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Machine-learning correction to density-functional crystal structure optimization

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Abstract

Density functional theory is routinely applied to predict crystal structures. The most common exchange-correlation functionals used to this end are the Perdew-Burke-Ernzerhof (PBE) approximation and its variant PBEsol. We investigate the performance of these functionals for the prediction of lattice parameters and show how to enhance their accuracy using machine learning. Our dataset is constituted by experimental crystal structures of the Inorganic Crystal Structure Database matched with PBE-optimized structures stored in the materials project database. We complement these data with PBEsol calculations. We demonstrate that the accuracy and precision of PBE/PBEsol volume predictions can be noticeably improved *a posteriori* by employing simple, explainable machine learning models. These models can improve PBE unit cell volumes to match the accuracy of PBEsol calculations, and reduce the error of the latter with respect to experiment by 35 %. Further, the error of PBE lattice constants is reduced by a factor of 3–5. A further benefit of our approach is the implicit correction of finite temperature effects without performing phonon calculations.

Keywords: machine learning, crystallographic structure, predictive

1 Introduction

Computational high-throughput studies form the basis for the discovery of new materials in modern material science. In solid state physics, these studies are mostly performed within Kohn-Sham density functional theory (DFT) [1–3]. While DFT formally provides an exact description of the many-body Schrödinger equation, it relies in practice on approximations for the exchange-correlation energy. In solid-state physics, one commonly utilizes the Perdew-Burke-Ernzerhof's PBE functional [4]. While PBE and its variants are successful in predicting structural and electronic properties of solids, they may yield, nevertheless, non-negligible deviations from experiments. Specifically, PBE underestimates atomic bond lengths, thus, overestimating lattice constants [5–7] and volumes. Variants of PBE such as the PBE for solids (PBEsol) [8] were designed to improve upon this problem [9]. However, they still do not achieve the desired accuracy in comparison with experiments.

The correctness of the lattice constants and the corresponding unit cell volumes is indispensable for a reliable prediction of bulk electronic properties [10–12] and when considering experimental realizations of composite materials. For instance, the lattice mismatch between growth substrates and films can be a source of major problems in experiments. Another reason to focus on lattice parameters is the fact that this is the material property for which it is possible to find the largest amount of experimental data, collected in the Inorganic Crystal Structure Database (ICSD) [13].

In this work, we demonstrate that machine learning methods can improve the lattice volume predictions based on PBE/PBEsol without increasing the computational effort. Machine learning enjoyed over the past few years great success in a wide variety of applications [14] ranging from property predictions of bandgaps [15–17] and elastic moduli [18] to the stability analysis of crystals [19, 20] and molecular force field estimations [21]. Recently, the prediction of lattice constants and volumes generated much interest [22–30]. The majority of these studies is, however, limited to a particular crystal structure. In contrast to previous studies which are mainly based on direct calculations, we are building our approach on first-principles calculations, aiming at improving their accuracy in comparison with corresponding experiments. Our approach is not limited to a specific crystal structure or a subset of chemical elements. We will focus here on applying explainable machine learning methods [31, 32] to correct errors of PBE/PBEsol calculations of crystal structures of newly predicted materials. Specifically, we will employ model agnostic supervised local explanations (MAPLEs) [33] in combination with a random forest model [34] to combine the high accuracy of tree models for small datasets and the interpretability of MAPLE models.

Before diving into detail, we can observe in figure 1 the primitive unit cell volumes V_{pred} , predicted from DFT calculations using PBE and PBEsol functionals, plotted against the experimental unit cell volumes V_{exp} . We remark that the primitive cell volume is the simplest quantity that can be directly compared, independently of the specific details of the crystal structure and

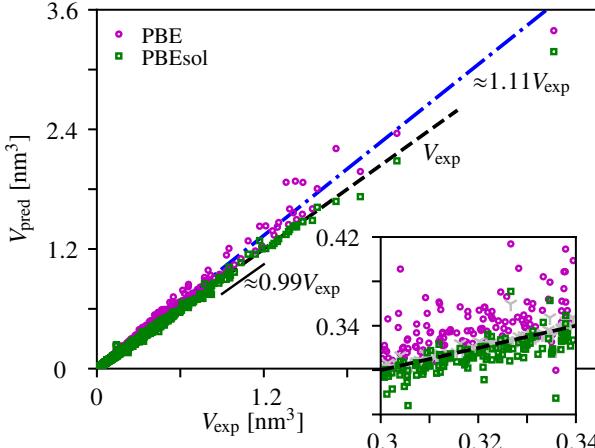
Machine-learning correction to density-functional crystal structure optimization


Fig. 1 (a) Correlation between measured primitive unit cell volumes V_{exp} and predicted ones V_{pred} . Ideal predictions match the black dashed line. The blue dash-dotted line depicts PBE's linear regression. The inset additionally considers the machine learning prediction $\text{pred} = \text{PBE+MAPLE}$ marked by gray tripods.

chemical composition. Their correlation gives a first impression about the accuracy (systematic error) and precision (variability) of the theoretically estimated unit cell volumes. Calculations with the PBE functional (magenta circles) significantly overestimates the measured volumes by roughly 11 %, while PBESol (green squares) provides a much better approximation of them.

On a closer look, one sees that V_{exp} constitutes a soft lower bound on the PBE volumes in the sense that about 90 % of the predicted volumes lay above it. This is a consequence of the tendency of PBE to underbind. This soft bound entails a skewness on the predicted PBE volume distribution, which we revisit later. The inset of figure 1 shows a close-up view of primitive unit cell volumes of about 0.32 nm^3 to better distinguish the individual data points. We additionally include in the inset the volumes obtained by correcting PBE calculations with machine learning (gray tripods) to anticipate visually the strong error reduction. We will discuss thoroughly the machine-learning corrections in the next sections.

The remaining article is organized as follows. In section 2, we present the employed machine learning models. Details on the experimental and theoretical datasets and their matching are discussed in Sec. 3. We analyze in section 4 our predictive models and compare their performance with the one of underlying DFT calculations. In section 5, we discuss the correction of the lattice constants. The last section is devoted to our conclusions.

2 Predictive models

Tree-ensemble-based models such as random forests [34] and gradient boosting [35, 36] are known to be suitable to the description of material properties for relatively small datasets [37, 38] but they are not restricted to them [39]. A drawback of employing multiple-decision trees is however their general lack of interpretability [32]. Appropriate combination with local linear models [40–42], as in model agnostic supervised local explanations (MAPLEs) [33], overcomes

4 Machine-learning correction to density-functional crystal structure optimization

this deficiency by providing local and example-based explanations. The former addresses causal relations between specific *input features* of an individual prediction (such as lattice constants) and its outcome by identifying their importances [33, 43, 44]. The latter asks instead for the contribution of specific *training points* [45–47].

In this work, we employ the MAPLE implementation of Plumb et al. [33] as well as tree models and utility functions from Ref. [48]. We evaluate the machine learning models by tenfold Monte-Carlo cross-validation. We choose this approach instead of using an independent testset, since our full dataset exhibits a large variance in structures/elements while being relatively small in size. In each independent run of the cross-validation scheme, the full dataset is randomly split at a ratio 1 : 9 without replacement into a test and a training set. The hyper-parameter optimization has been performed on a separate random splitting. Here, the number of trees forming the tree ensemble turns out to be the most important hyper parameter. The minimal number of samples controlling the splitting is of minor importance. The theoretical crystal structures calculated using DFT at the PBE and PBEsol level, respectively, serve as input parameters for the training, complemented with composition-specific features provided by Matminer [49].

By training the MAPLE models with the datasets discussed in Sec. 3, we find that the primitive-cell volume prediction is, indeed, to a large extent based on structural quantities, see Table A1 in the Appendix. Here, we use the average of the root-node impurity over the decision-tree ensemble as an estimator to quantify the relevance of the features. The binary splittings of an individual decision tree are such constructed that they minimize its impurity. In this sense, the first splitting and, therewith, the respective root-node feature has a major impact on the decision-tree structure and the model prediction. In particular, the splitting of the training set with respect to the root feature is in more than 50 % of the cases directly related to the crystal structure of the compounds, through, e.g., the volume V , the lattice constants a, b, c and the corresponding angles α, β, γ . Concerning the compositional features, the periodic table based features and averaged thermal properties of the elements play by far the largest role exceeding also two of the lattice angles in importance. Our models are available at Ref. [50].

3 Dataset

For our analysis and model training we consider roughly 2000 PBE-structures from the Materials Project (MP) [51]. The corresponding PBEsol calculations are available from Ref. [52]. The experimental crystal structures are extracted from the ICSD [13]. A mapping of ICSD- and MP-identifiers is provided in Table B2 of the Appendix.

We remark that experiments are conducted at finite temperature (2 K to 373 K) and pressure (≤ 1 bar) while DFT calculations describe equilibrium structures at zero temperature and pressure. In order to obtain PBE(sol)

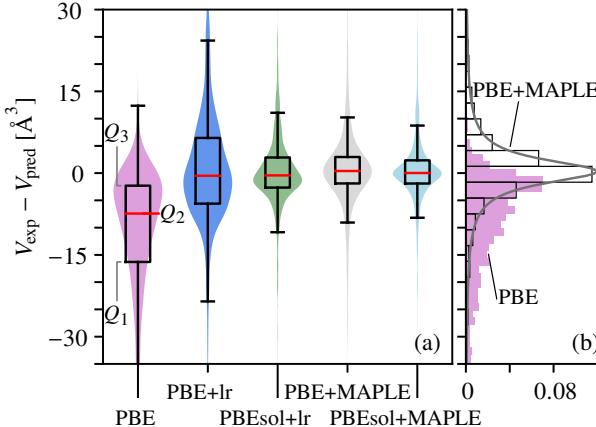


Fig. 2 Violin plot (a) and probability densities (b) of the volume residuals $V_{\text{exp}} - V_{\text{pred}}$ for the indicated test sets. The suffix ‘+lr’ indicates linear regression and Q_k is the k -th quartile.

crystal structures in the same thermodynamic conditions than experimental samples they should be corrected by expensive phonon calculations for thermal expansions and zero-point effects arising from finite lattice fluctuations [53–56]. For small molecules, the ambient pressure has additionally to be taken into account [57] but may be neglected for solids [53]. By training the predictive models on finite temperature volumes V_{exp} as target variables one has the advantage to implicitly include finite temperature corrections. In principle, the ambient temperature of the measurements could be included as an input parameter for machine learning. However it turns out that the resulting models are mostly independent of temperature, since the large majority of the experiments are performed at roughly the same temperature (about 293 K, median and mode). The mean value of the temperature distribution is indeed 271 K.

4 Volume predictions

In this section, we compare volume predictions obtained with various machine learning models. First, we give an overview of these predictions by discussing the central characteristics of their volume residuals. Then, we study their cross-validation error and address finally the convergence of the model training.

We show in figure 2(a) violin plots [58] of the volume residuals $V_{\text{exp}} - V_{\text{pred}}$. One sees clearly that the median of the DFT-PBE calculations (red line in magenta violin) of about $Q_2 \approx -7.4 \text{\AA}^3$ is, indeed, corrected by simple linear regression (blue violin). Also its interquartile range $\text{IQR} \equiv Q_3 - Q_1$ of about 14\AA^3 is roughly reduced by 2\AA^3 with the drawback that already well predicted volumes worsen. The skewness remains. Employing MAPLE cures the skewness and reduces the spreading further up to a third of the initial value (see gray violin). Intriguingly, its volume forecast is comparable to the simple linear regression prediction starting from PBEsol volumes. Beyond the median and the interquartile range, the violin shapes in Fig. 2(a) estimate the entire probability densities of the volume residuals. For the purpose of assessing their

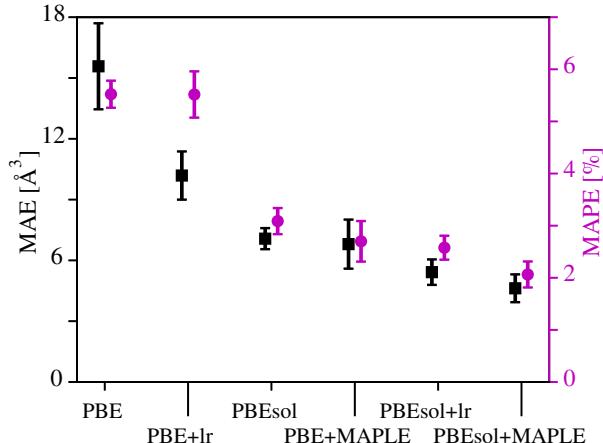


Fig. 3 Cross-validation errors for different models with standard deviations as error bars.

estimation quality, we compare the DFT-PBE estimate with the corresponding normalized histogram depicted in Fig. 2(b). The estimate captures well the curve progression but is less pronounced around its mode located at -1.3 \AA^3 . Additionally, we show in panel (b) the normalized histogram of the MAPLE prediction that corrects PBE volumes. As prefigured, it is considerably narrower and can be well approximated by a slightly biased Lorentzian (gray solid line) with a linewidth of roughly its interquartile range.

For a more quantitative comparison of the different models, we focus in the following on the cross-validation error. The cross-validation error of a specific model, is obtained by evaluating for each testset the error of its prediction with respect to the measured value, and taking the arithmetic mean of these errors. Additionally, we determine the standard deviation of the individual errors. As error metrics we chose the mean absolute error $\text{MAE} = \sum_{k=1}^n |y_{k,\text{exp}} - y_k| / n$ and the mean absolute percentage error $\text{MAPE} = 100 \sum_{k=1}^n |y_{k,\text{exp}} - y_k| / |ny_{k,\text{exp}}|$, where $y_{k,\text{exp}}$ (y_k) indicates the measured (predicted) property of the k -th sample. Since all experimental volumes are finite, MAPE is well defined. In figure 3, we show the cross-validation errors of the predicted primitive unit-cell volumes for different models. Their numerical mean values and standard deviations are listed in Table 1. As expected, DFT-PBE itself leads overall to the worst cross-validation errors while PBE corrected with linear regression (+lr) improves the MAE leaving the MAPE unchanged. The MAPLE model based on PBE volumes reduces the PBE-MAE by about 50 % and is slightly better than DFT-PBEsol volumes. However, PBEsol corrected with linear regression is once again better. Most importantly, the MAPLE model based on PBEsol shows the best MAE improving by roughly 35 % upon DFT calculations alone with this functional. The IQRs in Table 1 show the same tendency as the MAE and MAPE, supporting the conclusion regarding the possible improvements achievable with the MAPLE models. Additionally, we report therein the MAPLE models using the measured temperature as an input feature. They perform, however, very similarly to the models that do not

Machine-learning correction to density-functional crystal structure optimization

Table 1 Cross-validation errors of volume predictions and standard deviations for different DFT functionals and correction models. The superscript ‘*’ indicates the corresponding models including the temperature of the measurement as an additional feature.

model	MAE [\AA^3]		MAPE [%]		IQR [\AA^3]	
	mean	std	mean	std	mean	std
PBE	15.6	2.1	5.5	0.3	14.0	0.7
PBE+lr	10.2	1.2	5.5	0.4	11.9	1.1
PBEsol	7.1	0.5	3.1	0.3	6.9	0.7
PBE+MAPLE	6.8	1.2	2.7	0.4	5.1	0.8
PBE+MAPLE*	6.6	0.9	2.6	0.3	4.9	0.4
PBEsol+lr	5.4	0.6	2.6	0.2	5.5	0.5
PBEsol+MAPLE*	4.8	0.7	2.1	0.3	4.2	0.6
PBEsol+MAPLE	4.6	0.7	2.1	0.2	4.2	0.5

include such feature, as expected in view of the fact that most experiments were conducted at about the same temperature.

To assess the learning progress of the MAPLE models, we study in figure 4 the dependence of their MAE on the trainingset size n_{train} . The MAE’s are again obtained by tenfold cross-validation. As expected, they decrease polynomially with the trainingset size n_{train} [59, 60]. In particular, we find with $\text{MAE} \propto n_{\text{train}}^{-0.28}$ for PBE+MAPLE and $\text{MAE} \propto n_{\text{train}}^{-0.24}$ for PBEsol+MAPLE a similar learning behaviour for both predictive models. Including the total data available in the ICSD, the cross-validation error could be potentially reduced by 50 %. The relatively fast decay of the cross-validation errors with respect to the training-set size makes these correction procedures already applicable for small training sets. We would expect it to generalize to other material properties such as bulk moduli or formation energies for which very few experimental data are available and DFT results are a worse starting point.

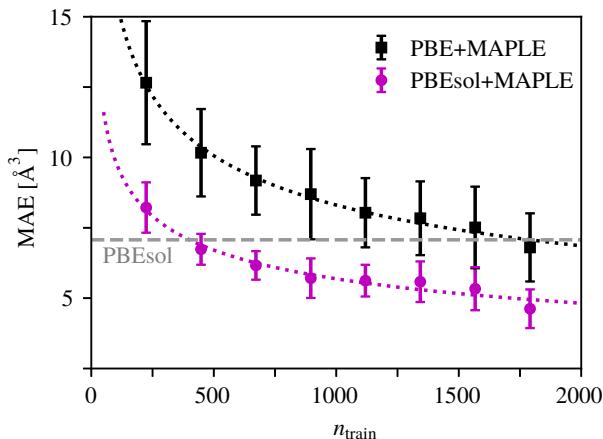


Fig. 4 Cross-validation errors for different models as a function of the training-set size n_{train} . The error bars indicate their standard deviation and the dotted lines correspond to their polynomial fit discussed in the main text. As reference, we indicate PBEsol’s MAE for the testset with the horizontal dashed line.

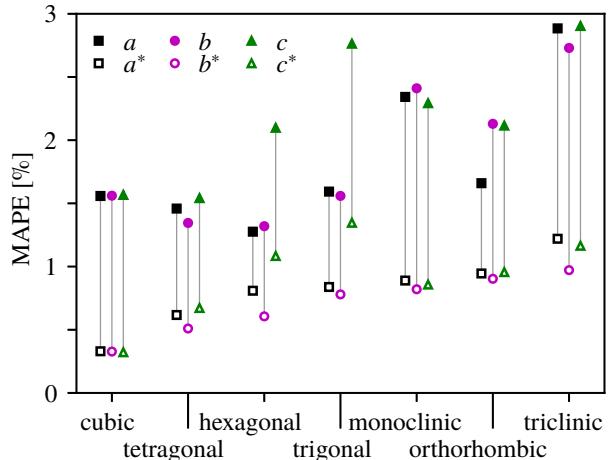


Fig. 5 Errors of the DFT-PBE lattice constants a , b , c and the rescaled ones a^* , b^* , c^* according to Eq. (1) with respect to experimental values from the ICSD for different crystal structures. The gray vertical lines serve as a guidance for the eye for tracking the individual improvements.

