5091
O	0.3209	9.7315	-1.8885
O	4.9607	8.8517	-4.5873
O	2.9617	8.2167	-0.8103
O	3.095	10.4708	-2.8159
O	4.8274	6.5977	-2.5818
O	0.4542	5.7179	-5.2806



Orthographic projections: views of BiO_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

125. $AlSiTe_3$ ($P\bar{3}1m$)

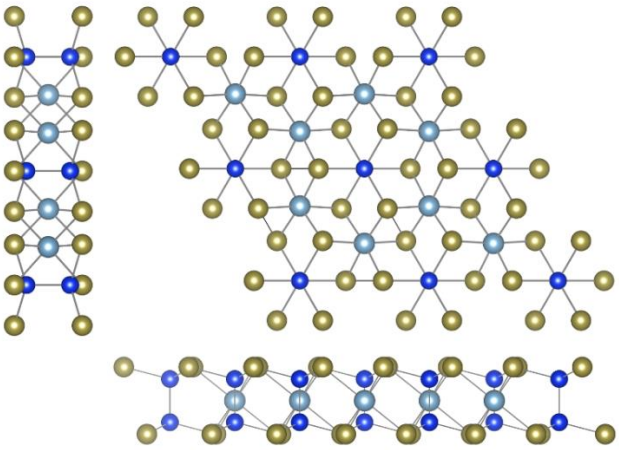
Formula	$AlSiTe_3$	**ID**	mp-31220
Measure	12.5	**Symbol**	$P\bar{3}1m$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	4.573	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.268	**Band Gap (eV)**	1.343

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $AlSiTe_3$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.45640000	-5.98666000	0.00000000
a_2	3.45640000	5.98666000	0.00000000
a_3	0.00000000	0.00000000	7.68409000

	x (Å)	*y* (Å)	*z* (Å)
Al	3.45640000	-1.99560000	3.84200000
Al	3.45640000	1.99560000	3.84200000
Si	0.00000000	0.00000000	2.69270000
Si	0.00000000	0.00000000	4.99130000
Te	2.22770000	3.85850000	5.62590000
Te	2.45740000	0.00000000	5.62590000
Te	2.22770000	-3.85850000	5.62590000
Te	4.45540000	0.00000000	2.05820000
Te	1.22870000	2.12820000	2.05820000
Te	1.22870000	-2.12820000	2.05820000



Orthographic projections: views of $AlSiTe_3$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

126. BiTeBr (P3m1)

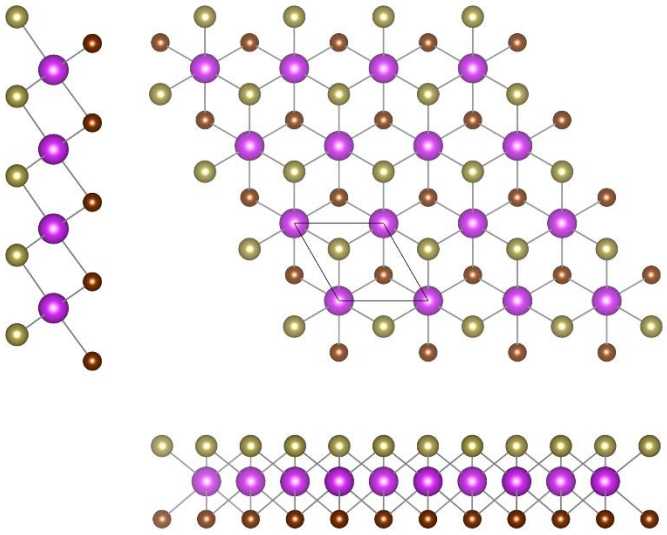
Formula	BiTeBr	**ID**	mp-33723
Measure	12.4	**Symbol**	P3m1
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	6.082	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.505	**Band Gap (eV)**	1.297

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of BiTeBr in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	2.17895000	-3.77405000	0.00000000
a_2	2.17895000	3.77405000	0.00000000
a_3	0.00000000	0.00000000	6.91433000

	x (Å)	*y* (Å)	*z* (Å)
Bi	0.00000000	0.00000000	0.03620000
Te	2.17900000	1.25800000	1.77720000
Br	2.17900000	-1.25800000	5.10090000



Orthographic projections: views of BiTeBr as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

127. LiC_6 (P6/mmm)

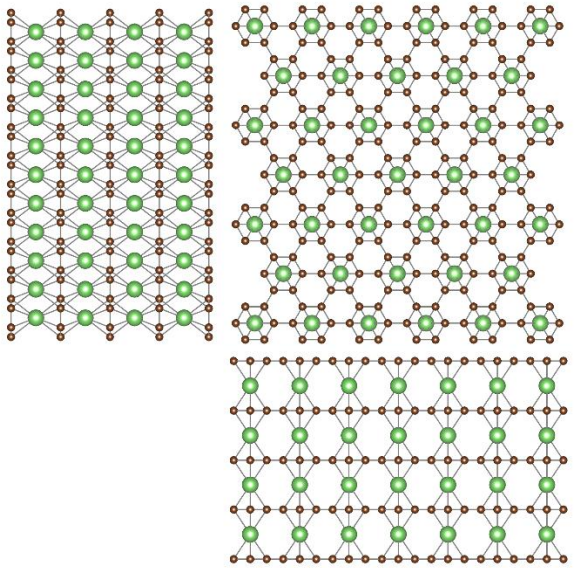
Formula	LiC_6	**ID**	mp-1001581
Measure	12.4	**Symbol**	P6/mmm
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.003
Density (g/cm^3)	2.164	**Energy-Above-Hull (eV/atom)**	0.002
Formation Energy (eV/atom)	-0.003	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of LiC_6 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	2.16165	-3.74408	0
a_2	2.16165	3.74408	0
a_3	0	0	3.74537

	x (Å)	*y* (Å)	*z* (Å)
Li	0	0	0
C	1.442	0	1.8727
C	1.4406	-2.4952	1.8727
C	1.4406	2.4952	1.8727
C	2.8813	0	1.8727
C	0.721	-1.2488	1.8727
C	0.721	1.2488	1.8727



Orthographic projections: views of LiC_6 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

128. $PdSe_2$ (Pbca)

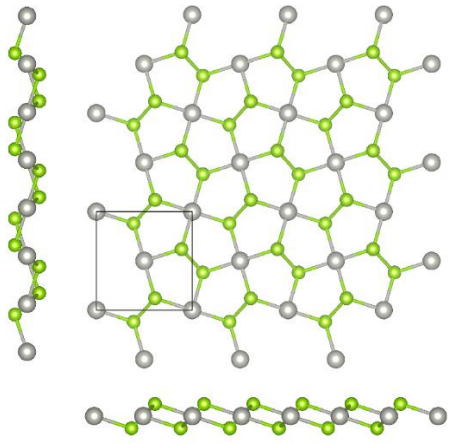
Formula	$PdSe_2$	**ID**	mp-2418
Measure	12.3	**Symbol**	Pbca
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	5.937	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.283	**Band Gap (eV)**	0.009