5 Lattice constants

This far, we have discussed volume corrections. To a certain extent, we can, therewith, also improve the lattice constants as we show in this section. To this end, we recall how the volume is calculated. The unit cell volume $V(\mathbf{a}, \mathbf{b}, \mathbf{c})$ is obtained from the triple product of the three lattice vectors \mathbf{a} , \mathbf{b} , \mathbf{c} and can be written as product $V = abc |\text{polsin}(\alpha, \beta, \gamma)|$ of a factor abc only depending on their lengths and a dimensionless factor $|\text{polsin}(\alpha, \beta, \gamma)|$ only depending on their interior angles.¹ The latter is for cubic crystal systems well predicted by PBE and PBEsol with a MAPE of the order of 0.02 % while lower symmetric systems does not exceed a MAPE of 0.6 %. Exploiting the simplification that all lattice constants coincide for cubic crystals, we can extract the lattice constant correction by the prescription

$$a \rightarrow a^* \equiv a \sqrt[3]{\frac{V_{\text{PBE(sol)}} + \text{MAPLE}}{V_{\text{PBE(sol)}}}} \quad (1)$$

for DFT calculations using PBE(sol). Therewith, the MAPE of the lattice vectors is roughly reduced by a factor of 5, see figure 5. If we use the same prescription as an approximate way to correct the lattice constants of non-cubic systems, we observe a consistent reduction of the MAPE of a factor of 3-5. In particular, we observe that when the three lattice parameters display different errors, the largest errors are those that get reduced more effectively, suppressing overall the MAPE of PBE lattice constants to less than 1 %.

¹The polar sine satisfies $\text{polsin}(\alpha, \beta, \gamma) \equiv \det([\mathbf{a}, \mathbf{b}, \mathbf{c}]) / abc = (1 + 2 \cos \alpha \cos \beta \cos \gamma - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma)^{1/2}$ [61].

6 Conclusions

We have investigated machine learning based unit cell volume corrections for density functional theory calculations. Model agnostic supervised local explanations improve both PBE’s and PBEsol’s volume prediction of the primitive unit cell. By applying MAPLE on PBE, one achieves overall improvements on the level of PBEsol calculations, hence, trivially reducing PBE’s volume deviations from experiments by about 50 %. This is of great convenience since all large solid state databases rely on PBE calculations. We provide our implementation at Ref. [50]. Furthermore, PBEsol+MAPLE outperforms PBEsol with a roughly 1.5 times smaller mean absolute error. The most relevant features contributing to the MAPLE models are, indeed, given by the lattice parameters calculated with DFT, while composition-specific features are significantly less important. A further benefit of our approach is the implicit correction of finite temperature effects rendering time-consuming phonon calculations unnecessary. Since the considered experiments are mostly performed at the same (room) temperature, our trained MAPLE models are, however, not expected to generalize well to other temperatures. We plan to address this point in future by training on datasets with a larger temperature variation.

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Declarations

The authors declare that there is no conflict of interest.

Appendix A Feature importances

The importance of the features for the MAPLE models is listed in Table A1.

Table A1 Most prominent feature importances for different MAPLE models. The superscript ‘*’ indicates the models using the measurement’s ambient temperature as an additional input parameter.

feature	importance [%]			
	PBE +MAPLE	PBEsol +MAPLE	PBE +MAPLE	PBEsol +MAPLE*
<i>V</i>	13.18	12.61	14.24	14.05
<i>b</i>	11.50	10.28	12.11	12.83
<i>a</i>	9.32	9.91	11.24	10.65
<i>c</i>	9.53	9.66	9.84	9.82
γ	5.61	6.58	5.80	6.82
mean melting point	6.81	6.54	6.52	6.67
mean group	6.07	6.09	4.93	4.34
mean block	5.40	5.36	5.46	5.59
maximum group	4.64	4.31	4.08	3.92
mean thermal conductivity	3.71	3.62	3.01	2.78
mean mendeleev number	3.37	3.35	3.65	3.67
β	2.63	2.94	2.74	2.58
α	2.03	2.39	1.84	2.19

Appendix B Mapping of crystal structures

The mapping between experimental structures stemming from ICSD and corresponding PBE structures from the materials project is listed hereafter in Table B2.

Table B2: Mapping between ICSD and MP entries.

composition	space group	MP-id	ICSD-id
AcBr ₃	P63/m	mp-27972	31578
AcCl ₃	P63/m	mp-27971	31569
AcClO	P4/nmm	mp-30273	31659
AcH ₂	Fm $\bar{3}$ m	mp-24147	56392
Ag(AuF ₄) ₂	P21/c	mp-18125	85416
Ag(Mo ₃ S ₄) ₂	R $\bar{3}$	mp-35109	605576
Ag(Mo ₃ Se ₄) ₂	R $\bar{3}$	mp-1103642	605584
Ag(TeMo) ₆	C2/m	mp-29607	40793
Ag ₂ F	P $\bar{3}$ m1	mp-1391	68438
Ag ₂ GeS ₃	Cmc21	mp-9900	41711
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Ag ₂ HgI ₄	I $\bar{4}$	mp-23485	25592
Ag ₂ HgO ₂	P43212	mp-29816	280333
Ag ₂ HgS ₂	P21/c	mp-9635	201713
Ag ₂ Mo ₂ O ₇	P $\bar{1}$	mp-27966	31027
Ag ₂ MoO ₄	Fd $\bar{3}$ m	mp-19318	238013
Ag ₂ O ₃	Fdd2	mp-546190	59193
Ag ₂ O	Pn $\bar{3}$ m	mp-353	247821
Ag ₂ PbO ₂	C2/c	mp-20210	24037
Ag ₂ PdCl ₄	Cmce	mp-28557	65239
Ag ₂ PdO ₂	Immm	mp-5495	51498
Ag ₂ SO ₃	P21/c	mp-30982	4433
Ag ₂ SO ₄	Fddd	mp-5625	27655
Ag ₂ S	P21/c	mp-610517	44507
Ag ₂ SeO ₃	P21/c	mp-16913	78388
Ag ₂ SeO ₄	Fddd	mp-11641	413089
Ag ₂ Se	P212121	mp-568936	260148
Ag ₂ Te ₂ O ₇	Imma	mp-13211	416281
Ag ₂ TeO ₃	P21/c	mp-18068	100694
Ag ₂ TeS ₃	Cc	mp-29163	85135
Ag ₂ Te	P21/c	mp-1592	73230
Ag ₂ W ₂ O ₇	P $\bar{1}$	mp-32537	31028
Ag ₃ AsS ₃	R3c	mp-4431	61806
Ag ₃ AsS ₄	Pmn21	mp-9538	86227
Ag ₃ AsSe ₃	R3c	mp-5145	76519
Ag ₃ BO ₃	R32	mp-27816	26521
Ag ₃ P ₁₁	Cm	mp-27821	26563
Ag ₃ PS ₄	Pmn21	mp-12459	416585
Ag ₃ PSe ₄	Pmn21	mp-30908	97760
Ag ₃ SBr	Cmcm	mp-1105645	174097
Ag ₃ SbS ₃	R3c	mp-4515	64986
Ag ₃ Sb	Pmm2	mp-2273	38820
Ag ₃ SnP ₇	P21/m	mp-29849	411041
Ag ₃ Sn	Pmmn	mp-611	154084
Ag ₅ (PbO ₃) ₂	P $\bar{3}$ 1m	mp-22286	155043
Ag ₅ IO ₆	R $\bar{3}$ c	mp-554648	415893
Ag ₅ SbS ₄	Cmc21	mp-4004	16987
Ag ₅ TePO ₄	P4/nmm	mp-1191803	420343
AgAs(SeF ₂) ₃	C2/m	mp-1191037	418700
AgAsSe ₂	R $\bar{3}$ m	mp-4483	20087
AgAuF ₄	I4/mcm	mp-16060	90071
AgBF ₄	Pnma	mp-12021	415320
AgBi(PS ₃) ₂	P $\bar{1}$	mp-556434	170639
AgBi(PSe ₃) ₂	R $\bar{3}$	mp-569126	195334

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AgBi(WO ₄) ₂	C2/m	mp-1192345	190732
AgBi ₂ F ₁₂	P $\bar{1}$	mp-28965	79879
AgBi ₃ S ₅	C2/m	mp-23474	200110
AgBiO ₃	R $\bar{3}$	mp-23548	89432
AgBiS ₂	R $\bar{3}$ m	mp-29678	44340
AgBr	Fm $\bar{3}$ m	mp-23231	65061
AgClO ₄	I $\bar{4}2$ m	mp-22993	9629
AgCl	Fm $\bar{3}$ m	mp-22922	64734
AgF ₂	P21/c	mp-7715	20453
AgF ₂	Pbca	mp-2284	6277
AgF	Fm $\bar{3}$ m	mp-7592	18008
AgH ₃ BrN	P21/m	mp-1102571	169137
AgHg ₃ SbO ₆	R $\bar{3}$ c	mp-12362	170764
AgIO ₄	I41/a	mp-30037	52380
AgI	P63mc	mp-22894	56553
AgI	P63mc	mp-580941	1899
AgI	F $\bar{4}3$ m	mp-22925	56552
AgNO ₂	Imm2	mp-5770	26750
AgNO ₃	R3c	mp-552185	374
AgP ₂	P21/c	mp-8200	35283
AgPPd ₅	P4/mmm	mp-1078079	605631
AgPPt ₅	P4/mmm	mp-1025385	605633
AgPdF ₆	P $\bar{1}$	mp-31215	51507
AgSb ₂ F ₁₂	P $\bar{1}$	mp-14653	65186
AgSbS ₂	C2/c	mp-3922	85130
AgSbTe ₂	P4/mmm	mp-12359	170662
AgSbTe ₂	R $\bar{3}$ m	mp-12360	170663
AgSnF ₆	P $\bar{1}$	mp-10809	51505
AgTe ₃	Im $\bar{3}$ m	mp-28246	37186
AgTe ₄ Au	P2/c	mp-3291	30874
Al ₂ (SO ₄) ₃	R $\bar{3}$	mp-4417	73249
Al ₂ CdS ₄	I $\bar{4}$	mp-5928	83526
Al ₂ CoO ₄	Fd $\bar{3}$ m	mp-36447	290133
Al ₂ FeO ₄	Fd $\bar{3}$ m	mp-30084	187920
Al ₂ O ₃	R $\bar{3}$ c	mp-1143	31545
Al ₂ S ₃	P61	mp-2654	73220
Al ₂ Te ₃	P21/c	mp-29502	406353
Al ₂ ZnO ₄	Fd $\bar{3}$ m	mp-2908	196109
Al ₂ ZnS ₄	Fd $\bar{3}$ m	mp-4842	35380
Al ₃ Ni ₂	P $\bar{3}$ m1	mp-1057	191103
Al ₅ Co ₂	P63/mmc	mp-196	109470
AlAgO ₂	P63/mmc	mp-9631	300020
AlAgO ₂	Pna21	mp-11794	99688

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AlAgS ₂	I $\bar{4}$ 2d	mp-5782	604692
AlAgSe ₂	I $\bar{4}$ 2d	mp-14091	604704
AlAgTe ₂	I $\bar{4}$ 2d	mp-14092	28746
AlAs	F $\bar{4}$ 3m	mp-2172	656315
AlBr ₃	P21/c	mp-23288	39768
AlCuO ₂	R $\bar{3}$ m	mp-3748	60844
AlCuS ₂	I $\bar{4}$ 2d	mp-4979	42124
AlCuSe ₂	I $\bar{4}$ 2d	mp-8016	28734
AlH ₁₂ (ClO ₂) ₃	R $\bar{3}$ c	mp-23743	22071
AlI ₃	P21/c	mp-30930	391247
AlN	P63mc	mp-661	602460
AlPO ₄	P3221	mp-3955	50100
AlP	F $\bar{4}$ 3m	mp-1550	52649
AlSb	F $\bar{4}$ 3m	mp-2624	609288
Ar	Fm $\bar{3}$ m	mp-23155	24788
As ₂ O ₃	Fd $\bar{3}$ m	mp-2184	409611
As ₂ O ₅	P212121	mp-1788	987
As ₂ Os	Pnnm	mp-2455	238253
As ₂ S ₃	P21/c	mp-641	15239
As ₂ Se ₃	P21/c	mp-909	44058
AsH ₉ C ₂ S(NO) ₄	P $\bar{1}$	mp-1200478	173457
AsI ₃	R $\bar{3}$	mp-23218	56571
AsS	P21/c	mp-542810	15238
As	R $\bar{3}$ m	mp-11	16516
Au ₂ O ₃	Fdd2	mp-27253	8014
Au ₂ Se ₂ O ₇	Pba2	mp-28095	37009
AuBrF ₆	P21	mp-30159	93481
AuCl ₃	P21/c	mp-27647	5467
AuClO	R $\bar{3}$	mp-27265	8190
B(HO) ₃	P $\bar{1}$	mp-23791	61354
B ₂ O ₃	P3121	mp-306	16021
B ₆ P	R $\bar{3}$ m	mp-28395	62748
BAsH ₄ NO ₄ F	Cc	mp-1191775	420517
BAsPbO ₅	P31	mp-22430	404328
BN	P63/mmc	mp-984	241875
BN	F $\bar{4}$ 3m	mp-1639	77271
BP	F $\bar{4}$ 3m	mp-1479	602964
B	R $\bar{3}$ m	mp-160	431643
Ba(AgGe) ₂	I4/mmm	mp-13910	25318
Ba(AgS) ₂	P $\bar{3}$ m1	mp-8579	50183
Ba(AuO ₂) ₂	I41/a	mp-9297	80327
Ba(CuS) ₂	Pnma	mp-5970	89573
Ba(NO ₃) ₂	Pa $\bar{3}$	mp-4396	35495

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Ba(P ₂ Au) ₂	Fddd	mp-1104130	425778
Ba(SbAu) ₂	P21/m	mp-570298	416298
Ba(ZnAs) ₂	I4/mmm	mp-570198	417000
Ba ₂ InBiS ₅	Cmc21	mp-864638	261678
Ba ₂ MnZn ₂ (AsO) ₂	I4/mmm	mp-19045	85659
Ba ₂ Pb	Pnma	mp-21246	416561
Ba ₂ ScFeAsO ₃	P4/nmm	mp-862301	420654
Ba ₂ SiO ₄	Pnma	mp-17612	291359
Ba ₂ Sn	Pnma	mp-1981	416562
Ba ₂ TaInO ₆	Fm $\bar{3}$ m	mp-1079630	261480
Ba ₂ ThCu ₂ Se ₅	C2/m	mp-1078405	195762
Ba ₂ TiO ₄	Pna21	mp-554529	29389
Ba ₃ MgTa ₂ O ₉	P $\bar{3}$ m1	mp-6325	240279
BaAg ₂	Imma	mp-1077322	240052
BaAgSb	P63/mmc	mp-1205316	56981
BaAgTeF	P4/nmm	mp-16742	419382
BaAg	Pnma	mp-11840	57342
BaAl ₂ O ₄	P63	mp-4202	291360
BaAu ₂	P6/mmm	mp-30363	260669
BaAu	Pnma	mp-570775	419559
BaBSbS ₄	Pnma	mp-866301	248221
BaBiBS ₄	C2/m	mp-861618	248222
BaBiClO ₂	Cmcm	mp-552806	79532
BaCO ₃	Pnma	mp-5504	166090
BaCl ₂	Pnma	mp-23199	262674
BaCu ₂ GeS ₄	P3121	mp-17947	10006
BaCu ₂ SnSe ₄	Ama2	mp-12364	170857
BaCuTeF	P4/nmm	mp-13287	245624
BaF ₂	Fm $\bar{3}$ m	mp-1029	64717
BaGe ₂	Pnma	mp-2139	409260
BaH ₂	Pnma	mp-23715	400343
BaHgS ₂	Pmc21	mp-28007	251739
BaI ₂	P $\bar{6}$ 2m	mp-568536	36210
BaLaAgSe ₃	Cmcm	mp-1101818	659172
BaMoO ₄	I41/a	mp-19276	194082
BaNdAgS ₃	Cmcm	mp-1095616	659170
BaO ₂	I4/mmm	mp-1105	80750
BaO	Fm $\bar{3}$ m	mp-1342	616005
BaPAu	P63/mmc	mp-985439	420340
BaPb ₃	R $\bar{3}$ m	mp-21446	419973
BaPb	Cmcm	mp-20136	58664
BaPrO ₃	Pnma	mp-22705	163752
BaSO ₄	Pnma	mp-3164	190065

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BaS	Fm $\bar{3}$ m	mp-1500	52690
BaSbAu	P63/mmc	mp-568895	280954
BaSe	Fm $\bar{3}$ m	mp-1253	52696
BaSi ₂	Pnma	mp-1477	185375
BaSn ₃ Au	I4mm	mp-1068048	238018
BaSn ₃	P63/mmc	mp-7759	419206
BaSnO ₃	Pm $\bar{3}$ m	mp-3163	239582
BaTeMo ₂ O ₉	P21	mp-19049	281503
BaTe	Fm $\bar{3}$ m	mp-1000	616165
BaUO ₄	Pbcm	mp-5611	239547
BaZnSO	Cmcm	mp-548469	171239
Be ₂ Ag	Fd $\bar{3}$ m	mp-603	57347
BeBr ₂	Ibam	mp-30139	92584
BeF ₂	P3121	mp-15951	261194
BeH ₂	Ibam	mp-768203	655664
BeI ₂	I41/acd	mp-30140	92587
BeO	P63mc	mp-2542	391224
BeSe	F $\bar{4}3$ m	mp-1541	616419
BeTe	F $\bar{4}3$ m	mp-252	616439
Be	P63/mmc	mp-87	1425
Bi ₂ CO ₅	Imm2	mp-30200	252588
Bi ₂ O ₃	P $\bar{4}21$ c	mp-23195	189995
Bi ₂ O ₃	P21/c	mp-23262	94229
Bi ₂ S ₃	Pnma	mp-22856	153946
Bi ₂ Se ₃	R $\bar{3}$ m	mp-541837	165226
Bi ₂ Te ₃	R $\bar{3}$ m	mp-34202	193330
BiBrO	P4/nmm	mp-23072	61225
BiCl ₃	Pnma	mp-22908	2866
BiClO	P4/nmm	mp-22939	195115
BiI ₃	R $\bar{3}$	mp-22849	53634
BiIO	P4/nmm	mp-22987	391354
BiI	C2/m	mp-27708	1558
BiSBr	Pnma	mp-23324	31389
BiSCl	Pnma	mp-23318	100173
BiSI	Pnma	mp-23514	23631
BiSeBr	Pnma	mp-569707	76649
BiSeI	Pnma	mp-23020	280311
Bi	R $\bar{3}$ m	mp-23152	64705
CNCl	C2/c	mp-571324	86484
CSCl ₂	P21/c	mp-554711	300291
C	P63/mmc	mp-48	230104
C	Fd $\bar{3}$ m	mp-66	190650
Ca(AuO ₂) ₂	I41/a	mp-2898	79801

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Ca(BO ₂) ₂	Pbcn	mp-3417	62430
Ca(CoGe) ₂	I4/mmm	mp-4259	81751
Ca(GaP) ₂	P63/mmc	mp-1078849	422525
Ca(GeIr) ₂	I4/mmm	mp-16259	52755
Ca(GeRu) ₂	I4/mmm	mp-19791	52761
Ca(InP) ₂	P63/mmc	mp-1079772	260562
Ca(MnSb) ₂	P $\bar{3}$ m1	mp-4150	41789
Ca(NiGe) ₂	I4/mmm	mp-2949	81755
Ca(PRh) ₂	I4/mmm	mp-8580	50185
Ca ₂ AgPd ₂	Immm	mp-1068053	429172
Ca ₂ AuN	Cmcm	mp-29175	85528
Ca ₂ CdPt ₂	Immm	mp-1069824	424554
Ca ₂ Co ₁₂ P ₇	P $\bar{6}$	mp-10923	94410
Ca ₂ FeN ₂	C2/m	mp-28770	72389
Ca ₂ GePd ₂	Fdd2	mp-1078326	251662
Ca ₂ MgPd ₂	Immm	mp-1068035	429174
Ca ₂ P ₂ O ₇	P21/c	mp-17922	22225
Ca ₂ PN ₃	Cmce	mp-8977	72532
Ca ₂ PbAu ₂	P4/mbm	mp-20723	409531
Ca ₂ Pb	Pnma	mp-30478	58920
Ca ₂ Si ₃ Ag	Fmmm	mp-29570	410522
Ca ₂ Si	Pnma	mp-2517	158275
Ca ₂ SnGe ₂	P4/mbm	mp-1078274	193226
Ca ₂ SnO ₄	Pbam	mp-4747	173626
Ca ₂ SnS ₄	Pnma	mp-866503	429695
Ca ₂ Sn	Pnma	mp-22735	659611
Ca ₂ V ₂ O ₇	P $\bar{1}$	mp-27614	421266
Ca ₂ VN ₃	C2/c	mp-17892	409644
Ca ₃ (BO ₃) ₂	R $\bar{3}$ c	mp-3575	23664
Ca ₃ (PO ₄) ₂	R $\bar{3}$ m	mp-3487	188081
Ca ₃ Al ₇ Ag ₂	R $\bar{3}$ m	mp-11430	104173
Ca ₃ Au ₄	R $\bar{3}$	mp-12699	54547
Ca ₃ Au	Pnma	mp-30366	58401
Ca ₃ C ₃ Cl ₂	Cmcm	mp-28160	33818
Ca ₃ GeO	Imma	mp-17193	413383
Ca ₃ MnN ₃	Cmcm	mp-14763	67888
Ca ₃ PCl ₃	Pm $\bar{3}$ m	mp-29342	202075
Ca ₃ SnO	Pm $\bar{3}$ m	mp-29241	100787
Ca ₃ Ti ₂ O ₇	Cmc21	mp-4163	259358
Ca ₃ UO ₆	R $\bar{3}$	mp-14252	35457
Ca ₃ V ₂ O ₈	C2/m	mp-1182001	412273
Ca ₄ In ₂ N	I41/amd	mp-20419	62535
Ca ₄ IrO ₆	R $\bar{3}$ c	mp-4100	81902

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Ca ₄ PdO ₆	R $\bar{3}$ c	mp-10299	88134
Ca ₄ Sb ₂ O	I4/mmm	mp-13660	16353
Ca ₅ Au ₄	P21/c	mp-571264	58406
Ca ₅ Si ₃	I4/mcm	mp-793	93699
Ca ₇ (H ₆ Cl) ₂	P $\bar{6}$	mp-984055	420927
CaAg ₂	Imma	mp-13270	417225
CaAgP	P $\bar{6}2$ m	mp-12277	10016
CaAgSb	Pnma	mp-11214	56982
CaAg	Cmcm	mp-538	57352
CaAl ₂	Fd $\bar{3}$ m	mp-2404	418966
CaAl ₄ O ₇	C2/c	mp-4867	14270
CaAu ₂	Imma	mp-443	55542
CaB ₆	Pm $\bar{3}$ m	mp-865	196516
CaBr ₂	Pnnm	mp-22888	56763
CaC ₂	I4/mmm	mp-2482	54186
CaCN ₂	R $\bar{3}$ m	mp-4124	418451
CaCO ₃	R $\bar{3}$ c	mp-3953	52151
CaCO ₃	Pnma	mp-4626	252901
CaCdAu	Pnma	mp-569628	420574
CaCdPt	Pnma	mp-1103046	426610
CaCl ₂	Pnnm	mp-23214	246416
CaCl ₂	Pbcn	mp-571642	56769
CaCoSi	P4/nmm	mp-1018658	428148
CaCuO ₂	P4/mmm	mp-4826	75868
CaF ₂	Fm $\bar{3}$ m	mp-2741	82707
CaFeO ₃	Pnma	mp-19115	92341
CaGaAu	Pnma	mp-11811	106273
CaH ₁₂ CO ₉	C2/c	mp-504880	195904
CaH ₂	Pnma	mp-23713	260873
CaH ₄ SO ₆	C2/c	mp-23690	92567
CaH ₆ C ₂ O ₇	P $\bar{1}$	mp-559469	159351
CaIn ₂ Au	Cmcm	mp-22602	408882
CaIn ₂ Pd	Cmcm	mp-22717	408881
CaIn ₄ Rh	Pmma	mp-21220	410891
CaInAu	Pnma	mp-20378	408579
CaMg(CO ₃) ₂	R $\bar{3}$	mp-6459	31333
CaMg ₂ N ₂	P $\bar{3}$ m1	mp-5795	79123
CaMg ₂ Ni ₉	R $\bar{3}$ m	mp-12695	54520
CaMg ₂	P63/mmc	mp-2432	412683
CaMgAsO ₄ F	C2/c	mp-7035	56862
CaMgPd	Pnma	mp-1102662	426616
CaMgSiO ₄	Pnma	mp-6493	202280
CaMnGe	P4/nmm	mp-20235	66956

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CaMnO ₃	Pnma	mp-19201	189134
CaMnSb ₂	P4/nmm	mp-21131	52705
CaMoO ₄	I41/a	mp-19330	194078
CaNbO ₃	Pnma	mp-4957	51202
CaNi ₅	P6/mmm	mp-774	54474
CaNiGe ₂	Cmcm	mp-13512	240342
CaO	Fm $\bar{3}$ m	mp-2605	261847
CaPPt	Pmc21	mp-28339	60826
CaPtO ₃	Cmcm	mp-4784	173278
CaRuO ₃	Pnma	mp-20947	165689
CaSO ₄	P6222	mp-3082	159702
CaSO ₄	Cmcm	mp-4406	183919
CaS	Fm $\bar{3}$ m	mp-1672	603165
CaSe	Fm $\bar{3}$ m	mp-1415	52788
CaSi ₂	R $\bar{3}$ m	mp-2700	193539
CaSi ₃ Ir	I4mm	mp-1068653	181447
CaSi ₃ Pt	I4mm	mp-1069604	181448
CaSi ₇ Ir ₃	R $\bar{3}$ c	mp-1191649	181449
CaSiNi ₂	P63/mmc	mp-10797	412411
CaSiO ₃	P $\bar{1}$	mp-4428	98727
CaSi	Cmcm	mp-1563	190659
CaSn ₂ Ir	Cmcm	mp-11957	410773
CaSnAu	Imm2	mp-1071278	195943
CaSnO ₃	Pnma	mp-4438	193658
CaSn	Cmcm	mp-2450	165193
CaTcO ₃	Pnma	mp-1188853	261342
CaTi ₂ O ₄	Cmcm	mp-3463	51183
CaTiO ₃	Pnma	mp-4019	180956
CaUO ₄	R $\bar{3}$ m	mp-3960	239453
CaV ₂ O ₅	Pmmn	mp-19305	82689
CaV ₂ O ₆	C2/m	mp-27624	21064
CaVO ₃	Pnma	mp-22608	88978
CaWO ₄	I41/a	mp-19426	5510
CaZn ₅	P6/mmm	mp-1734	418614
CaZnF ₄	I41/a	mp-5104	31366
CaZnSO	P63mc	mp-7204	245309
CaZrO ₃	Pnma	mp-4571	97463
Cd(AgI ₂) ₂	I42m	mp-1025377	190587
Cd(AuF ₄) ₂	P4/mcc	mp-29169	85413
Cd(CO ₂) ₂	P21/c	mp-555064	170029
Cd(GaS ₂) ₂	I $\bar{4}$	mp-4452	31354
Cd(GaSe ₂) ₂	I $\bar{4}$	mp-3772	30908
Cd(GaTe ₂) ₂	I $\bar{4}$	mp-13949	25646

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Cd(InS ₂) ₂	Fd $\bar{3}$ m	mp-559200	252372
Cd(InSe ₂) ₂	P $\bar{4}2$ m	mp-568032	151953
Cd(InSe ₂) ₂	I $\bar{4}$	mp-22304	151954
Cd ₂ AgAu	Fm $\bar{3}$ m	mp-31170	57337
CdAg	Pm $\bar{3}$ m	mp-2642	604907
CdAs ₂	I4122	mp-471	609931
CdCN ₂	R $\bar{3}$ m	mp-10969	95264
CdCO ₃	R $\bar{3}$ c	mp-4385	156740
CdCl ₂	R $\bar{3}$ m	mp-22881	86440
CdCu ₂ GeS ₄	Pmn21	mp-13982	26150
CdCu ₂ GeSe ₄	I $\bar{4}2$ m	mp-10967	95235
CdGeAs ₂	I $\bar{4}2$ d	mp-4953	42098
CdGeP ₂	I $\bar{4}2$ d	mp-3668	100467
CdHg ₄ (AsI ₂) ₂	P21	mp-570838	416973
CdI ₂	P $\bar{3}$ m1	mp-567259	43852
CdP ₄	P21/c	mp-7904	25605
CdSO ₄	Pmn21	mp-5679	100317
CdS	P63mc	mp-672	154186
CdSb ₂ Se ₃ Br ₂	C2/m	mp-567556	159464
CdSb	Pbca	mp-1321	52830
CdSe	P63mc	mp-1070	415785
CdSe	F $\bar{4}3$ m	mp-2691	187310
CdSiAs ₂	I $\bar{4}2$ d	mp-3078	22187
CdSiP ₂	I $\bar{4}2$ d	mp-4666	23696
CdSnAs ₂	I $\bar{4}2$ d	mp-3829	44258
CdSnO ₃	R $\bar{3}$	mp-754329	181930
CdSnP ₂	I $\bar{4}2$ d	mp-5213	44257
CdTe	F $\bar{4}3$ m	mp-406	161693
CdWO ₄	P2/c	mp-19387	248753
Ce(GeRh) ₂	I4/mmm	mp-5577	425230
Ce(PO ₃) ₃	C2221	mp-5843	240880
Ce(SiAu) ₂	I4/mmm	mp-5173	418530
Ce(SiAu ₂) ₂	Cmmm	mp-569496	418529
Ce(SiIr) ₂	P4/nmm	mp-21900	411678
Ce(SiPt) ₂	P4/nmm	mp-22438	61370
Ce(ZnAu ₂) ₂	I4/mmm	mp-1077954	426150
Ce ₂ CoSi ₃	P6/mmm	mp-20355	83895
Ce ₂ Ga ₁₀ Pd	I4/mmm	mp-12746	150461
Ce ₂ InGe ₂	P4/mbm	mp-20959	415108
Ce ₂ MgGe ₂	P4/mbm	mp-22511	413849
Ce ₂ Mo ₂ C ₃	C2/m	mp-13263	417827
Ce ₂ O ₃	P $\bar{3}$ m1	mp-2721	621706
Ce ₂ Si ₃ Rh	P6/mmm	mp-31163	164827

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Ce ₃ (Si ₄ Ni) ₂	Cmmm	mp-504613	16497
CeAgSb ₂	P4/nmm	mp-510280	79425
CeAgSn	P63mc	mp-31420	55819
CeB ₆	Pm $\bar{3}$ m	mp-21343	194311
CeBi ₂ Au	P4/nmm	mp-1078370	238705
CeC ₂	I4/mmm	mp-2839	17022
CeCd ₂ Ag	Fm $\bar{3}$ m	mp-31173	57363
CeClO	P4/nmm	mp-22952	412069
CeCoGeH	P4/nmm	mp-644499	98944
CeCoSi ₂	Cmcm	mp-7095	16501
CeCrGe ₃	P63/mmc	mp-20650	158977
CeCrS ₂ O	C2/m	mp-551214	14191
CeCrSe ₂ O	C2/m	mp-19375	54075
CeCuSO	P4/nmm	mp-635469	96344
CeCuSi	P63/mmc	mp-22740	173221
CeCuSn	P63mc	mp-22683	156394
CeGa ₆ Pd	P4/mmm	mp-580215	240161
CeGe ₃ Ir	I4mm	mp-13122	161868
CeGe ₃ Rh	I4mm	mp-13121	161867
CeGeAu	P63mc	mp-4219	57176
CeGeIr	Pnma	mp-20022	414509
CeIn ₂ Ir	Cmcm	mp-21278	414474
CeIn ₅ Rh	P4/mmm	mp-20294	150226
CeInAg ₂	Fm $\bar{3}$ m	mp-672191	57372
CeInIr	P $\bar{6}$ 2m	mp-20449	100002
CeInPd	P $\bar{6}$ 2m	mp-21387	59883
CeInPt	P $\bar{6}$ 2m	mp-640922	418186
CeMgPt	P $\bar{6}$ 2m	mp-19934	412400
CeMgSi ₂	I41/amd	mp-3545	246387
CeMnNi ₄	F43m	mp-5951	262477
CeMnSi	P4/nmm	mp-505331	85850
CeO ₂	Fm $\bar{3}$ m	mp-20194	184584
CePRuO	P4/nmm	mp-21372	80201
CeSi ₂ Ir ₃	Imma	mp-13475	79221
CeSi ₂ Mo ₂ C	P4/mmm	mp-1018666	189334
CeSi ₃ Ru	I4mm	mp-13120	161866
CeSiHRu	P4/nmm	mp-604496	161825
CeSiIr	P213	mp-21441	413854
CeSnIr	P $\bar{6}$ 2m	mp-20835	415903
CeSnPd	P $\bar{6}$ 2m	mp-19766	416969
CeSnPd	Pnma	mp-21490	106418
CeVO ₄	I41/amd	mp-19214	157326
CeZnPd	P $\bar{6}$ 2m	mp-13382	420208

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CeZnSbO	P4/nmm	mp-22620	85449
Cl ₂ O ₇	C2/c	mp-31050	63680
Cl ₂ O	I41/amd	mp-29537	407768
ClF ₃	Pnma	mp-556767	19079
ClF	P21/c	mp-29504	406442
ClO ₂	Pbca	mp-23207	67663
Co(PdSe) ₂	Ibam	mp-12464	416513
Co(SbO ₃) ₂	P42/mnm	mp-21908	203094
Co ₂ As	P $\bar{6}$ 2m	mp-18206	69999
Co ₂ B	I4/mcm	mp-493	5924
Co ₂ P ₂ O ₇	C2/m	mp-20283	74542
Co ₂ Te ₃ O ₈	C2/c	mp-18855	50702
Co ₃ (SnS) ₂	R $\bar{3}$ m	mp-19807	173764
Co ₃ C ₂ (SeO ₅) ₂	C2/m	mp-552260	56465
Co ₃ Sb ₄ (OF) ₆	I $\bar{4}$ 3m	mp-1105290	427045
Co ₃ Se ₄ (ClO ₅) ₂	C2/m	mp-1105151	425433
Co ₉ S ₈	Fm $\bar{3}$ m	mp-1513	40046
CoAgO ₂	P63/mmc	mp-1106049	261608
CoAs ₂	P21/c	mp-2715	174220
CoAs	Pnma	mp-583	48027
CoCO ₃	R $\bar{3}$ c	mp-21434	61066
CoCu ₂ GeS ₄	I $\bar{4}$ 2m	mp-6498	415927
CoCu ₂ SiS ₄	I $\bar{4}$ 2m	mp-11769	193981
CoCu ₂ SnS ₄	I $\bar{4}$ 2m	mp-11770	99294
CoCu ₂ SnSe ₄	I $\bar{4}$ 2m	mp-11771	99296
CoF ₂	P42/mnm	mp-555908	280604
CoF ₃	R $\bar{3}$ c	mp-559473	235863
CoH ₂ SO ₅	C2/c	mp-643547	71346
CoH ₂ SeO ₄	P21/c	mp-505469	408100
CoH ₂ SeO ₅	C2/c	mp-23967	66747
CoH ₄ (CO ₃) ₂	C2/c	mp-24296	59927
CoH ₄ (ClO) ₂	C2/m	mp-23853	22082
CoH ₆ (SeO ₄) ₂	P21/c	mp-744574	75134
CoH ₈ (IO ₅) ₂	P21/c	mp-25486	408060
CoH ₉ (CN ₂) ₃	R $\bar{3}$	mp-24037	2560
CoMoH ₂ SeO ₇	P $\bar{1}$	mp-866480	249955
CoMoP	Pnma	mp-22262	2421
CoP ₂ (H ₄ O ₅) ₂	P21/c	mp-24536	67490
CoP ₃	Im $\bar{3}$	mp-1944	92393
CoP ₄ (H ₅ O ₈) ₂	P $\bar{1}$	mp-696788	31310
CoP ₄ H ₁₆ (NO ₈) ₂	P $\bar{1}$	mp-24300	170045
CoPH ₁₆ NO ₁₀	Pmn21	mp-758833	170042
CoP	Pnma	mp-22270	43249

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CoPdO ₂	R̄3m	mp-18919	31917
CoPtO ₂	R̄3m	mp-1283971	31916
CoS ₂	Pā3	mp-2070	86351
CoSO ₄	Pnma	mp-19379	74161
CoSbS	Pmn21	mp-4962	40044
CoSbS	Pbca	mp-1191202	40045
CoSiH ₁₂ (OF) ₆	R̄3	mp-24122	2900
CoSi	P213	mp-7577	260982
CoSn	P6/mmm	mp-20536	55564
CoTeMoO ₆	P21212	mp-551806	93795
Cr(AgO ₂) ₂	Pnma	mp-542882	16298
Cr(CO) ₆	Pnma	mp-683501	59895
Cr(PO ₃) ₃	C2/c	mp-555540	56874
Cr ₂ (SO ₄) ₃	R̄3	mp-19361	150417
Cr ₂ Ag ₂ O ₇	P̄1	mp-562364	2433
Cr ₂ AgTe ₄	Fd̄3m	mp-20118	71695
Cr ₂ CuSe ₄	Fd̄3m	mp-3880	87477
Cr ₂ FeO ₄	Fd̄3m	mp-20168	250575
Cr ₂ HgO ₄	Fd̄3m	mp-21074	245275
Cr ₂ HgSe ₄	Fd̄3m	mp-5602	402408
Cr ₂ N	P̄31m	mp-8780	67400
Cr ₂ NiO ₄	Fd̄3m	mp-19303	84377
Cr ₂ O ₃	R̄3c	mp-19399	167291
Cr ₂ SiO ₄	Fddd	mp-18800	89069
Cr ₂ TeO ₆	P42/mnm	mp-21355	93212
Cr ₃ C ₂	Pnma	mp-20937	151477
Cr ₃ P	Ī4	mp-7806	23560
Cr ₃ Si	Pm̄3n	mp-729	53218
CrAgO ₂	R̄3m	mp-19378	4149
CrAgSe ₂	R3m	mp-3532	42397
CrAgTe ₂	R3m	mp-1018084	605002
CrB	Cmcm	mp-260	44249
CrBr ₂	C2/m	mp-567624	23903
CrCl ₂	Pnnm	mp-22857	192942
CrCl ₃	C2/m	mp-27630	22080
CrCl ₃	R̄3	mp-567504	22081
CrClO	Pmmn	mp-22946	4086
CrCuO ₂	R̄3m	mp-510625	163255
CrCuO ₂	P63/mmc	mp-505562	82065
CrCuS ₂	R3m	mp-5862	100594
CrF ₅	Pbcm	mp-639662	419661
CrFeO ₃	R̄3	mp-1078458	252042
CrGeTe ₃	R̄3	mp-541449	79268