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $PdSe_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	5.79442000	0.00000000	0.00000000
a_2	0.00000000	5.94542000	0.00000000
a_3	0.00000000	0.00000000	8.58506000

	x (Å)	*y* (Å)	*z* (Å)
Pd	2.89720000	0.00000000	4.29250000
Pd	0.00000000	2.97270000	4.29250000
Pd	2.89720000	2.97270000	0.00000000
Pd	0.00000000	0.00000000	0.00000000
Se	3.54210000	0.70960000	0.73740000
Se	0.64490000	2.26310000	7.84770000
Se	2.25230000	3.68230000	3.55520000
Se	5.14950000	5.23580000	5.02990000
Se	0.64490000	0.70960000	3.55520000
Se	3.54210000	2.26310000	5.02990000
Se	5.14950000	3.68230000	0.73740000
Se	2.25230000	5.23580000	7.84770000



Orthographic projections: views of $PdSe_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

129. CuI ($P\bar{3}m1$)

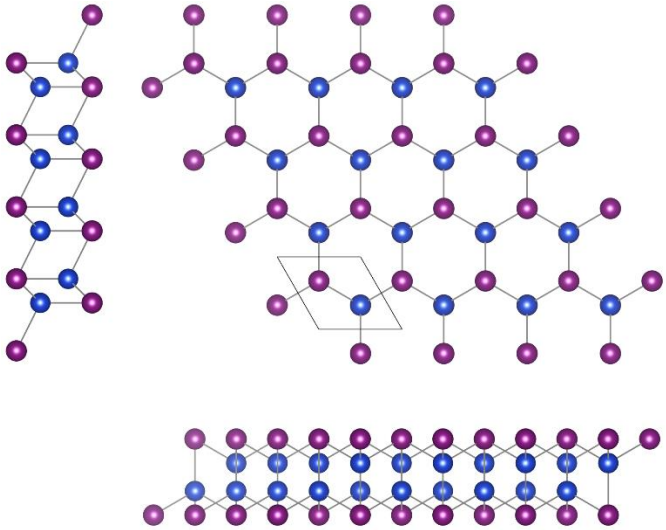
Formula	CuI	**ID**	mp-570081
Measure	12.3	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	5.687	**Energy-Above-Hull (eV/atom)**	0.001
Formation Energy (eV/atom)	-0.152	**Band Gap (eV)**	1.647

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CuI in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	2.07776000	-3.59878000	0.00000000
a_2	2.07776000	3.59878000	0.00000000
a_3	0.00000000	0.00000000	7.43662000

	x (Å)	*y* (Å)	*z* (Å)
Cu	2.07780000	-1.19960000	4.41780000
Cu	2.07780000	1.19960000	3.01880000
I	2.07780000	1.19960000	5.62020000
I	2.07780000	-1.19960000	1.81640000



Orthographic projections: views of CuI as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

130. NbI_2O (C2)

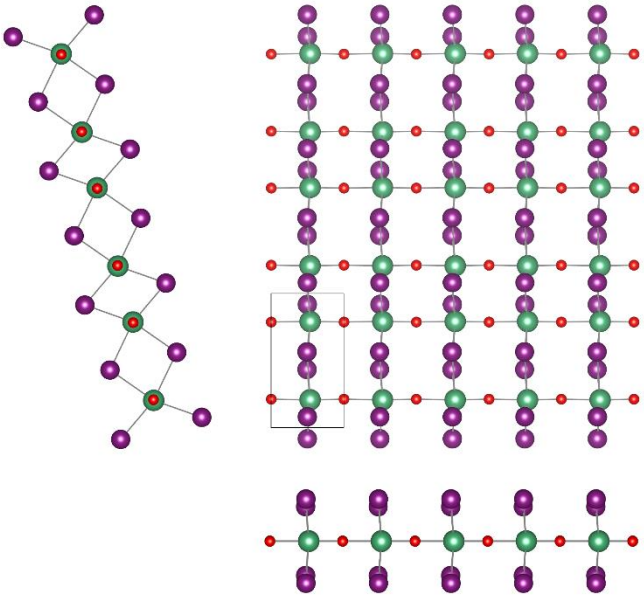
Formula	NbI_2O	**ID**	mp-549720
Measure	12.1	**Symbol**	C2
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	5.133	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.436	**Band Gap (eV)**	0.843

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of NbI_2O in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	0.00000000	16.07996000	0.00000000
a_2	3.97272000	0.00000000	0.00000000
a_3	0.00000000	-1.96329000	-7.34672000

	x (Å)	*y* (Å)	*z* (Å)
Nb	2.13150000	7.62630000	-1.53030000
Nb	0.14510000	-1.54960000	-5.81640000
Nb	0.14510000	15.66630000	-1.53030000
Nb	2.13150000	6.49040000	-5.81640000
I	3.96470000	2.21940000	-0.60120000
I	3.94800000	0.84320000	-4.15630000
I	1.96170000	5.23350000	-3.19040000
I	1.97830000	3.85730000	-6.74550000
I	1.97830000	10.25940000	-0.60120000
I	1.96170000	8.88310000	-4.15630000
I	3.94800000	13.27350000	-3.19040000
I	3.96470000	11.89730000	-6.74550000
O	0.00910000	7.61480000	-1.56380000
O	1.99540000	-1.53810000	-5.78300000
O	1.99540000	15.65480000	-1.56380000
O	0.00910000	6.50190000	-5.78300000



Orthographic projections: views of NbI_2O as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

131. Te_2Mo ($P2_1/m$)

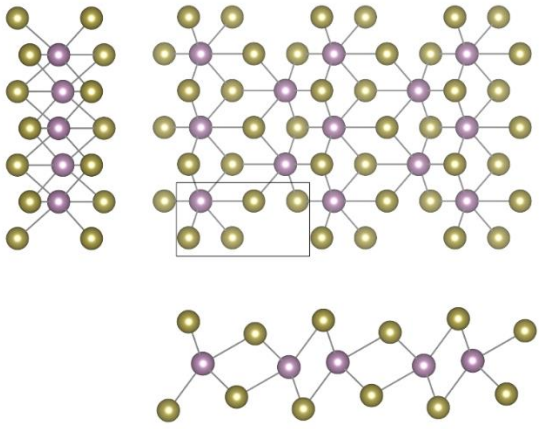
Formula	Te_2Mo	**ID**	mp-7459
Measure	12.0	**Symbol**	$P2_1/m$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	6.764	**Energy-Above-Hull (eV/atom)**	0.015
Formation Energy (eV/atom)	-0.261	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Te_2Mo in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	0.00000000	6.36619000	0.00000000
a_2	3.48688000	0.00000000	0.00000000
a_3	0.00000000	-0.64781000	-15.53442000

	x (Å)	*y* (Å)	*z* (Å)
Te	2.61520000	3.63710000	-1.47420000
Te	0.87170000	2.08130000	-14.06020000
Te	0.87170000	0.49540000	-2.06990000
Te	2.61520000	5.22300000	-13.46450000
Te	0.87170000	3.35290000	-5.69690000
Te	2.61520000	2.36550000	-9.83750000
Te	2.61520000	0.12950000	-6.29540000
Te	0.87170000	5.58890000	-9.23900000
Mo	2.61520000	1.15280000	-0.10060000
Mo	0.87170000	4.56560000	-15.43380000
Mo	0.87170000	1.70700000	-7.86830000
Mo	2.61520000	4.01140000	-7.66610000



Orthographic projections: views of Te_2Mo as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

132. ZnSe (P4/nmm)

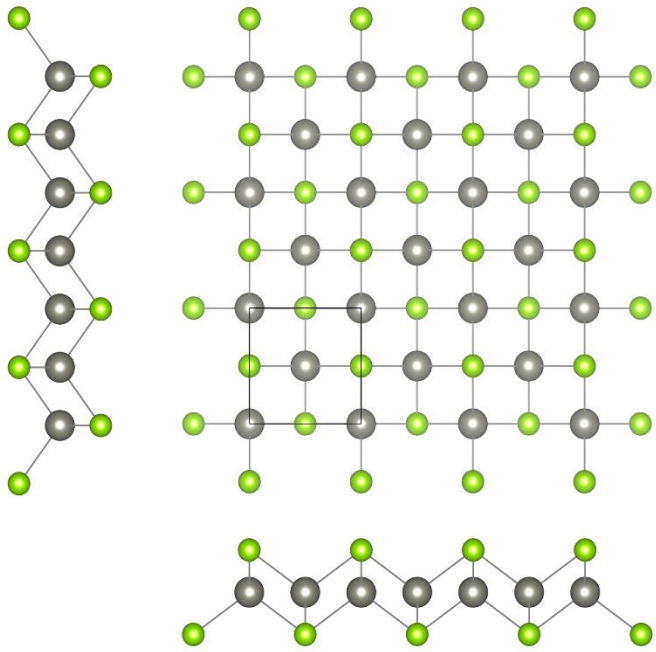
Formula	ZnSe	**ID**	mp-569679
Measure	12.0	**Symbol**	P4/nmm
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	4.681	**Energy-Above-Hull (eV/atom)**	0.160
Formation Energy (eV/atom)	-0.556	**Band Gap (eV)**	1.967

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of ZnSe in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	4.10770000	0.00000000	0.00000000
a_2	0.00000000	4.10770000	0.00000000
a_3	0.00000000	0.00000000	6.07035000

	x (Å)	*y* (Å)	*z* (Å)
Zn	0.00000000	0.00000000	0.00000000
Zn	2.05390000	2.05390000	0.00000000
Se	0.00000000	2.05390000	1.49500000
Se	2.05390000	0.00000000	4.57530000



Orthographic projections: views of ZnSe as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

133. $HfSe_3$ ($P2_1/m$)

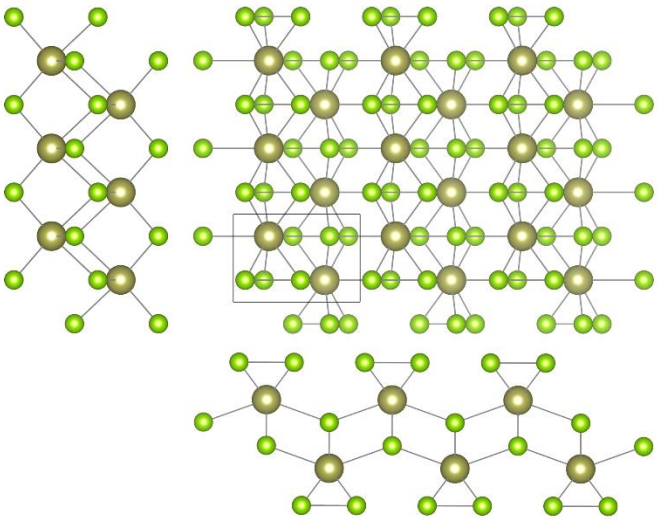
Formula	$HfSe_3$	**ID**	mp-15622
Measure	12.0	**Symbol**	$P2_1/m$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	6.660	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.013	**Band Gap (eV)**	0.611

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $HfSe_3$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	0.00000000	5.44820000	0.00000000
a_2	3.74952000	0.00000000	0.00000000
a_3	0.00000000	-1.09793000	-10.13890000

	x (Å)	*y* (Å)	*z* (Å)
Hf	0.93740000	3.53730000	-3.58880000
Hf	2.81210000	0.81300000	-6.55010000
Se	0.93740000	-0.38070000	-8.16570000
Se	2.81210000	4.73100000	-1.97320000
Se	2.81210000	3.53680000	-5.57060000
Se	0.93740000	0.81340000	-4.56830000
Se	2.81210000	2.34160000	-1.97460000
Se	0.93740000	2.00870000	-8.16430000



Orthographic projections: views of $HfSe_3$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

134. Br (Cmce)

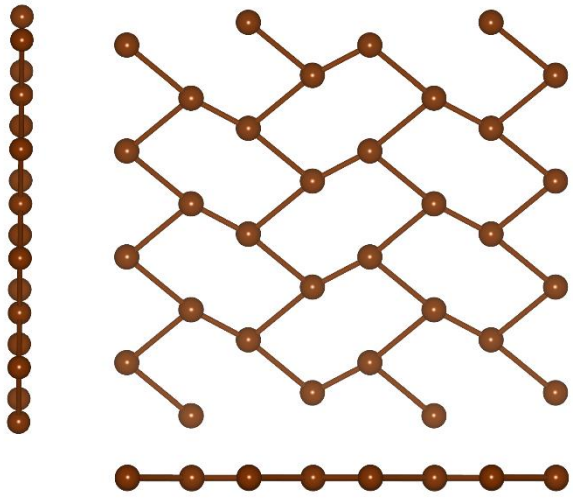
Formula	Br	**ID**	mp-23154
Measure	11.9	**Symbol**	Cmce
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	3.373	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	0.000	**Band Gap (eV)**	1.327

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Br in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	4.25865000	0.00000000	0.00000000
a_2	0.00000000	8.45219000	0.00000000
a_3	0.00000000	0.00000000	8.74380000

	x (Å)	*y* (Å)	*z* (Å)
Br	1.52260000	0.00000000	1.02960000
Br	2.73610000	0.00000000	7.71420000
Br	0.60670000	0.00000000	5.40150000
Br	3.65190000	0.00000000	3.34230000
Br	3.65190000	4.22610000	1.02960000
Br	0.60670000	4.22610000	7.71420000
Br	2.73610000	4.22610000	5.40150000
Br	1.52260000	4.22610000	3.34230000



Orthographic projections: views of Br as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

135. $Ca_2Cu(ClO)_2$ (I4/mmm)