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CrHgO ₄	P21/c	mp-19155	2224
CrHgO ₄	Cmcm	mp-19380	416147
CrInO ₃	Pnma	mp-756147	185586
CrO ₂	P42/mnm	mp-19177	167237
CrO ₃	Ama2	mp-510421	16031
CrP ₂	C2/m	mp-7291	2526
CrP ₄	C2/c	mp-7302	2790
CrPO ₄	Cmcm	mp-18906	62159
CrP	Pnma	mp-21048	43247
CrPb ₂ O ₅	C2/m	mp-22373	710043
CrPbO ₄	P21/c	mp-19146	40920
CrPdO ₂	R̄3m	mp-1063607	193885
CrSb ₂	Pnnm	mp-22498	42601
CrSi ₂	P6222	mp-1222	161434
CrSiTe ₃	R̄3	mp-3779	626809
CrWO ₄	Cmmm	mp-18785	8269
Cs ₂ AgBiBr ₆	Fm̄3m	mp-1078250	291597
Cs ₂ AgBiCl ₆	Fm̄3m	mp-1078258	291598
Cs ₂ Cd ₃ Te ₄	Ibam	mp-567386	90369
Cs ₂ Co ₃ S ₄	Ibam	mp-558911	65254
Cs ₂ CoSiO ₄	Cmc21	mp-542168	93878
Cs ₂ Hg ₃ I ₈	Cm	mp-540574	4074
Cs ₂ IrCl ₆	Fm̄3m	mp-28651	69142
Cs ₂ KCuF ₆	Fm̄3m	mp-6968	59102
Cs ₂ KU ₂ (Si ₂ O ₇) ₂	Cmmm	mp-862811	249936
Cs ₂ MgP ₄ (HO ₂) ₈	P̄1	mp-866620	260151
Cs ₂ MnV ₂ (BrO ₃) ₂	Cmm2	mp-572800	418761
Cs ₂ O ₃	Ī43d	mp-1213719	11275
Cs ₂ O	R̄3m	mp-7988	27919
Cs ₂ P ₂ H ₂ O ₇	C2/c	mp-643074	72982
Cs ₂ PdC ₂	P̄3m1	mp-505824	94396
Cs ₂ PdCl ₄	P4/mmm	mp-30314	95813
Cs ₂ PtC ₂	P̄3m1	mp-505825	94397
Cs ₂ SO ₄	Pnma	mp-505782	203160
Cs ₂ SnBr ₆	Fm̄3m	mp-641923	158957
Cs ₂ SnCl ₆	Fm̄3m	mp-608555	9023
Cs ₂ TeBr ₆	Fm̄3m	mp-23405	65058
Cs ₂ TeI ₆	Fm̄3m	mp-540957	38105
Cs ₂ Ti(AgS ₂) ₂	P42/mcm	mp-10488	280645
Cs ₂ UCl ₆	P̄3m1	mp-23077	202332
Cs ₂ VAgS ₄	Fddd	mp-8684	50460
Cs ₂ Zr(SiO ₃) ₃	P63/m	mp-6694	171578
Cs ₃ AuO	P63/mmc	mp-505212	78365

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Cs ₃ Bi ₂ Br ₉	P $\bar{3}$ m1	mp-27544	1142
Cs ₃ Bi ₂ I ₉	P63/mmc	mp-624214	23124
Cs ₃ Sb ₂ Br ₉	P $\bar{3}$ m1	mp-579560	39824
Cs ₃ Sb ₂ I ₉	P63/mmc	mp-23029	84989
Cs ₃ Sb	Fm $\bar{3}$ m	mp-10378	53243
CsAg ₃ S ₂	C2/m	mp-561902	1033
CsAg ₃ Se ₂	C2/m	mp-16234	52558
CsAgBr ₂	Cmcm	mp-23454	150301
CsAgCl ₂	Cmcm	mp-542772	37086
CsAgO	I4/mmm	mp-8666	25745
CsAsH ₆ (CSe) ₂	C2/c	mp-866612	171201
CsAu ₂ F ₇	C2/c	mp-554737	152057
CsAu ₃ S ₂	P $\bar{3}$ m1	mp-9384	82540
CsAu ₃ Se ₂	P $\bar{3}$ m1	mp-9386	82542
CsAuCl ₄	C2/c	mp-1095499	423233
CsAuSe	Cmcm	mp-574599	71655
CsAu	Pm $\bar{3}$ m	mp-2667	58427
CsBr	Pm $\bar{3}$ m	mp-22906	236387
CsCOF ₃	P21/c	mp-14734	69971
CsCSN	Pnma	mp-614311	60875
CsCeS ₂	R $\bar{3}$ m	mp-7015	73533
CsClO ₄	Pnma	mp-30206	63364
CsCl	Pm $\bar{3}$ m	mp-22865	257260
CsCoCl ₃	P63/mmc	mp-504708	27511
CsCoF ₃	R $\bar{3}$ m	mp-556943	410389
CsCr ₅ Se ₈	C2/m	mp-505149	73146
CsErZnSe ₃	Cmcm	mp-7155	280844
CsFeCl ₃	P63/mmc	mp-29400	300249
CsGeCl ₃	R3m	mp-22988	62557
CsH ₂ CO ₃	P21/c	mp-696986	39365
CsK ₂ CoO ₂	I4/mmm	mp-551244	74889
CsK ₂ PdF ₅	P4/mbm	mp-8959	72301
CsK ₂ Sb	Fm $\bar{3}$ m	mp-581024	53237
CsLaHgSe ₃	Cmcm	mp-11124	281441
CsLiCl ₂	P4/nmm	mp-23364	35397
CsLiCl ₂	C2/c	mp-1188344	423634
CsLiH ₄ SO ₅	Cm	mp-755891	200780
CsLiSO ₄	P21/c	mp-6726	63183
CsMgAs(H ₆ O ₅) ₂	F $\bar{4}$ 3m	mp-1193046	260150
CsMgCl ₃	P63/mmc	mp-23004	54167
CsMgP(H ₆ O ₅) ₂	F $\bar{4}$ 3m	mp-761178	281563
CsMnCl ₃	R $\bar{3}$ m	mp-23336	2555
CsNiCl ₃	P63/mmc	mp-22950	59371

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CsPH ₄ (NO) ₂	P43212	mp-767240	50237
CsPbBr ₃	Pnma	mp-567629	97851
CsScCl ₃	P63/mmc	mp-27359	10474
CsSmCdSe ₃	Cmcm	mp-510062	281436
CsSmHgSe ₃	Cmcm	mp-7212	281445
CsSmZnSe ₃	Cmcm	mp-505709	280840
CsSnBr ₃	Pm $\bar{3}$ m	mp-27214	4071
CsSnCl ₃	P21/c	mp-27394	14199
CsSnl ₃	Pnma	mp-568570	69996
CsTbZnTe ₃	Cmcm	mp-638078	170190
CsTeAu	Pmma	mp-573755	71653
CsTi ₂ Cl ₇	P21/m	mp-505663	411140
CsTiCl ₃	P63/mmc	mp-28283	49748
CsVCl ₃	P63/mmc	mp-22977	15932
CsWCl ₆	C2/c	mp-30974	1242
CsYCdSe ₃	Cmcm	mp-11116	281433
CsYHgSe ₃	Cmcm	mp-11123	281440
CsYZnSe ₃	Cmcm	mp-574620	280847
CsZn ₂ P ₂ HO ₈	Cmce	mp-699213	73955
Cu(HO) ₂	Cmc21	mp-505105	68459
Cu(IO ₃) ₂	P21	mp-27234	4327
Cu(IrS ₂) ₂	Fd $\bar{3}$ m	mp-15065	75531
Cu ₂ Ag(SeO ₅) ₂	C2/m	mp-1104157	65437
Cu ₂ Ag ₂ O ₃	I41/amd	mp-4362	51672
Cu ₂ AgPS ₄	Pmn21	mp-1105189	195307
Cu ₂ GeO ₄	I41/amd	mp-9600	100796
Cu ₂ GeS ₃	Cc	mp-15252	85138
Cu ₂ GeSe ₃	Imm2	mp-4728	160386
Cu ₂ GeSe ₃	Cc	mp-677105	192171
Cu ₂ GeTe ₃	Imm2	mp-12806	151872
Cu ₂ O	Pn $\bar{3}$ m	mp-361	172174
Cu ₂ P ₂ O ₇	C2/c	mp-3638	67316
Cu ₂ SO ₅	C2/m	mp-4386	61513
Cu ₂ S	P43212	mp-618991	16550
Cu ₂ Sb	P4/nmm	mp-1825	412295
Cu ₂ Se	Fm $\bar{3}$ m	mp-16366	56025
Cu ₂ SiS ₃	Cc	mp-15895	88235
Cu ₂ SiSe ₃	Cc	mp-15896	88236
Cu ₂ SnS ₃	Cc	mp-10519	91762
Cu ₂ SnSe ₃	Cc	mp-11658	97966
Cu ₂ SnTe ₃	Imm2	mp-13089	160882
Cu ₂ Te	P6/mmm	mp-1861	77055
Cu ₂ WS ₄	P $\bar{4}$ 2m	mp-8976	72529

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Cu ₂ WS ₄	I $\bar{4}$ 2m	mp-557373	98909
Cu ₃ (PO ₄) ₂	P $\bar{1}$	mp-4093	68811
Cu ₃ AsS ₄	Pmn21	mp-3345	413350
Cu ₃ AsSe ₄	I $\bar{4}$ 2m	mp-675626	610361
Cu ₃ N	Pm $\bar{3}$ m	mp-1933	40056
Cu ₃ PS ₄	Pmn21	mp-3934	412240
Cu ₃ PSe ₄	Pmn21	mp-5756	95412
Cu ₃ P	P63cm	mp-7463	15056
Cu ₃ SbS ₄	I $\bar{4}$ 2m	mp-5702	412239
Cu ₃ SbSe ₄	I $\bar{4}$ 2m	mp-9814	400652
CuAgO ₂	C2/m	mp-7237	95089
CuAgS	Pnma	mp-5014	66581
CuAgS	Cmcm	mp-8911	30233
CuAgTe ₂	Pmm2	mp-2977	42482
CuBS ₂	I $\bar{4}$ 2d	mp-12954	156413
CuBi(PSe ₃) ₂	P $\bar{3}$ 1c	mp-569715	195341
CuBiSeO	P4/nmm	mp-23116	189174
CuBr	F $\bar{4}$ 3m	mp-22913	78274
CuCl	F $\bar{4}$ 3m	mp-22914	78270
CuI	F $\bar{4}$ 3m	mp-22895	33724
CuP ₂	P21/c	mp-927	35282
CuPN ₂	I $\bar{4}$ 2d	mp-1078469	194793
CuPS ₃	P42/mnm	mp-1105187	430200
CuSO ₄	Pnma	mp-20525	259687
CuSbPbS ₃	Pmn21	mp-649774	427413
CuSbS ₂	Pnma	mp-4468	418753
CuSbSe ₂	Pnma	mp-20331	418754
CuSe ₂ Cl	P21/c	mp-31038	68292
CuSe ₂ O ₅	C2/c	mp-3199	603
CuSiO ₃	Pmma	mp-16053	89669
CuTe ₂ Cl	P21/c	mp-30971	641
CuTe ₂ I	P21/c	mp-31037	67253
CuTeO ₃	Pnma	mp-20977	29338
CuTeO ₄	P21/c	mp-22420	1672
CuWO ₄	P $\bar{1}$	mp-22773	182753
Cu	Fm $\bar{3}$ m	mp-30	7954
Dy ₂ Fe ₂ Si ₂ C	C2/m	mp-11705	67467
Dy ₂ O ₃	Ia $\bar{3}$	mp-2345	248578
Dy ₃ Co ₆ Sn ₅	Immm	mp-20703	152094
Dy ₃ GaCoS ₇	P63	mp-1192256	426875
Dy ₅ BiAu ₂	I4/mcm	mp-1181507	156957
Dy ₅ SbAu ₂	I4/mcm	mp-1181498	156952
DyAg ₂	I4/mmm	mp-2618	604335

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DyAgGe	P $\bar{6}$ 2m	mp-567574	81557
DyAgPb	P63mc	mp-510687	107106
DyAgSb ₂	P4/nmm	mp-10965	95133
DyAgSe ₂	P212121	mp-1181462	605083
DyAgSn	P63mc	mp-21198	418582
DyAgTe ₂	P $\bar{4}$ 21m	mp-4024	605089
DyAg	Pm $\bar{3}$ m	mp-2167	191694
DyCl ₃	Cmcm	mp-28448	40064
DyCoSn	Pnma	mp-22228	54584
DyCrO ₄	I41/amd	mp-18754	93788
DyCu ₄ Ag	F $\bar{4}$ 3m	mp-1072033	605006
DyCuS ₂	Pnma	mp-555044	172847
DyCuSn	P63mc	mp-22188	55581
DyFe ₂ SiC	Cmcm	mp-568668	40773
DyInAg ₂	Fm $\bar{3}$ m	mp-20898	57382
DySiAg	P $\bar{6}$ 2m	mp-1095130	605085
Er(CoSi) ₂	I4/mmm	mp-3239	55758
Er ₂ C(NO) ₂	P $\bar{3}$ m1	mp-6574	416880
Er ₂ CoSi ₂	C2/m	mp-568728	99214
Er ₂ MnC ₄	Ibam	mp-9267	73169
Er ₂ O ₃	Ia $\bar{3}$	mp-679	55832
Er ₂ ReC ₂	Pnma	mp-20799	69099
Er ₃ (CuSi) ₄	Immm	mp-5454	55650
Er ₃ CoSi ₃	C2/m	mp-568196	152534
Er ₃ GaCoS ₇	P63	mp-1191530	426877
Er ₅ BiAu ₂	I4/mcm	mp-1181438	156959
Er ₅ SbAu ₂	I4/mcm	mp-1188308	156954
Er ₆ CoTe ₂	P $\bar{6}$ 2m	mp-1079725	260931
ErAg ₂	I4/mmm	mp-30339	58252
ErAgSe ₂	P212121	mp-4044	15302
ErAgSn	P $\bar{6}$ 2m	mp-13265	417551
ErAgTe ₂	P $\bar{4}$ 21m	mp-12902	154791
ErAg	Pm $\bar{3}$ m	mp-2621	167893
ErCoC ₂	Amm2	mp-13501	55571
ErCoO ₃	Pnma	mp-562779	172049
ErCuS ₂	Pnma	mp-12454	172849
ErHCl	R $\bar{3}$ m	mp-24051	203143
ErIn ₅ Co	P4/mmm	mp-12872	153908
ErInAg ₂	Fm $\bar{3}$ m	mp-30340	58254
ErSCl	Pmmn	mp-27616	21009
ErSiAg	P62m	mp-1084844	605116
Eu(Ag ₂ Sb) ₂	R $\bar{3}$ m	mp-1078223	424312
Eu(CoP) ₂	I4/mmm	mp-20038	47200

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Eu(CuSn) ₂	C2/m	mp-1069357	182050
Eu(DySe ₂) ₂	Pnma	mp-645690	418589
Eu(GeAu) ₂	I4/mmm	mp-1068398	421997
Eu(SiAg) ₂	I4/mmm	mp-22653	605133
Eu(TmSe ₂) ₂	Pnma	mp-542964	418593
Eu ₂ H ₃ Cl	P $\bar{3}$ m1	mp-1018693	427476
EuAg ₅	P6/mmm	mp-542568	236629
EuAgAs	P63/mmc	mp-21330	24365
EuAgBi	P63/mmc	mp-23378	604830
EuAgP	P63/mmc	mp-20482	52567
EuCl ₂	Pnma	mp-22887	22039
EuCl ₃	P63/m	mp-569895	23148
EuCuSb	P63/mmc	mp-22292	422620
EuHCl	P4/nmm	mp-1070860	428162
Fe ₂ (SO ₄) ₃	P21/c	mp-540894	31341
Fe ₂ B	I4/mcm	mp-1915	391328
Fe ₂ CuGe ₂	Pmma	mp-21141	62330
Fe ₂ P	P $\bar{6}$ 2m	mp-778	246858
Fe ₂ SiO ₄	Pnma	mp-20313	10409
Fe ₃ C	Pnma	mp-510623	99002
Fe ₃ P	I $\bar{4}$	mp-18708	43365
FeAgO ₂	R $\bar{3}$ m	mp-19225	31919
FeAgO ₂	P63/mmc	mp-18966	2786
FeB	Pnma	mp-20787	391329
FeBr ₂	P $\bar{3}$ m1	mp-22880	409571
FeBr ₃	R $\bar{3}$	mp-23232	410924
FeCO ₃	R $\bar{3}$ c	mp-18969	21485
FeCl ₃	R $\bar{3}$	mp-23204	39764
FeClO	Pmmn	mp-540828	16013
FeCuO ₂	R $\bar{3}$ m	mp-510281	191496
FeCuS ₂	I $\bar{4}$ 2d	mp-3497	261882
FeF ₂	P42/mnm	mp-556911	9166
FeF ₃	R $\bar{3}$ c	mp-22398	235864
FeH ₄ (CO ₃) ₂	C2/c	mp-698316	161344
FeO	Fm $\bar{3}$ m	mp-1283030	180972
FeP ₂	Pnnm	mp-20027	15027
FeP	Pnma	mp-1005	43248
FeS ₂	Pa $\bar{3}$	mp-226	109377
FeSe	P63/mmc	mp-1090	169252
FeSi	P213	mp-871	41997
FeTe ₂	Pnnm	mp-19880	86518
FeWO ₄	P2/c	mp-19421	64733
Ga ₂ HgS ₄	I $\bar{4}$	mp-4809	67220

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Ga ₂ HgSe ₄	I $\bar{4}$	mp-4730	83712
Ga ₂ O ₃	R $\bar{3}$ c	mp-1243	27431
Ga ₂ S ₃	Cc	mp-539	409550
GaAg ₂	P $\bar{6}2m$	mp-578	151174
GaAgO ₂	Pna21	mp-1105293	193540
GaAgS ₂	I $\bar{4}2d$	mp-5342	605187
GaAgSe ₂	I $\bar{4}2d$	mp-5518	52570
GaAgTe ₂	I $\bar{4}2d$	mp-4899	71007
GaAs	F $\bar{4}3m$	mp-2534	107946
GaBr ₃	P21/c	mp-30953	413456
GaCl ₃	C2/m	mp-30952	413455
GaCuCl ₄	P $\bar{4}2c$	mp-29362	300103
GaCuI ₄	I $\bar{4}$	mp-29403	400817
GaCuO ₂	R $\bar{3}m$	mp-4280	60846
GaCuS ₂	I $\bar{4}2d$	mp-5238	66864
GaCuSe ₂	I $\bar{4}2d$	mp-4840	42097
GaCuTe ₂	I $\bar{4}2d$	mp-3839	74456
GaHCl ₂	C2/c	mp-1190111	165558
GaHgCl ₄	P1	mp-1103091	413579
GaI ₃	P21/c	mp-30954	413457
GaN	P63mc	mp-804	157398
GaP	F $\bar{4}3m$	mp-2490	77087
GaS	P63/mmc	mp-2507	173940
GaSb	F $\bar{4}3m$	mp-1156	635318
GaSe	P63/mmc	mp-1943	63122
GaTeCl	Pnnm	mp-27449	15582
GaTe	C2/m	mp-542812	8249
Gd(CrSi) ₂	I4/mmm	mp-610787	67472
Gd(SiAg) ₂	I4/mmm	mp-21287	605276
Gd ₂ CCl ₂	P3m1	mp-29394	400348
Gd ₂ CF ₂	P $\bar{3}m1$	mp-8301	33912
Gd ₂ CuO ₄	I4/mmm	mp-4860	65015
Gd ₂ Mo ₂ C ₃	C2/m	mp-12039	409822
Gd ₂ O ₃	Ia $\bar{3}$	mp-504886	184590
Gd ₃ Al ₇ Ag ₂	R $\bar{3}m$	mp-637182	99069
GdAg ₂	I4/mmm	mp-19783	104473
GdAgGe	P $\bar{6}2m$	mp-9341	605263
GdAg	Pm $\bar{3}m$	mp-542779	58265
GdCl ₃	P63/m	mp-23265	22270
GdClO	P4/nmm	mp-23050	59232
GdInAu	P $\bar{6}2m$	mp-1080496	104011
GdRuC ₂	Cmcm	mp-582826	80312
GdSnAu	P63mc	mp-20434	416419