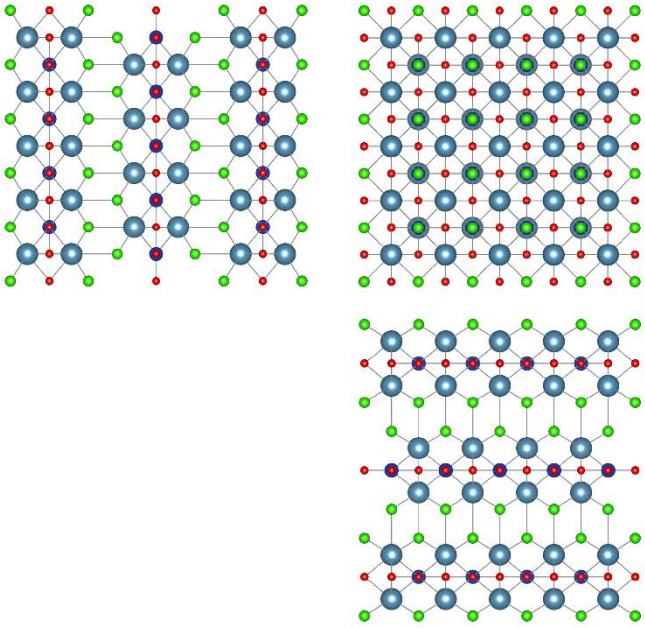
Formula	$Ca_2Cu(ClO)_2$	**ID**	mp-23143
Measure	11.7	**Symbol**	I4/mmm
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.013
Density (g/cm^3)	3.554	**Energy-Above-Hull (eV/atom)**	0.019
Formation Energy (eV/atom)	-2.408	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $Ca_2Cu(ClO)_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.88025	0	2.37597E-16
a_2	6.23991E-16	3.88025	2.37597E-16
a_3	0	0	15.30407

	x (Å)	*y* (Å)	*z* (Å)
Ca	0	0	6.0658
Ca	1.9401	1.9401	1.5862
Ca	1.9401	1.9401	13.7179
Ca	0	0	9.2383
Cu	0	0	0
Cu	1.9401	1.9401	7.652
Cl	0	0	2.7911
Cl	1.9401	1.9401	4.8609
Cl	1.9401	1.9401	10.4431
Cl	0	0	12.513
O	1.9401	0	0
O	0	1.9401	0
O	0	1.9401	7.652
O	1.9401	0	7.652



Orthographic projections: views of $Ca_2Cu(ClO)_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

136. $Mg_3Si_4(HO_6)_2$ ($P\bar{1}$)

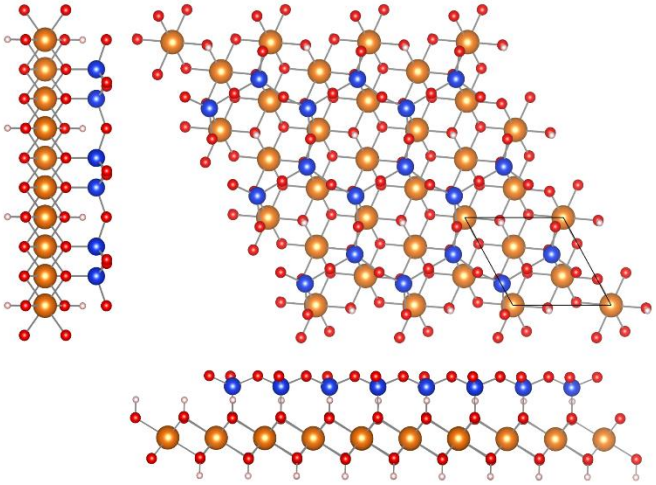
Formula	$Mg_3Si_4(HO_6)_2$	**ID**	mp-696497
Measure	11.7	**Symbol**	$P\bar{1}$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	2.694	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-3.000	**Band Gap (eV)**	5.232

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $Mg_3Si_4(HO_6)_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	5.32832000	0.00000000	0.00000000
a_2	2.65933000	4.63224000	0.00000000
a_3	0.98858000	1.39341000	9.47049000

	x (Å)	*y* (Å)	*z* (Å)
Mg	0.00000000	0.00000000	0.00000000
Mg	3.64990000	2.93960000	9.46960000
Mg	5.32630000	3.08600000	0.00090000
Mg	6.21140000	1.54590000	2.75620000
Si	2.76480000	4.47980000	6.71430000
Si	3.54710000	3.09020000	2.75410000
Si	5.42920000	2.93550000	6.71640000
Si	6.23010000	4.64470000	2.02090000
H	2.74620000	1.38090000	7.44960000
H	3.54410000	3.08340000	1.11590000
O	5.43220000	2.94230000	8.35460000
O	6.20710000	4.63350000	1.05140000
O	2.76920000	1.39220000	8.41910000
O	6.20850000	1.54620000	1.11830000
O	2.76770000	4.47950000	8.35220000
O	3.43090000	4.63390000	3.29840000
O	5.54530000	1.39180000	6.17210000
O	2.26960000	2.22380000	3.31490000
O	6.70660000	3.80190000	6.15560000
O	4.93730000	2.41990000	3.31260000
O	4.03890000	3.60570000	6.15790000



Orthographic projections: views of $Mg_3Si_4(HO_6)_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

137. TiBrN (Pmmn)

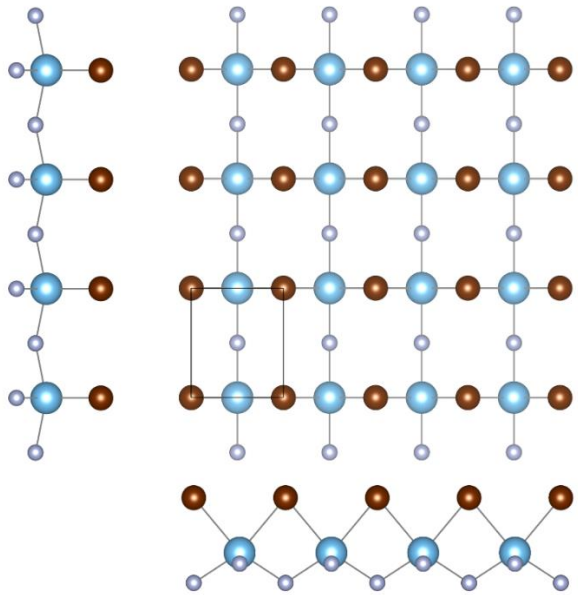
Formula	TiBrN	**ID**	mp-27849
Measure	11.6	**Symbol**	Pmmn
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	3.940	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.508	**Band Gap (eV)**	0.555

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of TiBrN in Cartesian coordinates.

	x (Å)	y (Å)	z (Å)
a_1	3.37770000	0.00000000	0.00000000
a_2	0.00000000	3.96139000	0.00000000
a_3	0.00000000	0.00000000	8.93237000

	x (Å)	y (Å)	z (Å)
Ti	0.00000000	1.98070000	8.18540000
Ti	1.68890000	0.00000000	0.74700000
Br	1.68890000	1.98070000	6.18390000
Br	0.00000000	0.00000000	2.74850000
N	0.00000000	0.00000000	8.58310000
N	1.68890000	1.98070000	0.34930000



Orthographic projections: views of TiBrN as seen from the x axis (left), the y axis (bottom) and the z axis (center). The primitive cell is also shown.