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GeAs ₂	Pbam	mp-17524	23872
GeAs	C2/m	mp-9548	86361
GeH ₃ Cl	Cmc21	mp-28369	62109
GeO ₂	P42/mnm	mp-470	92551
GeS	Pnma	mp-2242	1256
GeSe ₂	P21/c	mp-540625	425644
GeSe	Pnma	mp-700	41738
Ge	Fd $\bar{3}$ m	mp-32	184252
H ₁₀ C ₂ N ₂ O ₅	P21212	mp-697408	64925
H ₃ CS	P21/c	mp-559204	249028
H ₃ NCl	Pa $\bar{3}$	mp-1200750	23145
H ₄ CSN ₂	P21/c	mp-23993	955
H ₄ NCl	P $\bar{4}$ 3m	mp-34337	428519
H ₄ NF	P63mc	mp-23794	23766
H ₅ ClO ₂	P21/c	mp-24381	15353
H ₈ S(NO ₂) ₂	Pna21	mp-24468	266695
Hf ₂ Ag ₃ F ₁₄	C2/m	mp-28550	65178
Hf ₂ CuSb ₃	P $\bar{4}$ m2	mp-19928	93243
Hf ₄ CuSi ₄	C2/m	mp-1079688	421374
HfBrN	Pmmn	mp-568346	95720
HfC	Fm $\bar{3}$ m	mp-21075	159873
HfCl ₄	P2/c	mp-29422	402054
HfCuGe	I4/mmm	mp-1077453	290194
HfCuSn	P63mc	mp-1018713	190121
HfF ₄	C2/c	mp-31033	66008
HfGaAu	P $\bar{6}$ m2	mp-12952	156265
HfInCu ₂	Fm $\bar{3}$ m	mp-600125	54594
HfNCl	R $\bar{3}$ m	mp-541911	261541
HfO ₂	P21/c	mp-352	173158
HfS ₂	P $\bar{3}$ m1	mp-985829	601164
HfSe ₂	P $\bar{3}$ m1	mp-985831	195308
Hg(AuF ₄) ₂	P4/mcc	mp-29170	85414
Hg ₂ P ₃ Cl	C2/c	mp-28875	74771
Hg ₂ PCl ₂	C2/m	mp-29679	50594
Hg ₂ SO ₄	P2/c	mp-7461	248726
Hg ₃ (ClO) ₂	P21/c	mp-22999	2137
Hg ₃ (SCl) ₂	I213	mp-23418	28159
HgBr	I4/mmm	mp-23177	23721
HgCl ₂	Pnma	mp-22855	76648
HgCl	I4/mmm	mp-22897	65441
HgF	I4/mmm	mp-706	72354
HgI ₂	P42/nmc	mp-23192	181575
HgI	I4/mmm	mp-22859	262368

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HgO	Pnma	mp-1224	14124
HgSO ₄	Pmn21	mp-3228	100316
HgS	P3121	mp-634	81923
HgS	F $\bar{4}$ m	mp-1123	81917
HgSeO ₃	P21/c	mp-557224	412547
HgSe	F $\bar{4}$ 3m	mp-820	290038
Ho(CuGe) ₂	I4/mmm	mp-4539	627697
Ho(CuSi) ₂	I4/mmm	mp-4105	55786
Ho ₂ CF ₂	P $\bar{3}$ m1	mp-9006	56887
Ho ₂ Co ₁₂ P ₇	P $\bar{6}$	mp-3706	84086
Ho ₂ O ₃	Ia $\bar{3}$	mp-812	82422
Ho ₅ BiAu ₂	I4/mcm	mp-1188851	156958
Ho ₅ SbAu ₂	I4/mcm	mp-1181047	156953
Ho ₆ GaCo ₂	Immm	mp-11844	102434
HoAg ₂	I4/mmm	mp-2120	605354
HoAgSn	P63mc	mp-4311	418581
HoAgTe ₂	P $\bar{4}$ 21m	mp-12904	154795
HoAg	Pm $\bar{3}$ m	mp-2778	605351
HoCoO ₃	Pnma	mp-20570	172048
HoCrO ₄	I41/amd	mp-19076	169872
HoCrO ₄	I41/a	mp-19055	169873
HoCuS ₂	Pnma	mp-12453	172848
HoGa ₅ Co	P4/mmm	mp-4856	655672
HoInAg ₂	Fm $\bar{3}$ m	mp-30342	58280
ICl	P21/c	mp-567998	411014
In(GaAu) ₂	P63/mmc	mp-1080559	190987
In ₂ Ag	I4/mcm	mp-19974	58282
In ₂ HgSe ₄	I $\bar{4}$	mp-20731	25649
In ₂ HgTe ₄	I $\bar{4}$	mp-19765	25652
In ₂ S ₃	I41/amd	mp-22216	183879
In ₂ Se ₃	R $\bar{3}$ m	mp-20830	640498
In ₅ AgTe ₈	P $\bar{4}$ 2m	mp-569813	151871
InAg(PS ₃) ₂	P $\bar{3}$ 1c	mp-22661	202185
InAg(PSe ₃) ₂	P $\bar{3}$ 1c	mp-20902	71968
InAg ₃	Pm $\bar{3}$ m	mp-30343	58283
InAgO ₂	R $\bar{3}$ m	mp-22660	202429
InAgS ₂	I $\bar{4}$ 2d	mp-19833	51617
InAgS ₂	Pna21	mp-21459	52578
InAgSe ₂	I $\bar{4}$ 2d	mp-20554	52583
InAgTe ₂	I $\bar{4}$ 2d	mp-22386	236191
InAs	F $\bar{4}$ 3m	mp-20305	41444
InBi ₂ S ₄ Cl	C2/m	mp-559521	484
InBi ₂ Se ₄ Br	C2/m	mp-571169	159465

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InBr ₃	C2/m	mp-570219	65198
InBr	Cmcm	mp-22870	62239
InCl	P213	mp-23276	2429
InCl	Cmcm	mp-571555	425449
InCo ₃ SnS ₂	R̄3m	mp-1077901	425136
InCuO ₂	R̄3m	mp-20930	91058
InCuS ₂	Ī42d	mp-22736	186714
InCuSe ₂	Ī42d	mp-22811	252780
InCuTe ₂	Ī42d	mp-22261	74460
InI	Cmcm	mp-23202	65464
InN	P63mc	mp-22205	109463
InPS ₄	Ī4	mp-20790	1699
InP	F̄3m	mp-20351	41443
InS	Pnnm	mp-19795	81338
InSb ₂ S ₄ Br	C2/m	mp-559864	159467
InSb ₂ S ₄ Cl	C2/m	mp-556541	159468
InSb ₂ Se ₄ Br	C2/m	mp-570321	159466
InSb	F̄43m	mp-20012	162196
InSe	R3m	mp-22691	23002
Ir(Cl ₂ F ₃) ₂	P21/c	mp-29870	411351
IrCl ₃	Fddd	mp-568208	25716
IrO ₂	P42/mnm	mp-2723	84577
K(CuSe) ₂	Ī4/mmm	mp-567657	98403
K(In ₃ Au ₂) ₂	P̄6m2	mp-567545	249520
K(InAu ₂) ₂	Ī4/mcm	mp-21134	249221
K(SnAu) ₃	Pmmn	mp-570936	249645
K ₂ AgAs	Cmcm	mp-7642	1154
K ₂ AgF ₄	P21/c	mp-1104293	421461
K ₂ Au ₃	Immm	mp-8700	65113
K ₂ BiAu	Cmcm	mp-1084770	380341
K ₂ CN ₂	C2/m	mp-10408	411094
K ₂ CO ₃	P21/c	mp-3963	66943
K ₂ CO ₃	C2/c	mp-554072	662
K ₂ Ca(CO ₃) ₂	R̄3m	mp-6494	29442
K ₂ Co(SeO ₃) ₂	R̄3m	mp-19189	71536
K ₂ CoH ₄ (SeO ₅) ₂	P̄1	mp-644334	98686
K ₂ CoP ₂ (H ₃ O ₄) ₂	C2/m	mp-1188582	59884
K ₂ CoP ₄ (HO ₂) ₈	P̄1	mp-1195899	261585
K ₂ CoSe ₂	Ibam	mp-8768	67390
K ₂ CrO ₄	Pnma	mp-19232	2402
K ₂ Cu ₂ Te ₅	Cmcm	mp-29828	280533
K ₂ CuP	Cmcm	mp-8446	61082
K ₂ Ge ₂ PbS ₆	C2/c	mp-561132	170601

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K ₂ Hg ₃ (GeS ₄) ₂	C2	mp-11131	281506
K ₂ La ₂ Ti ₃ O ₁₀	I4/mmm	mp-6548	74193
K ₂ MgCl ₄	I4/mmm	mp-27207	4035
K ₂ OsCl ₆	Fm $\bar{3}$ m	mp-23533	68764
K ₂ PAuS ₄	P21/m	mp-9509	85679
K ₂ PAu	Cmcm	mp-9687	300201
K ₂ PHO ₄	Pna21	mp-733468	74543
K ₂ PdCl ₄	P4/mmm	mp-22956	65034
K ₂ PdCl ₆	Fm $\bar{3}$ m	mp-23067	65037
K ₂ PtCl ₄	P4/mmm	mp-22934	2722
K ₂ PtCl ₆	Fm $\bar{3}$ m	mp-23513	280465
K ₂ ReCl ₆	Fm $\bar{3}$ m	mp-22947	68763
K ₂ RuCl ₆	Fm $\bar{3}$ m	mp-23471	8055
K ₂ SO ₄	Pnma	mp-4529	79781
K ₂ SbAu	Cmcm	mp-867335	380340
K ₂ Si ₂ O ₅	Cc	mp-29825	280480
K ₂ Si ₄ O ₉	P63/m	mp-8380	31201
K ₂ Sn(AuS ₂) ₂	P $\bar{1}$	mp-557121	74022
K ₂ SnCl ₆	Fm $\bar{3}$ m	mp-23499	604
K ₂ TcCl ₆	Fm $\bar{3}$ m	mp-27632	22096
K ₂ TeI ₆	P21/c	mp-27688	23649
K ₂ V ₂ CoO ₇	P $\bar{4}21$ m	mp-1190373	195619
K ₂ VAgS ₄	Fddd	mp-8900	66840
K ₂ WCl ₆	Fm $\bar{3}$ m	mp-568914	409840
K ₂ ZnTe ₂	Ibam	mp-12535	420088
K ₃ Ag ₃ As ₂	R $\bar{3}$ m	mp-14206	32016
K ₃ AuO	Pm $\bar{3}$ m	mp-9200	79086
K ₃ Cr(HO) ₆	R $\bar{3}$ c	mp-504994	62653
K ₃ Cu(CN) ₄	R3c	mp-6610	36070
K ₃ Cu ₂ F ₇	I4/mmm	mp-20982	15373
K ₃ Cu ₃ P ₂	R $\bar{3}$ m	mp-7439	12163
K ₃ Ge ₄ Au	Pmmn	mp-17112	413728
K ₃ Sb	P63/mmc	mp-14017	656327
K ₃ Sb	Fm $\bar{3}$ m	mp-10159	44677
K ₄ Ge ₂ Au ₇	R $\bar{3}$ m	mp-9201	79111
K ₅ CuSb ₂	R $\bar{3}$ m	mp-27999	32032
K ₆ CdTe ₄	P63mc	mp-17698	420087
KAg ₂ PS ₄	I $\bar{4}2$ m	mp-12532	420033
KAg ₃ Se ₂	C2/m	mp-9782	402643
KAgO	I4/mmm	mp-3074	37324
KAgSe	P4/nmm	mp-16236	52586
KAs ₄ BrO ₆	P6/mmm	mp-23083	16890
KAu ₂	P63/mmc	mp-30401	58520

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KAu ₅	P6/mmm	mp-1298	106286
KAuS	Cmcm	mp-7077	202178
KAuSe	Cmcm	mp-9881	40759
KB ₆	Pm $\bar{3}$ m	mp-1076	98985
KBr	Fm $\bar{3}$ m	mp-23251	187220
KCO ₂	Pbam	mp-560616	165561
KCeS ₂	R $\bar{3}$ m	mp-7329	351
KClO ₃	P21/m	mp-23022	31120
KClO ₄	Pnma	mp-23526	35111
KCl	Fm $\bar{3}$ m	mp-23193	165593
KCo(PO ₃) ₃	P $\bar{6}$ c2	mp-1192408	193216
KCoF ₃	Pm $\bar{3}$ m	mp-559946	189368
KCr ₄ O ₈	I4/m	mp-18881	183639
KCr ₅ S ₈	C2/m	mp-12178	2568
KCrO ₂	R $\bar{3}$ m	mp-546552	182236
KCu ₃ S ₂	C2/m	mp-9868	100001
KCu ₄ AsS ₄	P21	mp-557728	420017
KCuO ₂	Cmcm	mp-3982	202997
KCuS	Pnma	mp-28270	49008
KHCO ₂	Cmcm	mp-643989	151294
KHCO ₃	P21/c	mp-634431	2076
KIn ₉ Co ₂	P6/mmm	mp-571263	260251
KMgAs(H ₆ O ₅) ₂	Pmn21	mp-1200428	427801
KNa ₂ Sb	Fm $\bar{3}$ m	mp-15724	44332
KNiAsO ₄	R $\bar{3}$	mp-559672	63544
KScAs ₂ (HO ₄) ₂	C2/c	mp-695800	59820
KSiBiS ₄	P21/c	mp-866651	421485
KTaO ₃	Pm $\bar{3}$ m	mp-3614	280424
KTeAu	P63/mmc	mp-3553	71651
KThCuS ₃	Cmcm	mp-12365	170864
KTi ₂ F ₇	Cmmm	mp-976271	174209
KTlCl ₄	I41/a	mp-27385	14105
Kr	Fm $\bar{3}$ m	mp-612118	43726
La(C ₂ N ₃) ₃	Cmcm	mp-31321	391272
La(CoP) ₂	I4/mmm	mp-4402	87582
La(CuGe) ₂	I4/mmm	mp-20322	81756
La(SiAg) ₂	I4/mmm	mp-16237	52587
La ₂ C ₂ Cl	C2/c	mp-567694	419171
La ₂ CoIrO ₆	P21/c	mp-18862	79495
La ₂ Cu ₂ O ₅	Pbam	mp-5696	82389
La ₂ CuO ₄	I4/mmm	mp-19735	74150
La ₂ MgCu ₂	P4/mbm	mp-11086	411709
La ₂ MnCoO ₆	P21/c	mp-19208	196225

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La ₂ O ₃	P $\bar{3}$ m1	mp-1968	56771
La ₃ (CrN ₃) ₂	I4/mmm	mp-569565	162677
La ₃ InC	Pm $\bar{3}$ m	mp-29056	80956
La ₃ Si ₃ Cl ₂	C2/m	mp-29559	408031
La ₄ C ₂ Cl ₅	Immm	mp-569637	418410
LaAl ₂ Ag ₃	P6/mmm	mp-16766	57329
LaAuO ₃	Pbcm	mp-28853	73873
LaBi ₂ Au	P4/nmm	mp-1078401	238704
LaBr ₃	P63/m	mp-23263	65478
LaCO	C2/m	mp-27311	462
LaCdAu	P $\bar{6}$ 2m	mp-542251	411543
LaCl ₃	P63/m	mp-22896	23146
LaClO	P4/nmm	mp-23025	40297
LaCo ₅ P ₃	Cmcm	mp-9552	86373
LaCr ₄ (CuO ₄) ₃	Im $\bar{3}$	mp-1106068	248607
LaCrGe ₃	P63/mmc	mp-13005	158976
LaCrO ₃	Pnma	mp-19281	251092
LaCrO ₄	P21/c	mp-18456	81938
LaCrS ₂ O	Pnma	mp-18885	14192
LaCuO ₂	R $\bar{3}$ m	mp-20072	18102
LaCuO ₃	R $\bar{3}$ c	mp-3474	9428
LaCuS ₂	P21/c	mp-4841	24375
LaCuSO	P4/nmm	mp-6088	96343
LaCuSeO	P4/nmm	mp-552488	96758
LaCuSi	P63/mmc	mp-4835	84207
LaCuTeO	P4/nmm	mp-546790	416522
LaInAg ₂	Fm $\bar{3}$ m	mp-568917	58290
LaNb ₂ CuBrO ₇	P4/mmm	mp-624909	88033
LaRhC ₂	P41	mp-3380	63063
LaTeCl	P4/nmm	mp-1018752	426280
LaTeCl	Pnma	mp-1103189	426279
LaZnAsO	P4/nmm	mp-549589	420204
LaZnPO	P4/nmm	mp-7060	85777
Li(Co ₃ P ₂) ₂	P $\bar{6}$ m2	mp-8864	69692
Li(CoO ₂) ₂	P2/m	mp-552024	159792
Li ₂ AgPb	F $\bar{4}$ 3m	mp-30349	58314
Li ₂ AgSb	F $\bar{4}$ 3m	mp-16238	52589
Li ₂ AgSn ₂	I41/amd	mp-1080714	426085
Li ₂ AgSn	Fm $\bar{3}$ m	mp-30350	58317
Li ₂ AlAg	F $\bar{4}$ 3m	mp-31168	57330
Li ₂ CN ₂	I4/mmm	mp-9610	200369
Li ₂ Co(WO ₄) ₂	P $\bar{1}$	mp-552307	92852
Li ₂ CoCl ₄	Cmmm	mp-22980	73227