138. Bi_2Se_3 ($R\bar{3}m$)

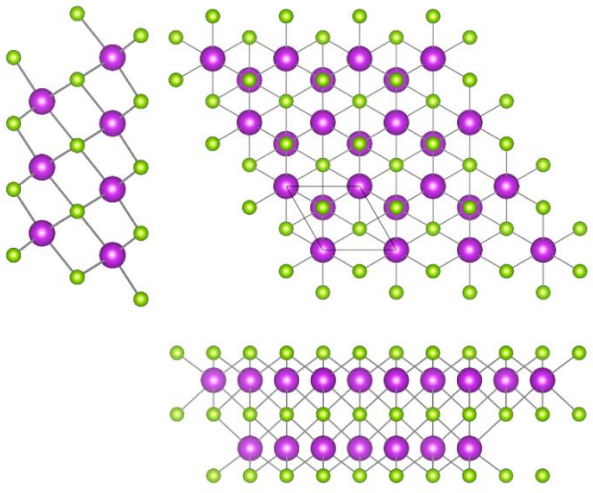
Formula	Bi_2Se_3	**ID**	mp-541837
Measure	11.5	**Symbol**	$R\bar{3}m$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	7.056	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.388	**Band Gap (eV)**	0.543

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Bi_2Se_3 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	2.09488000	-3.62844000	0.00000000
a_2	2.09488000	3.62844000	0.00000000
a_3	0.00000000	0.00000000	30.41115000

	x (Å)	*y* (Å)	*z* (Å)
Bi	2.09490000	1.20950000	1.94650000
Bi	2.09490000	1.20950000	8.19050000
Bi	0.00000000	0.00000000	12.08360000
Bi	0.00000000	0.00000000	18.32760000
Bi	2.09490000	-1.20950000	22.22060000
Bi	2.09490000	-1.20950000	28.46460000
Se	0.00000000	0.00000000	0.00000000
Se	2.09490000	-1.20950000	3.51190000
Se	0.00000000	0.00000000	6.62520000
Se	2.09490000	-1.20950000	10.13710000
Se	2.09490000	1.20950000	13.64890000
Se	2.09490000	-1.20950000	16.76220000
Se	2.09490000	1.20950000	20.27410000
Se	0.00000000	0.00000000	23.78600000
Se	2.09490000	1.20950000	26.89930000



Orthographic projections: views of Bi_2Se_3 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

139. ZrSiTe (P4/nmm)

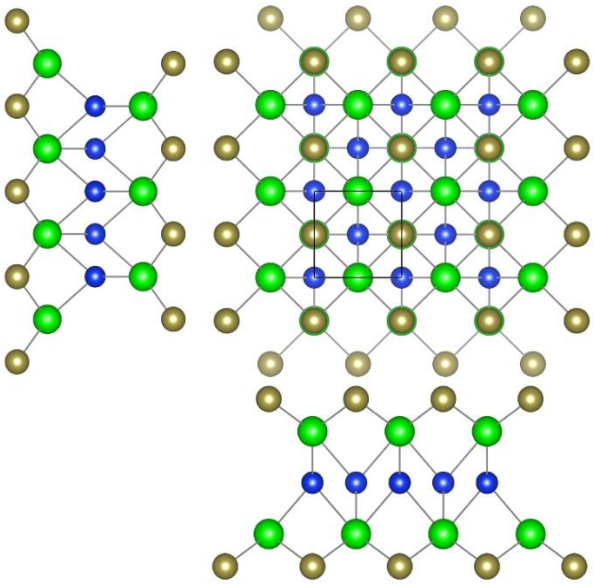
Formula	ZrSiTe	**ID**	mp-19917
Measure	11.5	**Symbol**	P4/nmm
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	6.063	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.800	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of ZrSiTe in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.69862000	0.00000000	0.00000000
a_2	0.00000000	3.69862000	0.00000000
a_3	0.00000000	0.00000000	9.88709000

	x (Å)	*y* (Å)	*z* (Å)
Zr	0.00000000	1.84930000	2.80500000
Zr	1.84930000	0.00000000	7.08210000
Si	1.84930000	1.84930000	4.94350000
Si	0.00000000	0.00000000	4.94350000
Te	1.84930000	0.00000000	1.45280000
Te	0.00000000	1.84930000	8.43430000



Orthographic projections: views of ZrSiTe as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

140. PbI_2 ($R\bar{3}m$)

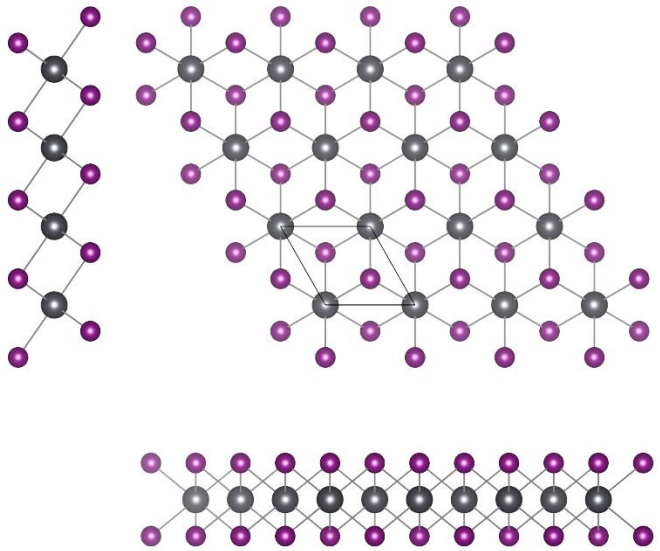
Formula	PbI_2	**ID**	mp-540789
Measure	11.5	**Symbol**	$R\bar{3}m$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.001
Density (g/cm^3)	5.461	**Energy-Above-Hull (eV/atom)**	0.003
Formation Energy (eV/atom)	-0.665	**Band Gap (eV)**	2.413

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of PbI_2 in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	2.32711000	-4.03066000	0.00000000
a_2	2.32711000	4.03066000	0.00000000
a_3	0.00000000	0.00000000	44.83567000

	x (Å)	*y* (Å)	*z* (Å)
Pb	0.00000000	0.00000000	0.00000000
Pb	2.32710000	1.34360000	7.47260000
Pb	2.32710000	-1.34360000	14.94520000
Pb	4.65420000	0.00000000	22.41780000
Pb	2.32710000	1.34360000	29.89040000
Pb	2.32710000	-1.34360000	37.36310000
I	2.32710000	-1.34360000	9.35440000
I	0.00000000	0.00000000	5.59080000
I	2.32710000	-1.34360000	1.87780000
I	0.00000000	0.00000000	13.06740000
I	2.32710000	1.34360000	24.29970000
I	2.32710000	-1.34360000	20.53600000
I	2.32710000	1.34360000	16.82300000
I	2.32710000	-1.34360000	28.01260000
I	0.00000000	0.00000000	39.24490000
I	2.32710000	1.34360000	35.48120000
I	0.00000000	0.00000000	31.76830000
I	2.32710000	1.34360000	42.95780000



Orthographic projections: views of PbI_2 as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

141. $ZrSe_2$ ($P\bar{3}m1$)

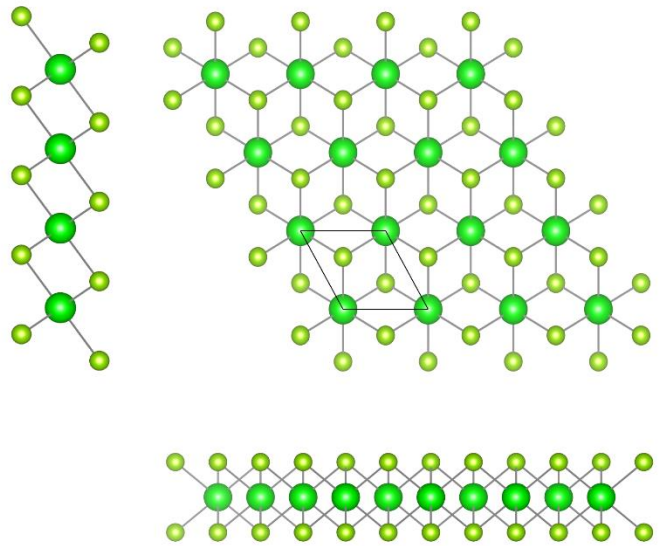
Formula	$ZrSe_2$	**ID**	mp-2076
Measure	11.3	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	4.935	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.329	**Band Gap (eV)**	0.343