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Li ₂ CrCl ₄	C2/m	mp-567474	403035
Li ₂ CuO ₂	Immm	mp-4711	238945
Li ₂ CuP	P63/mmc	mp-12029	240250
Li ₂ CuSn ₂	I41/amd	mp-1078460	426084
Li ₂ InAg	F $\bar{4}$ 3m	mp-30344	58292
Li ₂ O	Fm $\bar{3}$ m	mp-1960	257372
Li ₂ SO ₄	P21/c	mp-4556	58
Li ₂ SiO ₃	Cmc21	mp-5012	100402
Li ₂ Sn ₂ Au	I41/amd	mp-31496	55349
Li ₂ TiO ₃	C2/c	mp-2931	257005
Li ₂ ZnCl ₄	Fd $\bar{3}$ m	mp-22961	202743
Li ₃ (CuO ₂) ₂	C2/m	mp-545467	66509
Li ₃ Ag ₂ Ge ₃	Pn $\bar{3}$ m	mp-29166	85306
Li ₃ AuS ₂	Ibam	mp-15999	280535
Li ₃ N	P6/mmm	mp-2251	156888
Li ₄ NCI	R $\bar{3}$ m	mp-29149	84649
Li ₅ CrCl ₈	Cmmm	mp-23361	67742
Li ₅ NCl ₂	R $\bar{3}$ m	mp-29151	84763
Li ₆ FeCl ₈	Fm $\bar{3}$ m	mp-28828	73217
Li ₈ CeO ₆	R $\bar{3}$	mp-8611	61219
LiAg ₂ Sn	Fm $\bar{3}$ m	mp-2927	151446
LiAg ₃ O ₂	Ibam	mp-27227	4204
LiAg	I41/amd	mp-1018026	247146
LiAg	Pm $\bar{3}$ m	mp-2426	605515
LiAsH ₂ OF ₆	Imma	mp-697263	59367
LiAsH ₆ (OF ₂) ₃	P63mc	mp-556562	416608
LiAsS ₂	Cc	mp-555874	419061
LiAsSe ₂	Cc	mp-1078724	248116
LiAuF ₆	R $\bar{3}$	mp-1079483	165209
LiAuI ₄	P21/c	mp-29520	406967
LiAuS	Fddd	mp-29829	280534
LiBr	Fm $\bar{3}$ m	mp-23259	52236
LiC ₂ N ₃	P2/c	mp-1190940	425113
LiCa ₂ HC ₃	P4/mbm	mp-1104693	261184
LiCaSb	Pnma	mp-16264	428106
LiCaSi ₂	Pnma	mp-13916	25327
LiCe ₂ HO ₃	Immm	mp-24149	56745
LiCl	Fm $\bar{3}$ m	mp-22905	26909
LiCoO ₂	R $\bar{3}$ m	mp-22526	51767
LiCrS ₂	P $\bar{3}$ m1	mp-4226	26233
LiCuO	I4/mmm	mp-5127	40156
LiF	Fm $\bar{3}$ m	mp-1138	62361
LiGaTe ₂	I $\bar{4}$ 2d	mp-5048	162555

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LiH ₂ ClO ₅	C2/c	mp-1195620	430214
LiH ₄ CN ₃	P21/c	mp-1196875	425947
LiH	Fm $\bar{3}$ m	mp-23703	173177
LiI	Fm $\bar{3}$ m	mp-22899	414244
LiIn(IO ₃) ₄	P $\bar{1}$	mp-973966	422056
LiInAg ₂	Fm $\bar{3}$ m	mp-567787	171472
LiInSe ₂	Pna21	mp-20310	60838
LiMgAs	F $\bar{4}$ 3m	mp-12558	107954
LiNbO ₃	R3c	mp-3731	28294
LiSnAu	P63/mmc	mp-11977	412208
LiZnAs	F $\bar{4}$ 3m	mp-9124	74504
LiZnN	F $\bar{4}$ 3m	mp-7575	16790
LiZnP	F $\bar{4}$ 3m	mp-10182	642242
Lu ₂ (CN ₂) ₃	R32	mp-568116	240311
Lu ₂ CCl ₂	R $\bar{3}$ m	mp-573376	62227
LuAg ₄	I4/m	mp-568953	58321
LuAgO ₂	R $\bar{3}$ m	mp-1018025	246823
LuAgPb	P $\bar{6}$ 2m	mp-16747	107278
LuAgSn	P63mc	mp-12505	418580
LuAgSn	P $\bar{6}$ 2m	mp-3608	416377
LuCoO ₃	Pnma	mp-550950	172052
LuCrO ₄	I41/amd	mp-19360	95967
LuCuS ₂	Pnma	mp-12457	172852
LuGeAu	P63mc	mp-9351	81734
LuHCl	R $\bar{3}$ m	mp-23896	62226
LuSiAg	P $\bar{6}$ 2m	mp-1079794	605536
LuSiAu	P $\bar{6}$ m2	mp-9024	71999
LuSnAu	F $\bar{4}$ 3m	mp-5177	415825
Mg(Co ₃ P ₂) ₂	P $\bar{6}$ m2	mp-10924	94412
Mg(CoGe) ₆	P6/mmm	mp-12398	415256
Mg ₂ Cu	Fddd	mp-2481	174173
Mg ₂ Ge	Fm $\bar{3}$ m	mp-408	81735
Mg ₂ Ni	P6222	mp-2137	162120
Mg ₂ Si	Fm $\bar{3}$ m	mp-1367	180944
Mg ₂ Sn	Fm $\bar{3}$ m	mp-2343	104870
Mg ₃ Sb ₂	P $\bar{3}$ m1	mp-2646	245692
MgAg ₃	Pm $\bar{3}$ m	mp-30351	58323
MgAg	Pm $\bar{3}$ m	mp-2696	58322
MgCN ₂	R $\bar{3}$ m	mp-9166	75039
MgCO ₃	R $\bar{3}$ c	mp-5348	63663
MgCdAg ₂	Fm $\bar{3}$ m	mp-30727	104404
MgCl ₂	R $\bar{3}$ m	mp-23210	86439
MgCoGe	P4/nmm	mp-1018808	418853

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MgCr ₂ O ₄	Fd $\bar{3}$ m	mp-19202	97201
MgCu ₂	Fd $\bar{3}$ m	mp-1038	174174
MgCuSb	F $\bar{4}3$ m	mp-3522	412294
MgF ₂	P42/mnm	mp-1249	8120
MgGaAu ₂	P63/mmc	mp-1079175	192087
MgGaAu	P $\bar{6}2$ m	mp-1080605	192086
MgMn ₂ O ₄	I41/amd	mp-27510	290600
MgMoO ₄	C2/m	mp-19047	20418
MgO	Fm $\bar{3}$ m	mp-1265	9863
MgSiP ₂	I $\bar{4}2$ d	mp-2961	22189
MgTe	P63mc	mp-1039	642882
MgV ₂ O ₆	C2/m	mp-1176494	10391
MgWO ₄	P2/c	mp-18875	67901
MgZn ₂ H ₁₂ (BrO) ₆	Immm	mp-697121	49914
Mn ₂ CrSbO ₆	P21/c	mp-1105510	238799
Mn ₂ Sb	P4/nmm	mp-20664	415627
Mn ₂ SiO ₄	Pnma	mp-18928	88026
Mn ₃ (CuO ₄) ₂	C2/m	mp-504567	971
Mn ₄ Si ₇	P $\bar{4}c$ 2	mp-680339	183036
Mn ₅ Si ₃	P63/mcm	mp-1111	166772
MnCO ₃	R $\bar{3}$ c	mp-18814	8433
MnCl ₂	R $\bar{3}$ m	mp-28233	33752
MnCrF ₅	C2/c	mp-555156	939
MnF ₂	P42/mnm	mp-560902	68735
MnO	Fm $\bar{3}$ m	mp-1281224	162039
MnP	Pnma	mp-2662	43246
MnS ₂	Pa $\bar{3}$	mp-1455	36545
MnSO ₄	Cmcm	mp-22554	23839
MnS	P63mc	mp-2562	44765
MnS	Fm $\bar{3}$ m	mp-2065	41331
MnSi	P213	mp-1431	244205
MnSn ₂	I4/mcm	mp-20086	171198
MnTe ₂	Pa $\bar{3}$	mp-21893	12956
MoCl ₅	P $\bar{1}$	mp-569436	84620
MoO ₂	P42/mnm	mp-510536	244050
MoO ₃	Pnma	mp-20589	151750
MoPbO ₄	I41/a	mp-22169	239428
MoS ₂	P63/mmc	mp-2815	95569
MoSe ₂	P63/mmc	mp-1634	601045
NCIO	Pnma	mp-505727	411511
Na(CuS) ₄	P3m1	mp-29069	81306
Na ₂ AgF ₄	P21/c	mp-1104717	425149
Na ₂ AgSb	Cmcm	mp-7392	10010

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Na ₂ BiAu	Cmcm	mp-1078709	380339
Na ₂ CO ₃	C2/m	mp-3070	281361
Na ₂ CoGeO ₄	Pc	mp-545646	200680
Na ₂ CrO ₄	Cmcm	mp-18779	26330
Na ₂ Cu(CO ₃) ₂	P21/c	mp-6090	60858
Na ₂ CuF ₄	P21/c	mp-3237	67249
Na ₂ CuP	Cmcm	mp-7639	1153
Na ₂ LiAu ₃	P63/mmc	mp-12815	152090
Na ₂ Mg(CO ₃) ₂	R $\bar{3}$	mp-6026	100482
Na ₂ MgCl ₄	Pbam	mp-28657	69343
Na ₂ MnCl ₄	Pbam	mp-27280	9136
Na ₂ PdC ₂	P $\bar{3}m$ 1	mp-4823	50172
Na ₂ PtC ₂	P $\bar{3}m$ 1	mp-4366	411389
Na ₂ SO ₄	Fddd	mp-4770	81506
Na ₂ TeSe ₃	C2/c	mp-573581	430312
Na ₂ Ti ₃ O ₇	P21/m	mp-3488	250000
Na ₃ AgO ₂	Ibam	mp-3527	24817
Na ₃ AlF ₆	P21/c	mp-3416	99659
Na ₃ AuO ₂	P42/mnm	mp-28365	62066
Na ₃ AuS ₂	R $\bar{3}c$	mp-15567	202329
Na ₃ ClO	Pm $\bar{3}m$	mp-28602	67319
Na ₃ Co(NO ₂) ₆	R $\bar{3}$	mp-19310	280729
Na ₃ Co ₂ SbO ₆	C2/m	mp-19087	245538
Na ₃ CrF ₆	P21/c	mp-560929	27070
Na ₃ Sb	P63/mmc	mp-7956	26882
Na ₄ TlAu	Fmmm	mp-31470	107428
Na ₄ V ₂ O ₇	C2/c	mp-648893	35635
Na ₅ CoSO ₂	P4/mmm	mp-19027	412978
NaAg ₂	Fd $\bar{3}m$	mp-30352	58337
NaAg ₃ O ₂	Ibam	mp-27303	9627
NaAsS ₂	P21/c	mp-5942	854
NaAuSe ₂	P21/c	mp-29139	84004
NaBr	Fm $\bar{3}m$	mp-22916	41440
NaClO ₄	Cmcm	mp-22968	200405
NaCl	Fm $\bar{3}m$	mp-22862	181148
NaCoO ₂	P63/mmc	mp-867515	246585
NaCoPO ₄	P21/c	mp-562796	280175
NaCoSO ₄ F	C2/c	mp-1205341	262275
NaCr(GeO ₃) ₂	C2/c	mp-21213	260079
NaCrO ₂	R $\bar{3}m$	mp-578604	253188
NaCuO ₂	C2/m	mp-4541	80561
NaCuSe	P4/nmm	mp-7433	12155
NaCuTe	P4/nmm	mp-7434	12156

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NaErCl ₄	P2/c	mp-29083	82364
NaF	Fm $\bar{3}$ m	mp-682	262837
NaGeAu	Imm2	mp-9249	78866
NaH ₃ C ₂ O ₅	P $\bar{1}$	mp-696174	186554
NaHCO ₂	C2/c	mp-23684	151256
NaI	Fm $\bar{3}$ m	mp-23268	61502
NaIn ₂ Au	Cmcm	mp-21352	107505
NaLa ₂ TaO ₆	P21/c	mp-13019	159206
NaSb(PS ₃) ₂	P21	mp-561303	155270
NaSbCl ₆	P42/m	mp-28177	36517
NaSb	P21/c	mp-7944	26473
NaSn	I41/acd	mp-11051	409434
NaTaO ₃	Pnma	mp-3858	239690
NaTe ₃	P $\bar{3}$ c1	mp-28478	61355
NaZr ₂ CoF ₁₁	C2/m	mp-22091	81221
Nb(SeCl) ₂	P $\bar{1}$	mp-27361	10483
Nb ₂ CS ₂	P $\bar{3}$ m1	mp-5745	95113
Nb ₂ CS ₂	R $\bar{3}$ m	mp-4384	95112
Nb ₃ AgO ₈	Ibam	mp-16837	67244
NbBr ₅	Pnma	mp-28601	67298
NbC	Fm $\bar{3}$ m	mp-910	237582
NbCl ₃ O	P42/mnm	mp-27815	26471
NbCoP	Pnma	mp-21449	49727
NbCu ₃ S ₄	P $\bar{4}$ 3m	mp-5621	170784
NbCu ₃ Se ₄	P $\bar{4}$ 3m	mp-4043	73956
NbCuTe ₂	P21/m	mp-31510	414338
NbF ₅	C2/m	mp-18687	26647
NbI ₅	P $\bar{1}$	mp-569578	10457
Nd(AgGe) ₂	I4/mmm	mp-4229	154452
Nd(C ₂ N ₃) ₃	Cmcm	mp-31320	391269
Nd(CoGe) ₂	I4/mmm	mp-4999	81749
Nd(CuGe) ₂	I4/mmm	mp-3177	52765
Nd(SiAg) ₂	I4/mmm	mp-31204	106695
Nd ₂ (SO ₄) ₃	C2/c	mp-29265	200393
Nd ₂ CuO ₄	I4/mmm	mp-4158	203228
Nd ₂ MgCu ₂	P4/mbm	mp-16638	411710
Nd ₂ MoC ₂	P42/mnm	mp-603912	417666
Nd ₂ S ₃	Pnma	mp-438	72290
Nd ₂ WC ₂	P42/mnm	mp-569275	417667
Nd ₄ Cu ₂ O ₇	C2/m	mp-556595	86841
NdAgAs ₂	Pnma	mp-864793	420612
NdAgPb	P63mc	mp-20880	107102
NdAgSn	P63mc	mp-4808	155736

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NdCl ₃	P63/m	mp-23183	23147
NdClO	P4/nmm	mp-23058	59231
NdCoC ₂	Cc	mp-8761	67375
NdCoGe	P4/nmm	mp-20531	85861
NdCoO ₃	Pnma	mp-22599	164821
NdCrGe ₃	P63/mmc	mp-13008	158979
NdCrO ₃	Pnma	mp-19269	38022
NdCrO ₄	I41/amd	mp-19126	93786
NdCu ₄ Ag	F $\bar{4}3m$	mp-1077428	605036
NdCuO ₂	R $\bar{3}m$	mp-4886	83052
NdCuS ₂	P21/c	mp-10495	415079
NdCuSO	P4/nmm	mp-542314	96346
NdCuSe ₂	P21/c	mp-3739	95827
NdCuTeO	P4/nmm	mp-974307	416523
NdF ₃	P63cm	mp-18511	63049
NdLuSe ₃	Cmcm	mp-13327	249621
NdMgCu ₄	F $\bar{4}3m$	mp-1071051	194977
NdRhC ₂	Amm2	mp-8540	63064
NdTeCl	P4/nmm	mp-1018818	426777
Ne	Fm $\bar{3}m$	mp-111	43427
Ni(AgO) ₂	R $\bar{3}m$	mp-19405	172559
Ni(AuF ₄) ₂	P21/c	mp-22552	50212
Ni(CO) ₄	Pa $\bar{3}$	mp-1203274	24662
Ni ₂ P	P $\bar{6}2m$	mp-21167	27162
Ni ₃ P	I $\bar{4}$	mp-2296	98373
Ni ₃ S ₂	R32	mp-362	23114
Ni ₃ Sn	P63/mmc	mp-20112	411928
Ni ₄ B ₃	C2/c	mp-569404	187403
NiAgO ₂	R $\bar{3}m$	mp-19069	73974
NiAgO ₂	P63/mmc	mp-19284	415451
NiAgSe ₂	R3m	mp-1018020	605616
NiCO ₃	R $\bar{3}c$	mp-19147	61067
NiCl ₂	R $\bar{3}m$	mp-27396	14208
NiF ₂	P42/mnm	mp-559798	73457
NiO	Fm $\bar{3}m$	mp-19009	28834
NiP ₃	Im $\bar{3}$	mp-2301	92394
NiSO ₄	Cmcm	mp-18749	33737
NiS	P63/mmc	mp-594	42494
NiSb	P63/mmc	mp-810	190179
NiWO ₄	P2/c	mp-21179	235272
NpCl ₄	I41/amd	mp-23161	75482
OsCl ₄	Cmmm	mp-571035	1165
OsO ₄	C2/c	mp-540783	63

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OsS ₂	Pa $\bar{3}$	mp-20905	300224
P ₁₀ Au ₇ I	P $\bar{6}2m$	mp-27370	12162
P ₂ H ₁₂ C ₄ O ₃	C2/c	mp-1199137	170836
P ₂ O ₅	Pnma	mp-2173	79698
P ₂ Os	Pnnm	mp-2319	238252
P ₂ PbAu ₂	Cmcm	mp-30108	412224
P ₃ Au ₂	C2/m	mp-27258	8058
P ₃ N ₅	C2/c	mp-567907	56876
P ₄ N ₃ Cl ₁₁	R3	mp-28792	71913
P ₄ S ₃	Pnma	mp-1468	31348
PCl ₃	Pnma	mp-23230	32027
PH ₃ CS ₃	P21/c	mp-559616	320555
P	Cmce	mp-157	417180
PaCl ₄	I41/amd	mp-27291	9309
Pb(ClO ₃) ₂	Fdd2	mp-28513	40286
PbBr ₂	Pnma	mp-28077	36170
PbC ₂ (SN) ₂	C2/c	mp-20605	143
PbCClO ₂	C2/m	mp-552056	99805
PbCN ₂	Pnma	mp-19727	410915
PbCO ₃	Pnma	mp-19893	166089
PbCl ₂	Pnma	mp-23291	27736
PbCl ₄	C2/c	mp-570355	280975
PbClF	P4/nmm	mp-22964	82884
PbF ₂	Fm $\bar{3}m$	mp-315	86738
PbI ₂	P $\bar{3}m1$	mp-22893	68819
PbICl	Pnma	mp-23053	32642
PbO ₂	P42/mnm	mp-20725	8491
PbO	P4/nmm	mp-19921	62840
PbSO ₄	Pnma	mp-3472	190064
PbS	Fm $\bar{3}m$	mp-21276	62190
PbSeO ₃	P21/m	mp-20716	98376
PbSeO ₄	P21/c	mp-22342	40921
PbSe	Fm $\bar{3}m$	mp-2201	62195
PbWO ₄	P21/c	mp-504591	250592
PbWO ₄	I41/a	mp-22410	81550
Pb	Fm $\bar{3}m$	mp-20483	96501
Pd(AuF ₄) ₂	P21/c	mp-8585	50213
Pd(PbCl ₃) ₂	P21/c	mp-28982	78873
Pd(Se ₃ Cl) ₂	P21/c	mp-29469	405207
Pd ₂ Cl ₂ O	I41/amd	mp-28323	61333
PdCl ₂	R $\bar{3}$	mp-29487	404624
PdCl ₂	Pnnm	mp-569008	421213
PdF ₂	P42/mnm	mp-1058	73165

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PdS ₂	Pbca	mp-13682	648747
PdS	P42/m	mp-20250	61063
Pr(AgGe) ₂	I4/mmm	mp-5564	154449
Pr(C ₂ N ₃) ₃	Cmcm	mp-567763	391270
Pr(CoP) ₂	I4/mmm	mp-5054	73649
Pr(CoSi) ₂	I4/mmm	mp-5112	55923
Pr(SiAg) ₂	I4/mmm	mp-31203	106694
Pr ₂ Co ₂ I	P63/mmc	mp-567727	416273
Pr ₂ MoC ₂	P42/mnm	mp-31258	413345
Pr ₂ O ₃	P $\bar{3}$ m1	mp-2063	61179
Pr ₂ WC ₂	P42/mnm	mp-568326	417668
Pr ₄ C ₂ Cl ₅	Immm	mp-570498	418384
PrAgAs ₂	Pnma	mp-4308	174359
PrAgSb ₂	P4/nmm	mp-1079478	190195
PrAgSn	P63mc	mp-31421	55820
PrAg	Pm $\bar{3}$ m	mp-2525	58345
PrAl ₂ Ag	R $\bar{3}$ m	mp-1101762	604688
PrAu ₆	C2/c	mp-569032	2125
PrBi ₂ Au	P4/nmm	mp-1078315	238707
PrCl ₃	P63/m	mp-23211	62251
PrCoC ₂	Cc	mp-567341	78551
PrCoGe ₃	I4mm	mp-13125	161875
PrCoO ₃	Pnma	mp-20090	164818
PrCr ₂ Si ₂ C	P4/mmm	mp-21402	152143
PrCrGe ₃	P63/mmc	mp-13007	158978
PrCuO ₂	R $\bar{3}$ m	mp-13694	246822
PrCuS ₂	P21/c	mp-16684	95829
PrCuSO	P4/nmm	mp-6166	96345
PrCuSe ₂	P21/c	mp-11792	99677
PrInAg ₂	Fm $\bar{3}$ m	mp-570683	58297
PrLuSe ₃	Cmcm	mp-13326	249620
PrTeCl	P4/nmm	mp-1018941	426284
Pt(SCl ₃) ₂	P $\bar{1}$	mp-28722	66013
Pt ₅ Se ₄	P21/c	mp-29767	87926
Pt	Fm $\bar{3}$ m	mp-126	243678
PuCl ₃	P63/m	mp-22918	4060
PuO ₂	Fm $\bar{3}$ m	mp-1959	55456
Rb(InAu ₂) ₂	I4/mcm	mp-20804	249220
Rb ₂ Au ₃	Immm	mp-11814	106288
Rb ₂ Cu ₂ SnS ₄	Ibam	mp-18006	74020
Rb ₂ MnCl ₄	I4/mmm	mp-22978	1139
Rb ₂ Na ₄ Co ₂ O ₅	P42/mnm	mp-18151	64680
Rb ₂ NbCuS ₄	Fddd	mp-15221	84304

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Rb ₂ NbCuSe ₄	Fddd	mp-15222	84305
Rb ₂ O ₃	I ₄ 3d	mp-2571	427458
Rb ₂ PdC ₂	P ₃ m1	mp-10918	94394
Rb ₂ SO ₄	Pnma	mp-3372	203159
Rb ₂ SnCl ₆	Fm ₃ m	mp-23059	65059
Rb ₂ TeBr ₆	Fm ₃ m	mp-23383	49521
Rb ₂ TeI ₆	P4/mnc	mp-28070	36009
Rb ₂ Ti(CuS ₂) ₂	P42/mcm	mp-7129	280644
Rb ₂ TlAu ₃	Pmma	mp-867851	249924
Rb ₂ VAgS ₄	Fddd	mp-8901	66841
Rb ₂ VCuS ₄	Fddd	mp-15219	84302
Rb ₃ Au ₇	Cmmm	mp-31144	106290
Rb ₃ AuO	Pm ₃ m	mp-4405	75499
Rb ₃ Sb ₂ Br ₉	P ₃ m1	mp-28222	39823
Rb ₄ Sn ₂ Au ₇	R ₃ m	mp-30416	58581
RbAg ₂ SbS ₄	P3221	mp-17756	82145
RbAg ₃ S ₂	C ₂ /m	mp-1205335	1034
RbAg ₃ Se ₂	C ₂ /m	mp-10477	90795
RbAg ₃ Te ₂	C ₂ /m	mp-10481	90872
RbAg ₅ Se ₃	P4/nbm	mp-29685	50738
RbAgO	I ₄ /mmm	mp-8603	49753
RbAu ₅	P6/mmm	mp-1209	106289
RbAuF ₄	I ₄ /mcm	mp-3419	33952
RbAuS	Cmcm	mp-9010	71654
RbAuSe	Cmcm	mp-9731	402190
RbAu	Pm ₃ m	mp-30373	58428
RbBr	Fm ₃ m	mp-22867	22167
RbCO ₂	Pbam	mp-556872	165563
RbCeS ₂	R ₃ m	mp-3535	73546
RbClO ₃	R3m	mp-23011	10283
RbClO ₄	Pnma	mp-28433	63363
RbCl	Fm ₃ m	mp-23295	18016
RbCr ₅ S ₈	C ₂ /m	mp-7295	2567
RbCr ₅ Se ₈	C ₂ /m	mp-28818	73145
RbCu ₃ S ₂	C ₂ /m	mp-10985	409646
RbF	Fm ₃ m	mp-11718	53828
RbI	Fm ₃ m	mp-22903	22168
RbNbAsClO ₅	P4/nmm	mp-556645	85758
RbNiCl ₃	P6 ₃ /mmc	mp-23486	15010
RbTiCl ₃	P6 ₃ /mmc	mp-28282	49747
RbV(CuS ₂) ₂	Ama2	mp-15998	280516
Re(TeCl ₆) ₂	P ₁	mp-28633	68656
Re ₂ O ₇	P212121	mp-1016092	15217

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ReAgO ₄	I41/a	mp-7094	280086
ReCl ₃	R $\bar{3}$ m	mp-23174	62222
ReCl ₄	P2/c	mp-27340	10293
ReCl ₆	R $\bar{3}$	mp-1078114	425145
ReO ₂	P42/mnm	mp-12875	154021
ReS ₂	P $\bar{1}$	mp-572758	81814
ReSe ₂	P $\bar{1}$	mp-541582	81813
ReSi ₂	I4/mmm	mp-12605	38274
RuCl ₃	P63/mcm	mp-22850	414040
RuF ₅	P21/c	mp-540829	165397
RuO ₂	P42/mnm	mp-825	172178
RuS ₂	Pa $\bar{3}$	mp-2030	68472
RuSe ₂	Pa $\bar{3}$	mp-1922	68473
S(ClO) ₂	Fdd2	mp-28405	62970
SCl ₂ O	P21/c	mp-28406	62971
SCl	Fdd2	mp-28096	37016
Sb ₂ (SO ₄) ₃	P21/c	mp-27339	618
Sb ₂ O ₃	Fd $\bar{3}$ m	mp-1999	240206
Sb ₂ O ₃	Pccn	mp-2136	240207
Sb ₂ Os	Pnnm	mp-2695	238254
Sb ₂ Pt	Pa $\bar{3}$	mp-562	43105
Sb ₂ S ₃	Pnma	mp-2809	171850
Sb ₂ Se ₃	Pnma	mp-2160	194836
Sb ₂ Te ₃	R $\bar{3}$ m	mp-1201	193341
Sb ₃ ClO ₄	P2/c	mp-29591	410039
Sb ₄ Cl ₂ O ₅	P21/c	mp-23419	2233
SbCl ₃	Pnma	mp-22872	8258
SbCl ₅	P63/mmc	mp-23176	250363
SbClF ₈	P $\bar{1}$	mp-27314	9899
SbF ₃	Ama2	mp-1880	16142
SbI ₃	R $\bar{3}$	mp-23281	26082
SbSBr	Pnma	mp-22971	88584
SbSI	Pnma	mp-23041	85301
SbSeI	Pnma	mp-22996	35470
Sb	R $\bar{3}$ m	mp-104	64697
Sc ₂ O ₃	Ia $\bar{3}$	mp-216	169172
Sc ₂ S ₃	Fddd	mp-401	22236
Sc ₃ Co ₂ Ge ₃	Cmcm	mp-31191	106479
Sc ₃ Co ₂ Si ₃	Cmcm	mp-9901	41745
Sc ₃ CoC ₄	Immm	mp-5075	173167
Sc ₃ GaC	Pm $\bar{3}$ m	mp-8577	50162
Sc ₃ InC	Pm $\bar{3}$ m	mp-8578	50163
Sc ₃ IrC ₄	Immm	mp-1092328	415137

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Sc ₃ OsC ₄	Immm	mp-867215	420075
Sc ₃ RhC ₄	Immm	mp-1078784	415136
Sc ₃ RuC ₄	Immm	mp-8996	72864
Sc ₄ OsCl ₄	C2/c	mp-1105775	421532
Sc ₇ Cl ₁₂	R $\bar{3}$	mp-23186	36424
ScAg(PSe ₃) ₂	P $\bar{3}$ 1c	mp-13383	195336
ScAg ₄	I4/m	mp-30354	605794
ScAgGe	P $\bar{6}$ 2m	mp-1080424	428469
ScAgSe ₂	P $\bar{3}$ m1	mp-12908	155115
ScAlAg ₂	Fm $\bar{3}$ m	mp-31169	57333
ScCl ₃	R $\bar{3}$	mp-23309	74517
ScCoC ₂	P4/nmm	mp-615314	62598
ScCrC ₂	P63/mmc	mp-1188534	80374
ScCrO ₃	Pnma	mp-18961	185585
ScCuO ₂	R $\bar{3}$ m	mp-4636	55689
ScCuO ₂	P63/mmc	mp-3642	60847
ScCuS ₂	P3m1	mp-6980	15298
ScCuSi	Pnma	mp-20083	86391
ScGeAu	P63mc	mp-9350	81733
ScH ₃ (CO ₂) ₃	R $\bar{3}$ c	mp-1193413	281595
ScHCl	R $\bar{3}$ m	mp-24081	40981
ScInAg ₂	Fm $\bar{3}$ m	mp-30347	58298
ScInCu ₄	F43m	mp-13240	416528
ScN	Fm $\bar{3}$ m	mp-2857	644666
ScNiSb	F $\bar{4}$ 3m	mp-3432	40296
ScSbPd	F $\bar{4}$ 3m	mp-569779	415944
ScSiAu	P $\bar{6}$ m2	mp-9023	71998
ScSnAu	F $\bar{4}$ 3m	mp-2894	415827
ScTlS ₂	P63/mmc	mp-13312	418474
ScTlSe ₂	R $\bar{3}$ m	mp-13313	418475
ScTlTe ₂	R $\bar{3}$ m	mp-13314	418476
Sc	P63/mmc	mp-67	164088
SeCl ₄	C2/c	mp-540675	15578
SeCl	P21/c	mp-504825	37018
Si(AgO) ₄	P42/n	mp-556164	418314
Si ₂ Mo	I4/mmm	mp-2592	182115
Si ₂ W	I4/mmm	mp-1620	73599
Si ₃ N ₄	P63/m	mp-988	170004
Si ₇ (Ni ₂ Au) ₂	C2/m	mp-1103787	429212
SiAg ₂ O ₃	P212121	mp-28195	36589
SiAg ₂ S ₃	P21/c	mp-1190974	180764
SiAgPt ₅	P4/mmm	mp-1025220	605693
SiC	R3m	mp-11713	24168

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SiC	P63mc	mp-11714	24170
SiC	P63mc	mp-7140	86253
SiC	P63mc	mp-7631	156190
SiC	F $\bar{4}$ 3m	mp-8062	603798
SiCl ₂	P212121	mp-29174	85526
SiI ₄	Pa $\bar{3}$	mp-635441	91745
SiMo ₃	Pm $\bar{3}$ n	mp-1275	35755
SiNi	P213	mp-1095177	187621
SiO ₂	P3121	mp-7000	154289
SiP ₂	Pbam	mp-9996	43098
SiP	Cmc21	mp-2798	87149
SiPbO ₃	P2/c	mp-21723	250220
SiS ₂	Ibam	mp-1602	291208
Si	Fd $\bar{3}$ m	mp-149	51688
Sm(AgGe) ₂	I4/mmm	mp-972680	165008
Sm(SiAg) ₂	I4/mmm	mp-567600	106696
Sm ₂ (CN ₂) ₃	C2/m	mp-568498	240312
Sm ₂ Cr ₂ C ₃	C2/m	mp-1078035	380337
Sm ₂ CuO ₄	I4/mmm	mp-4210	72243
Sm ₂ Mo ₂ C ₃	C2/m	mp-13264	417828
Sm ₂ O ₃	C2/m	mp-1745	241936
Sm ₂ SCl ₄	C2/c	mp-29880	89534
Sm ₃ Co ₆ Sn ₅	Immm	mp-22002	55511
Sm ₄ Mg ₃ Co ₂	P2/m	mp-571606	416491
SmAgAs ₂	P4/nmm	mp-1205313	420613
SmAgPb	P63mc	mp-570855	107103
SmAg	Pm $\bar{3}$ m	mp-2475	58350
SmBi ₂ Au	P4/nmm	mp-1080419	238708
SmCoGe	Pnma	mp-20777	76520
SmCoO ₃	Pnma	mp-20016	90969
SmCrGe ₃	P63/mmc	mp-13009	158980
SmCrO ₃	Pnma	mp-1105788	237360
SmCuS ₂	P21/c	mp-5081	415080
SmCuSe ₂	P21/c	mp-11793	237036
SmCuSeO	P4/nmm	mp-9194	75572
SmCuSn	P63mc	mp-12791	151170
SmGa ₅ Co	P4/mmm	mp-19988	249519
SmInAg ₂	Fm $\bar{3}$ m	mp-568719	58299
SmRhC ₂	Amm2	mp-8758	67328
SmSiAg	P $\bar{6}$ 2m	mp-972524	605842
SmSnAu	P63mc	mp-4304	416418
Sn(CO ₂) ₂	C2/c	mp-542769	150101
SnBr ₂	Pnma	mp-29862	411177

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SnCl ₂	Pnma	mp-29179	15452
SnClF	Pnma	mp-27373	647
SnHgO ₃	R $\bar{3}$ c	mp-13554	260029
SnO	P4/nmm	mp-2097	15516
SnP ₇ Au ₃	P21/m	mp-3245	240776
SnS ₂	P $\bar{3}$ m1	mp-1170	100610
SnSO ₄	Pnma	mp-542967	186951
SnS	Pnma	mp-2231	52108
SnSe ₂	P $\bar{3}$ m1	mp-665	43594
SnSe	Pnma	mp-691	186650
SnTe	Fm $\bar{3}$ m	mp-1883	52489
Sn	I41/amd	mp-84	252800
Sn	Fd $\bar{3}$ m	mp-117	40039
Sr(Ag ₂ Sb) ₂	R $\bar{3}$ m	mp-1077980	424311
Sr(AgGe) ₂	I4/mmm	mp-7879	25317
Sr(AuO ₂) ₂	I41/a	mp-9298	80328
Sr(ClO ₃) ₂	Fdd2	mp-28477	61157
Sr(CuGe) ₂	I4/mmm	mp-3241	424224
Sr(CuO) ₂	I41/amd	mp-13900	25002
Sr(GaAu) ₂	P4/nmm	mp-12780	370004
Sr(SiAg) ₂	I4/mmm	mp-7880	25330
Sr ₂ CeO ₄	Pbam	mp-15743	237186
Sr ₂ CoTeO ₆	P21/c	mp-561642	153002
Sr ₂ CrO ₄	I4/mmm	mp-18854	245595
Sr ₂ CrSbO ₆	C2/m	mp-1084823	290789
Sr ₂ Cu ₂ O ₅	Pbam	mp-21129	82019
Sr ₂ Cu ₃ O ₅	Cmmm	mp-552089	50089
Sr ₂ Cu ₃ O ₅	Immm	mp-5700	416905
Sr ₂ CuO ₃	Immm	mp-5456	202993
Sr ₂ LiCoN ₂	P42/mnm	mp-569001	72387
Sr ₂ NCl	R $\bar{3}$ m	mp-23033	410769
Sr ₂ PbO ₄	Pbam	mp-20944	4418
Sr ₂ SiO ₄	P21/c	mp-18510	243631
Sr ₂ Ti ₂ As ₂ OF ₂	I4/mmm	mp-1079747	167013
Sr ₂ TiO ₄	I4/mmm	mp-5532	194713
Sr ₂ VFeAsO ₃	P4/nmm	mp-1106248	248695
Sr ₃ (CoO ₃) ₂	R $\bar{3}$ c	mp-1192011	182288
Sr ₃ BiN	Pm $\bar{3}$ m	mp-570008	152053
Sr ₃ CrN ₃	P63/m	mp-12906	154803
Sr ₃ SbN	Pm $\bar{3}$ m	mp-1013534	152052
Sr ₃ Ti ₂ O ₇	I4/mmm	mp-3349	63704
Sr ₃ ZnCoO ₆	R $\bar{3}$ c	mp-1191185	189230
Sr ₇ (H ₆ Cl) ₂	P $\bar{6}$	mp-23827	418948

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SrAg ₂	Imma	mp-30356	58359
SrAg ₅	P6/mmm	mp-2410	58361
SrAgAs	P63/mmc	mp-6954	49742
SrAgP	P63/mmc	mp-10667	52596
SrAgSF	P4/nmm	mp-1078562	183709
SrAgTeF	P4/nmm	mp-1080438	183711
SrAl ₂ O ₄	P21	mp-3094	291361
SrAu ₂	Imma	mp-434	55543
SrBiClO ₂	Cmcm	mp-547244	84636
SrBr ₂	P4/n	mp-32711	262673
SrC ₂ (SN) ₂	C2/c	mp-10927	94427
SrCN ₂	Pnma	mp-9167	182046
SrCO ₃	Pnma	mp-3822	166088
SrCdAu	Pnma	mp-1095513	426612
SrCl ₂	Fm $\bar{3}$ m	mp-23209	196826
SrClF	P4/nmm	mp-22957	2349
SrCrO ₄	P21/c	mp-510607	40922
SrCu ₂ O ₃	Cmmm	mp-5938	416903
SrF ₂	Fm $\bar{3}$ m	mp-981	40414
SrGaCu ₂	R $\bar{3}$ m	mp-30580	102938
SrGe ₂	Pnma	mp-1244	152799
SrGeAu ₃	P4/nmm	mp-1078860	262386
SrH ₁₂ (ClO ₃) ₂	P321	mp-23885	59143
SrHCl	P4/nmm	mp-23860	37200
SrHfO ₃	Pnma	mp-3378	86830
SrI ₂	Pbca	mp-23181	15101
SrInAu	Pnma	mp-22529	391422
SrMoO ₄	I41/a	mp-18834	239418
SrO	Fm $\bar{3}$ m	mp-2472	163625
SrPbO ₃	Pnma	mp-20489	78682
SrSO ₄	Pnma	mp-5285	190063
SrS	Fm $\bar{3}$ m	mp-1087	249177
SrSeO ₄	P21/c	mp-4092	40923
SrSe	Fm $\bar{3}$ m	mp-2758	52429
SrSi ₃ Au	I4mm	mp-1067925	194347
SrSnO ₃	Pnma	mp-2879	238971
SrTiO ₃	Pm $\bar{3}$ m	mp-551830	94573
SrWO ₄	I41/a	mp-19163	291536
SrZnASF	P4/nmm	mp-1080135	189934
SrZnCl ₄	I41/a	mp-23034	410191
SrZrS ₃	Pnma	mp-5193	154104
Ta(ICl) ₂	Immm	mp-28683	69688
Ta ₂ AgF ₁₂	P $\bar{1}$	mp-28375	62543