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $ZrSe_2$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.90234000	-3.29495000	0.00000000
a_2	1.90234000	3.29495000	0.00000000
a_3	0.00000000	0.00000000	6.68691000

	x (Å)	*y* (Å)	*z* (Å)
Zr	0.00000000	0.00000000	0.00000000
Se	1.90230000	-1.09830000	5.09430000
Se	1.90230000	1.09830000	1.59260000



Orthographic projections: views of $ZrSe_2$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

142. ScHCl ($R\bar{3}m$)

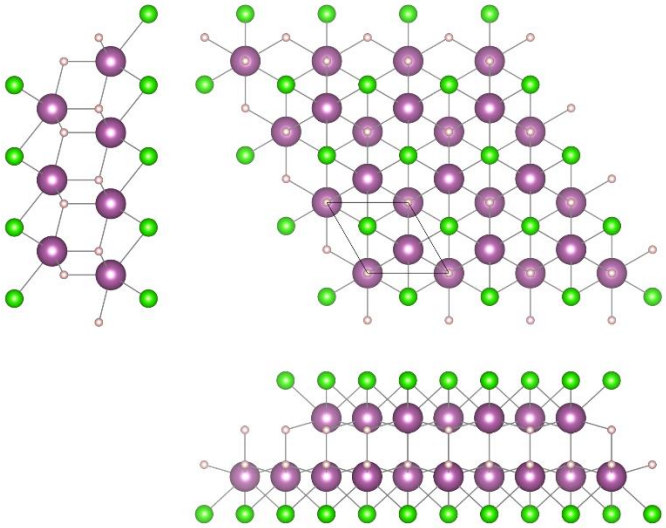
Formula	ScHCl	**ID**	mp-24081
Measure	11.2	**Symbol**	$R\bar{3}m$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	2.742	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-1.609	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of ScHCl in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.75506000	-3.03985000	0.00000000
a_2	1.75506000	3.03985000	0.00000000
a_3	0.00000000	0.00000000	27.72360000

	x (Å)	*y* (Å)	*z* (Å)
Sc	1.75510000	-1.01330000	5.87720000
Sc	0.00000000	0.00000000	3.36400000
Sc	1.75510000	1.01330000	15.11840000
Sc	1.75510000	-1.01330000	12.60520000
Sc	0.00000000	0.00000000	24.35960000
Sc	1.75510000	1.01330000	21.84640000
H	1.75510000	-1.01330000	3.87310000
H	0.00000000	0.00000000	5.36810000
H	1.75510000	1.01330000	13.11430000
H	1.75510000	-1.01330000	14.60930000
H	0.00000000	0.00000000	22.35550000
H	1.75510000	1.01330000	23.85050000
Cl	1.75510000	1.01330000	1.74900000
Cl	1.75510000	1.01330000	7.49220000
Cl	0.00000000	0.00000000	10.99020000
Cl	0.00000000	0.00000000	16.73340000
Cl	1.75510000	-1.01330000	20.23140000
Cl	1.75510000	-1.01330000	25.97460000



Orthographic projections: views of ScHCl as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

143. GaTe (C2/m)

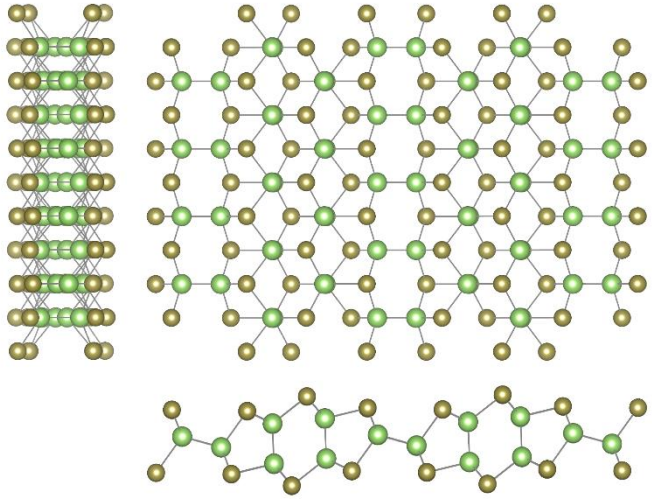
Formula	GaTe	**ID**	mp-542812
Measure	11.0	**Symbol**	C2/m
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	5.008	**Energy-Above-Hull (eV/atom)**	0.003
Formation Energy (eV/atom)	-0.361	**Band Gap (eV)**	1.035

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of GaTe in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	0.00000000	18.22634000	0.00000000
a_2	4.15018000	0.00000000	0.00000000
a_3	0.00000000	-3.06941000	-10.37979000

	x (Å)	*y* (Å)	*z* (Å)
Ga	0.00000000	13.90000000	-6.06180000
Ga	2.07510000	10.37010000	-4.31800000
Ga	0.00000000	11.73930000	-7.24150000
Ga	2.07510000	12.53080000	-3.13830000
Ga	2.07510000	14.26290000	-9.51960000
Ga	0.00000000	10.00720000	-0.86020000
Ga	2.07510000	4.78680000	-6.06180000
Ga	0.00000000	1.25690000	-4.31800000
Ga	2.07510000	2.62620000	-7.24150000
Ga	0.00000000	3.41760000	-3.13830000
Ga	0.00000000	5.14970000	-9.51960000
Ga	2.07510000	0.89410000	-0.86020000
Te	0.00000000	12.53140000	-9.81770000
Te	2.07510000	11.73870000	-0.56210000
Te	0.00000000	14.24870000	-3.39650000
Te	2.07510000	10.02140000	-6.98330000
Te	2.07510000	15.35510000	-7.01740000
Te	0.00000000	8.91500000	-3.36240000
Te	2.07510000	3.41820000	-9.81770000
Te	0.00000000	2.62550000	-0.56210000
Te	2.07510000	5.13550000	-3.39650000
Te	0.00000000	0.90820000	-6.98330000
Te	0.00000000	6.24190000	-7.01740000
Te	2.07510000	-0.19810000	-3.36240000



Orthographic projections: views of GaTe as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

144. $TaTe_4Ir$ ($Pmn2_1$)

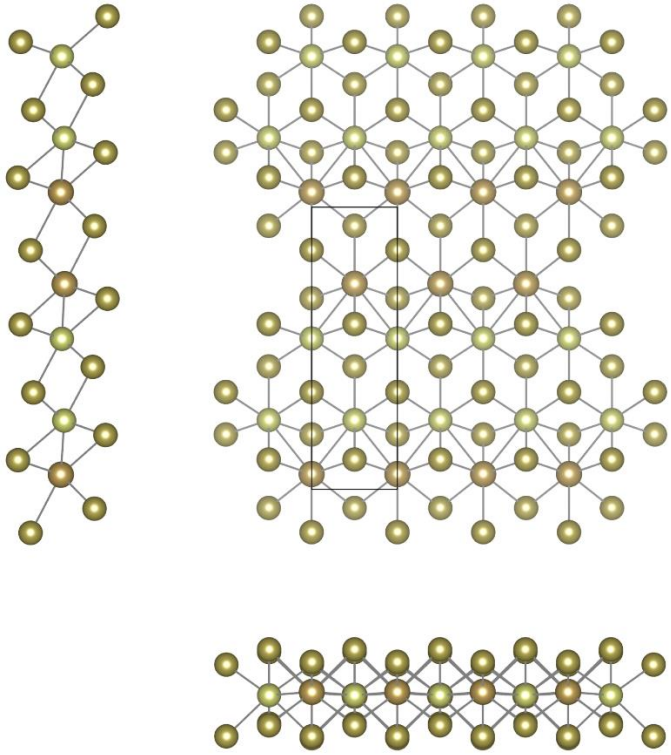
Formula	$TaTe_4Ir$	**ID**	mp-17287
Measure	10.9	**Symbol**	$Pmn2_1$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.001
Density (g/cm^3)	8.616	**Energy-Above-Hull (eV/atom)**	0.000
Formation Energy (eV/atom)	-0.367	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $TaTe_4Ir$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.83814000	0.00000000	0.00000000
a_2	0.00000000	12.63317000	0.00000000
a_3	0.00000000	0.00000000	14.04698000

	x (Å)	*y* (Å)	*z* (Å)
Ta	0.00000000	0.68270000	0.04730000
Ta	1.91910000	11.95050000	7.07080000
Ta	0.00000000	3.43070000	6.90080000
Ta	1.91910000	9.20240000	13.92430000
Te	1.91910000	1.33310000	1.96270000
Te	0.00000000	11.30010000	8.98620000
Te	1.91910000	1.91810000	8.42220000
Te	0.00000000	10.71510000	1.39870000
Te	1.91910000	4.08300000	4.98880000
Te	0.00000000	8.55020000	12.01230000
Te	1.91910000	5.50160000	12.66820000
Te	0.00000000	7.13160000	5.64470000
Te	0.00000000	0.83540000	5.56750000
Te	1.91910000	11.79780000	12.59100000
Te	0.00000000	2.45590000	12.09870000
Te	1.91910000	10.17730000	5.07520000
Te	0.00000000	4.35740000	1.27360000
Te	1.91910000	8.27570000	8.29710000
Te	0.00000000	5.23420000	8.86470000
Te	1.91910000	7.39900000	1.84120000
Ir	0.00000000	6.75700000	0.00110000
Ir	1.91910000	5.87620000	7.02460000
Ir	0.00000000	9.53000000	6.92030000
Ir	1.91910000	3.10320000	13.94380000



Orthographic projections: views of $TaTe_4Ir$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

145. $MoCl_3$ (C2/m)

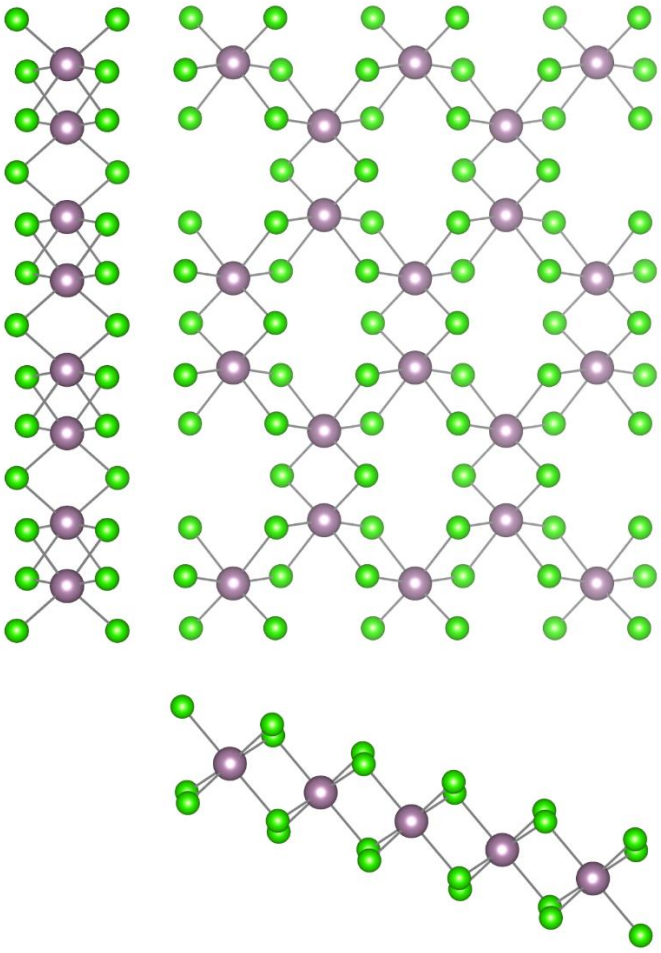
Formula	$MoCl_3$	**ID**	mp-22853
Measure	10.9	**Symbol**	C2/m
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	3.211	**Energy-Above-Hull (eV/atom)**	0.083
Formation Energy (eV/atom)	-1.226	**Band Gap (eV)**	0.146

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $MoCl_3$ in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	0.00000000	6.28236000	0.00000000
a_2	10.03611000	0.00000000	0.00000000
a_3	0.00000000	-2.09712000	-6.63631000

	x (Å)	*y* (Å)	*z* (Å)
Mo	3.54960000	3.14120000	0.00000000
Mo	6.48650000	3.14120000	0.00000000
Mo	8.56760000	0.00000000	0.00000000
Mo	1.46850000	0.00000000	0.00000000
Cl	0.00000000	0.93410000	-1.65330000
Cl	0.00000000	3.25110000	-4.98310000
Cl	1.71040000	-0.03060000	-5.31880000
Cl	1.71040000	4.21580000	-1.31750000
Cl	8.32570000	4.21580000	-1.31750000
Cl	8.32570000	-0.03060000	-5.31880000
Cl	5.01810000	4.07530000	-1.65330000
Cl	5.01810000	0.11000000	-4.98310000
Cl	6.72850000	3.11060000	-5.31880000
Cl	6.72850000	1.07460000	-1.31750000
Cl	3.30760000	1.07460000	-1.31750000
Cl	3.30760000	3.11060000	-5.31880000



Orthographic projections: views of $MoCl_3$ as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

146. GaGeTe ($R\bar{3}m$)

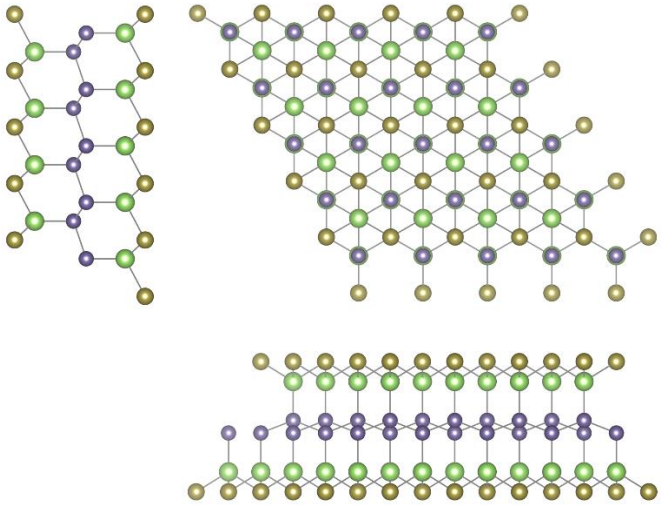
Formula	GaGeTe	**ID**	mp-8211
Measure	10.8	**Symbol**	$R\bar{3}m$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	4.989	**Energy-Above-Hull (eV/atom)**	0.008
Formation Energy (eV/atom)	-0.235	**Band Gap (eV)**	0.284

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of GaGeTe in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	2.06320000	-3.57357000	0.00000000
a_2	2.06320000	3.57357000	0.00000000
a_3	0.00000000	0.00000000	36.56015000

	x (Å)	*y* (Å)	*z* (Å)
Ga	0.00000000	0.00000000	9.31260000
Ga	2.06320000	-1.19120000	2.87420000
Ga	2.06320000	-1.19120000	21.49930000
Ga	2.06320000	1.19120000	15.06090000
Ga	2.06320000	1.19120000	33.68600000
Ga	0.00000000	0.00000000	27.24760000
Ge	0.00000000	0.00000000	11.78500000
Ge	2.06320000	-1.19120000	0.40170000
Ge	2.06320000	-1.19120000	23.97170000
Ge	2.06320000	1.19120000	12.58850000
Ge	2.06320000	1.19120000	36.15840000
Ge	0.00000000	0.00000000	24.77520000
Te	0.00000000	0.00000000	4.14460000
Te	2.06320000	-1.19120000	8.04210000
Te	2.06320000	-1.19120000	16.33130000
Te	2.06320000	1.19120000	20.22890000
Te	2.06320000	1.19120000	28.51800000
Te	0.00000000	0.00000000	32.41560000



Orthographic projections: views of GaGeTe as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

147. GeAs (C2/m)

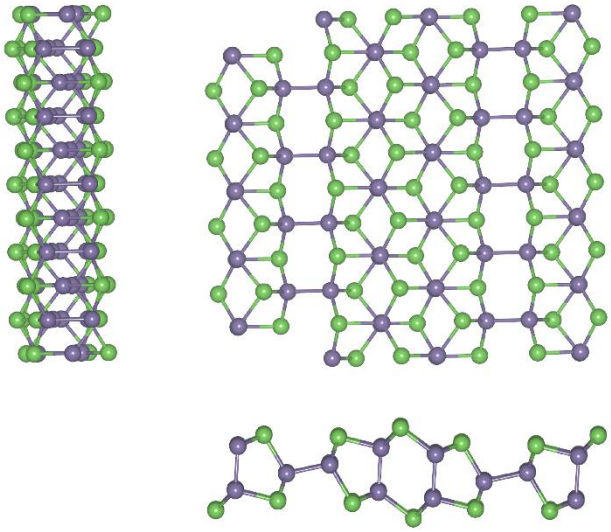
Formula	GeAs	**ID**	mp-9548
Measure	10.6	**Symbol**	C2/m
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.000
Density (g/cm^3)	4.813	**Energy-Above-Hull (eV/atom)**	0.002
Formation Energy (eV/atom)	-0.031	**Band Gap (eV)**	0.639

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of GeAs in Cartesian coordinates.

	x (Å)	y (Å)	z (Å)
a_1	0.00000000	16.64960000	0.00000000
a_2	3.83326000	0.00000000	0.00000000
a_3	0.00000000	-2.53277000	-9.57296000

	x (Å)	y (Å)	z (Å)
Ge	0.00000000	10.32300000	-7.56220000
Ge	1.91660000	12.11860000	-2.01070000
Ge	0.00000000	8.17010000	-8.80990000
Ge	1.91660000	14.27150000	-0.76310000
Ge	1.91660000	7.95000000	-5.66100000
Ge	0.00000000	14.49160000	-3.91190000
Ge	1.91660000	1.99820000	-7.56220000
Ge	0.00000000	3.79380000	-2.01070000
Ge	1.91660000	-0.15470000	-8.80990000
Ge	0.00000000	5.94670000	-0.76310000
Ge	0.00000000	-0.37480000	-5.66100000
Ge	1.91660000	6.16680000	-3.91190000
As	1.91660000	11.88990000	-7.85170000
As	0.00000000	10.55170000	-1.72130000
As	1.91660000	6.84030000	-7.92050000
As	0.00000000	15.60140000	-1.65240000
As	0.00000000	9.49810000	-5.22790000
As	1.91660000	12.94350000	-4.34500000
As	0.00000000	3.56510000	-7.85170000
As	1.91660000	2.22690000	-1.72130000
As	0.00000000	-1.48450000	-7.92050000
As	1.91660000	7.27660000	-1.65240000
As	1.91660000	1.17330000	-5.22790000
As	0.00000000	4.61870000	-4.34500000



Orthographic projections: views of GeAs as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

148. $NbTe_2$ ($P\bar{3}m1$)

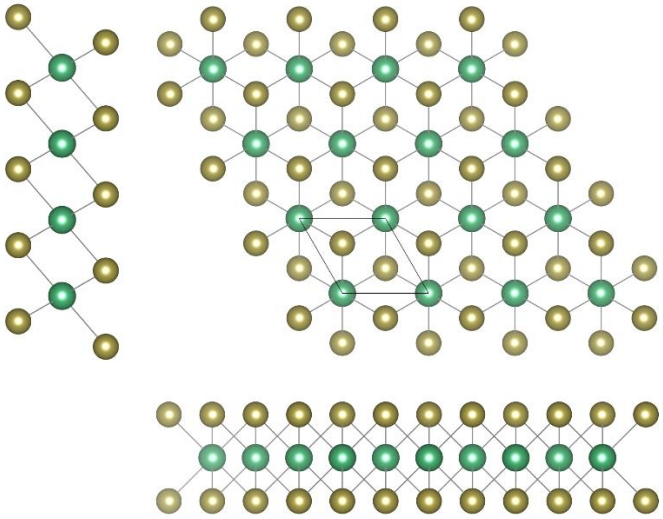
Formula	$NbTe_2$	**ID**	mp-1018150
Measure	10.5	**Symbol**	$P\bar{3}m1$
Magnetic Ordering	NM	**Tot. Magnetization (μ_B/cell)**	0.011
Density (g/cm^3)	6.804	**Energy-Above-Hull (eV/atom)**	0.036
Formation Energy (eV/atom)	-0.425	**Band Gap (eV)**	0.000

Crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of $NbTe_2$in Cartesian coordinates.

	x (Å)	*y* (Å)	*z* (Å)
a_1	1.84652000	-3.19826000	0.00000000
a_2	1.84652000	3.19826000	0.00000000
a_3	0.00000000	0.00000000	7.19333000

	x (Å)	*y* (Å)	*z* (Å)
Nb	0.00000000	0.00000000	0.00000000
Te	1.84650000	-1.06610000	5.35220000
Te	1.84650000	1.06610000	1.84110000



Orthographic projections: views of $NbTe_2$as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center). The primitive cell is also shown.

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