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Ta ₂ C	P $\bar{3}$ m1	mp-7088	409555
Ta ₂ CoO ₆	P42/mnm	mp-31517	203095
TaAgO ₃	R $\bar{3}$ c	mp-9890	40831
TaAgS ₃	Cmcm	mp-5821	84910
TaC	Fm $\bar{3}$ m	mp-1086	159875
TaCl ₄	C2/m	mp-29465	402406
TaCl ₅	C2/m	mp-29831	409433
TaCrP	Pnma	mp-1095419	196498
TaCu ₃ S ₄	P $\bar{4}3$ m	mp-10748	185524
TaCuN ₂	R $\bar{3}$ m	mp-8927	71136
TaF ₅	C2/m	mp-561197	431296
TaNO	P21/c	mp-4165	192423
TaSi ₂	P6222	mp-517	43596
TaTlS ₃	Pnma	mp-10795	412385
Tb(CoSi) ₂	I4/mmm	mp-3292	55924
Tb(CuGe) ₂	I4/mmm	mp-4521	627844
Tb(CuSi) ₂	I4/mmm	mp-3456	55784
Tb(SiAg) ₂	I4/mmm	mp-4614	98341
Tb ₂ Co ₂ I	P63/mmc	mp-567614	418080
Tb ₃ (CoGe ₂) ₂	C2/m	mp-22643	62292
Tb ₃ (MnC ₃) ₂	P63/m	mp-28827	73214
Tb ₃ GaCoS ₇	P63	mp-1192199	426678
Tb ₄ Mg ₃ Co ₂	P2/m	mp-569343	417036
Tb ₅ SbAu ₂	I4/mcm	mp-1179018	156951
TbAg ₂	I4/mmm	mp-30358	605886
TbAgPb	P63mc	mp-31447	107105
TbAgSe ₂	I41md	mp-979271	605827
TbAgSn	P63mc	mp-31422	55822
TbAgTe ₂	P $\bar{4}21$ m	mp-3551	154793
TbAg	Pm $\bar{3}$ m	mp-2268	605891
TbCl ₂ F	C2/c	mp-560119	418279
TbCl ₃	P63/m	mp-568170	63541
TbCl ₃	Cmcm	mp-23293	63542
TbCl	R $\bar{3}$ m	mp-27923	23352
TbCoGe	Pnma	mp-21144	52986
TbCoO ₃	Pnma	mp-19802	172046
TbCoSi	Pnma	mp-22206	88213
TbCrO ₄	I41/amd	mp-19272	166175
TbCu ₄ Ag	F $\bar{4}3$ m	mp-1072264	605048
TbCuS ₂	P21/c	mp-5737	415075
TbH ₂ ClO ₂	P21/m	mp-1102075	260832
TbInAg ₂	Fm $\bar{3}$ m	mp-22382	58301
TbMgCo ₄	F $\bar{4}3$ m	mp-1070837	195971

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Tc ₂ O ₇	Pbca	mp-27485	140217
TcCl ₃	C2/m	mp-1078708	262639
TcO ₂	P42/mnm	mp-1205302	254200
Te ₂ AuI	Pmma	mp-27527	16325
Te ₂ Mo	P63/mmc	mp-602	644476
Te ₂ Ru	Pa $\bar{3}$	mp-1848	65169
Te ₃ As ₂	C2/m	mp-484	196146
TeCl ₄	C2/c	mp-569561	411157
TeO ₂	P212121	mp-8377	90733
TePb	Fm $\bar{3}$ m	mp-19717	63098
TeRhCl	C2/m	mp-22945	405714
Te	P3121	mp-19	161690
Th(CoSi) ₂	I4/mmm	mp-7072	68210
Th(CuP) ₂	P3m1	mp-9581	100270
Th(CuSi) ₂	I4/mmm	mp-5948	68212
Th(SO ₄) ₂	Pbca	mp-1202893	423489
ThAg ₂	P6/mmm	mp-309	58368
ThBr ₄	I41/amd	mp-23160	72425
ThCl ₄	I41/a	mp-567431	6055
ThF ₄	C2/c	mp-31034	66009
ThI ₄	P21/c	mp-27697	23942
ThRu ₃ C	Pm $\bar{3}$ m	mp-22394	79241
ThSO	P4/nmm	mp-8136	31654
ThSeO	P4/nmm	mp-7950	26654
ThTeO	P4/nmm	mp-3718	65950
Ti(CuS) ₄	I $\bar{4}$ 2m	mp-29091	82558
Ti ₂ Ag	I4/mmm	mp-979115	605939
Ti ₂ CrO ₅	C2/c	mp-19369	65219
Ti ₂ CuS ₄	Fd $\bar{3}$ m	mp-3951	170227
Ti ₂ CuSb ₃	P4m2	mp-505804	93241
Ti ₂ GaC	P63/mmc	mp-12537	419117
Ti ₂ O ₃	R $\bar{3}$ c	mp-458	28353
Ti ₂ SnC	P63/mmc	mp-3871	86812
Ti ₃ O ₅	C2/m	mp-556480	75193
Ti ₃ SiC ₂	P63/mmc	mp-5659	86213
TiAg ₂ (IO ₃) ₆	R $\bar{3}$	mp-1194095	420852
TiAl ₃	I4/mmm	mp-542915	58189
TiB ₂	P6/mmm	mp-1145	56723
TiBr ₄	Pa $\bar{3}$	mp-569814	39241
TiC	Fm $\bar{3}$ m	mp-631	159871
TiCl ₃	P31c	mp-567330	39428
TiClO	Pmmn	mp-22992	155833
TiCoO ₃	R $\bar{3}$	mp-19424	48107

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TiCoSb	F $\bar{4}$ 3m	mp-5967	169138
TiCrP	P $\bar{6}$ 2m	mp-11580	96721
TiF ₄	Pnma	mp-28974	78737
TiFeO ₃	R $\bar{3}$	mp-19417	247547
TiFe	Pm $\bar{3}$ m	mp-305	633925
TiI ₄	C2/c	mp-541013	39820
TiNCl	Pmmn	mp-27850	261525
TiNiO ₃	R $\bar{3}$	mp-18732	171584
TiO ₂	P42/mnm	mp-2657	167953
TiO ₂	I41/amd	mp-390	92363
TiSi ₂	Fddd	mp-2582	1089
Ti	P63/mmc	mp-46	253841
Tl(CoS) ₂	I4/mmm	mp-5501	100438
Tl ₂ Au ₄ S ₃	Pmmn	mp-29898	51235
Tl ₂ CN ₂	P $\bar{1}$	mp-570443	417297
Tl ₂ CO ₃	C2/m	mp-543045	4239
Tl ₂ Cu ₂ SnS ₄	Ibam	mp-18240	171221
Tl ₂ MoCl ₆	Fm $\bar{3}$ m	mp-29562	408777
Tl ₂ PAuS ₄	P21/m	mp-9510	85680
Tl ₂ PdCl ₄	P4/mmm	mp-29889	89601
Tl ₂ SO ₄	Pnma	mp-4112	59944
Tl ₂ S	R3	mp-667	59735
Tl ₂ TeBr ₆	P4/mnc	mp-31076	99127
Tl ₂ TeI ₆	P21/c	mp-31077	99128
Tl ₂ TeS ₃	Pnma	mp-17172	391285
Tl ₂ Te	C2/c	mp-582753	280923
Tl ₂ WCl ₆	Fm $\bar{3}$ m	mp-29556	409229
Tl ₃ AsSe ₃	R3m	mp-7684	15148
Tl ₄ CdI ₆	P4/mnc	mp-570339	60756
TlAgI ₂	I4/mcm	mp-27801	26318
TlAgS	Pnma	mp-1095594	605754
TlAgSe	Pnma	mp-29238	100710
TlAgTeO ₃	Iba2	mp-1191720	169995
TlAgTe	Pnma	mp-5874	52609
TlBr	Pm $\bar{3}$ m	mp-22875	61532
TlCO ₂	P21/c	mp-556745	170127
TlCl	Pm $\bar{3}$ m	mp-23167	5253
TlCr ₅ S ₈	C2/m	mp-541823	78157
TlCr ₅ Se ₈	C2/m	mp-3407	37123
TlGaTe ₂	I4/mcm	mp-3785	16243
TlII	Pm $\bar{3}$ m	mp-23197	61520
TlII	Fm $\bar{3}$ m	mp-571102	60491
TlII	Cmcm	mp-22858	258845

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TlInSe ₂	I4/mcm	mp-568517	180272
TlInTe ₂	I4/mcm	mp-22791	16245
TlV ₂ AgO ₆	C2/c	mp-18853	201934
Tm ₂ C(NO) ₂	P3m1	mp-13039	416883
Tm ₃ (CuGe) ₄	Immm	mp-568519	99159
TmAg ₂	I4/mmm	mp-30359	58373
TmAgGe	P62m	mp-1078772	164587
TmAgPb	P62m	mp-20522	107277
TmAgS ₂	I41md	mp-1079656	423922
TmAgSe ₂	P212121	mp-1188652	605834
TmAgSn	P63mc	mp-6917	417550
TmAgSn	P62m	mp-2990	239160
TmAgTe ₂	P421m	mp-1078600	605918
TmAgTe ₂	P3m1	mp-12953	156301
TmAg	Pm3m	mp-2796	58372
TmCl ₃	R3c	mp-28044	35398
TmCoO ₃	Pnma	mp-561954	172050
TmCu ₄ Ag	F43m	mp-1025116	605053
TmCuS ₂	Pnma	mp-12455	172850
TmSiAg	P62m	mp-1079093	605849
TmSnAu	F43m	mp-3462	416420
U(Cr ₃ P ₂) ₂	P6m2	mp-29005	72375
U(CrC) ₄	I4/m	mp-2971	40319
U(CuP) ₂	P3m1	mp-21478	78476
U(CuSi) ₂	I4/mmm	mp-22374	246933
U(SO ₄) ₂	Pbca	mp-1200785	423491
U ₂ C ₃	I43d	mp-2625	26477
U ₂ Cl ₅ O ₂	Cmmm	mp-27661	23084
U ₃ Si ₂	P4/mbm	mp-21346	73695
UAl ₄	Imma	mp-574122	240127
UB ₁₂	Fm3m	mp-22319	189924
UBr ₃	P63/m	mp-23255	4070
UBrO ₂	Cmcm	mp-27536	1107
UC ₂	I4/mmm	mp-2486	26478
UCO ₅	Imm2	mp-29761	87760
UC	Fm3m	mp-2489	26476
UCl ₃	P63/m	mp-23208	202333
UCl ₄	I41/amd	mp-23235	202331
UCl ₆	P3m1	mp-23250	746
UF ₆	Pnma	mp-2275	36218
UGe ₂	Cmmm	mp-1237	236995
UI ₃	Cmcm	mp-23244	201171
UI ₄	C2/c	mp-655360	41417

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UO ₂	Fm $\bar{3}$ m	mp-1597	246851
V ₂ CoP ₂ (H ₄ O ₇) ₂	I4/m	mp-24174	281336
V ₂ CuS ₄	Fd $\bar{3}$ m	mp-5178	190442
V ₂ O ₃	R $\bar{3}$ c	mp-18937	95761
V ₂ O ₅	Pmmn	mp-25279	267173
V ₂ Pb ₂ O ₇	P21/c	mp-22005	2901
V ₂ Pb ₃ O ₈	C2	mp-19903	67605
V ₃ Ag ₂ TeS ₆	P $\bar{6}$ 2m	mp-1102112	251064
V ₃ Si	Pm $\bar{3}$ n	mp-2567	87329
V ₄ Ag ₂ O ₁₁	C2/m	mp-19402	93453
V ₄ Cu ₃ S ₈	R3m	mp-29211	100053
VAg ₃ O ₄	C2/c	mp-18889	249417
VAgHgO ₄	C2	mp-18901	414429
VAgO ₃	Cm	mp-559736	82079
VC	Fm $\bar{3}$ m	mp-1282	159870
VCl ₅	P $\bar{1}$	mp-1101909	425146
VClO	Pmmn	mp-23061	1981
VCoSi	Pnma	mp-21371	409847
VCu ₃ Se ₄	P $\bar{4}$ 3m	mp-21855	409449
VCuO ₃	R $\bar{3}$	mp-504580	19046
VF ₃	R $\bar{3}$ c	mp-559931	69167
V	Im $\bar{3}$ m	mp-146	171003
W(CO) ₆	Pnma	mp-541695	300206
WC	P $\bar{6}$ m2	mp-1894	246150
WCl ₄	C2/m	mp-980949	165263
WCl ₅	C2/m	mp-27160	2398
WCl ₆	R $\bar{3}$	mp-571518	425147
WO ₂	P42/mnm	mp-19372	80829
WOF ₄	C2/m	mp-540636	10393
WS ₂	P63/mmc	mp-224	202366
WSe ₂	P63/mmc	mp-1821	40752
Xe	Fm $\bar{3}$ m	mp-611517	43428
Y(CoGe) ₂	I4/mmm	mp-4908	81748
Y(CoSi) ₂	I4/mmm	mp-5129	427109
Y(CuGe) ₂	I4/mmm	mp-4520	52764
Y ₂ Au	Pnma	mp-979911	262044
Y ₂ C(NO) ₂	P $\bar{3}$ m1	mp-546864	245332
Y ₂ Cl ₃	C2/m	mp-27678	23337
Y ₂ MgCu ₂	P4/mbm	mp-4901	411711
Y ₂ MnCrO ₆	P21/c	mp-1106099	188476
Y ₂ O ₃	Ia $\bar{3}$	mp-2652	86814
Y ₃ Au ₂	P4/mbm	mp-1080493	262043
Y ₃ InC	Pm $\bar{3}$ m	mp-19817	80955

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Y ₄ C ₇	P21/c	mp-9530	86049
Y ₄ Cl ₅	C2/m	mp-23382	68014
Y ₄ GaCo ₄	C2/m	mp-21875	20953
YAg ₂	I4/mmm	mp-999544	605961
YAgPb	P $\bar{6}$ 2m	mp-21505	107275
YAgSb ₂	P4/nmm	mp-1078739	190094
YAgTe ₂	P $\bar{4}$ 21m	mp-12903	154792
YAg	Pm $\bar{3}$ m	mp-2474	58376
YCl	C2/m	mp-23062	400298
YCl	R $\bar{3}$ m	mp-540884	61107
YCr ₄ (CuO ₄) ₃	Im $\bar{3}$	mp-1105560	248615
YCrO ₃	Pnma	mp-18725	185525
YCrO ₄	I41/a	mp-555657	157934
YCuO ₂	P63/mmc	mp-2918	35580
YCUP ₂	P4/nmm	mp-30208	95177
YCuS ₂	Pnma	mp-12843	92458
YCu	Pm $\bar{3}$ m	mp-712	187860
YF ₃	Pnma	mp-2416	6023
YGeAu	P63mc	mp-10098	405323
YI ₃	R $\bar{3}$	mp-571442	170773
YMgAg	P $\bar{6}$ 2m	mp-30737	104477
YMgCu ₄	F $\bar{4}$ 3m	mp-13172	191559
YNiSb	F $\bar{4}$ 3m	mp-11520	105331
YSbPt	F $\bar{4}$ 3m	mp-4964	44970
YSiAg	P $\bar{6}$ 2m	mp-1091398	605850
YSnAu	P63mc	mp-567197	415826
Zn(AgI ₂) ₂	Pmn21	mp-1104888	190588
Zn(CrS ₂) ₂	Fd $\bar{3}$ m	mp-4194	164169
Zn(GaSe ₂) ₂	I $\bar{4}$	mp-15776	44887
Zn(GaTe ₂) ₂	I $\bar{4}$	mp-15777	290911
Zn(InTe ₂) ₂	I $\bar{4}$	mp-20832	25650
Zn ₂ AgAu	Fm $\bar{3}$ m	mp-31171	57340
Zn ₂ NCl	Pna21	mp-1189171	425734
Zn ₂ SiO ₄	R $\bar{3}$	mp-3789	257027
Zn ₃ As ₂	P42/nbc	mp-680580	87576
Zn ₃ N ₂	Ia $\bar{3}$	mp-9460	84918
Zn ₃ P ₂	P42/nmc	mp-2071	250159
Zn ₃ TeAs ₂ Pb ₃ O ₁₄	P321	mp-558298	85574
ZnAgF ₃	Pm $\bar{3}$ m	mp-14099	28950
ZnAs ₂	P21/c	mp-7262	2021
ZnBr ₂	I41/acd	mp-647579	30803
ZnCN ₂	I $\bar{4}$ 2d	mp-29826	280523
ZnCO ₃	R $\bar{3}$ c	mp-9812	100679

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ZnCl ₂	Pna21	mp-22889	2459
ZnCr ₂ O ₄	Fd $\bar{3}$ m	mp-19410	196119
ZnCu ₂ GeSe ₄	I $\bar{4}$ 2m	mp-10824	93409
ZnCu ₂ SiS ₄	Pmn21	mp-977414	261367
ZnCu ₂ SnS ₄	I $\bar{4}$ 2m	mp-1025500	184478
ZnF ₂	P42/mnm	mp-1873	280605
ZnGeAs ₂	I $\bar{4}$ 2d	mp-4008	68324
ZnGeN ₂	Pna21	mp-2979	15144
ZnGeP ₂	I $\bar{4}$ 2d	mp-4524	23706
ZnO	P63mc	mp-2133	162843
ZnP ₂	P21/c	mp-1392	250015
ZnS	P63mc	mp-560588	67453
ZnS	F $\bar{4}$ 3m	mp-10695	291064
ZnSb	Pbca	mp-753	43265
ZnSe	F $\bar{4}$ 3m	mp-1190	77091
ZnSiAs ₂	I $\bar{4}$ 2d	mp-3595	68323
ZnSiP ₂	I $\bar{4}$ 2d	mp-4763	23680
ZnSnAs ₂	I $\bar{4}$ 2d	mp-5190	250389
ZnSnP ₂	I $\bar{4}$ 2d	mp-4175	22179
ZnSnSb ₂	I $\bar{4}$ 2d	mp-4756	651588
ZnTe	F $\bar{4}$ 3m	mp-2176	77072
ZnWO ₄	P2/c	mp-18918	166208
Zn	P63/mmc	mp-79	421013
Zr(CuP) ₂	P $\bar{3}$ m1	mp-8219	35585
Zr ₂ Ag	I4/mmm	mp-2221	605999
Zr ₂ CoP	P21/m	mp-29152	84825
Zr ₂ InCo ₂	P4/mbm	mp-22150	404847
Zr ₃ (Cu ₂ Si ₃) ₂	I4/mmm	mp-27961	30732
Zr ₄ In ₅ Co ₂	P2/m	mp-607475	55578
ZrBrN	R3m	mp-541912	51771
ZrCl ₂	R $\bar{3}$	mp-571537	41539
ZrCl ₂	R3m	mp-23162	30052
ZrCl ₄	P2/c	mp-569175	26049
ZrCl	R $\bar{3}$ m	mp-27440	868
ZrCoF ₆	Fm $\bar{3}$ m	mp-554222	83724
ZrCoP	Pnma	mp-8418	49726
ZrCr ₅ P ₃	P21/m	mp-18686	409488
ZrCuSn	Pnma	mp-1101867	190123
ZrGaAu	P $\bar{6}$ m2	mp-12951	156264
ZrI ₄	P2/c	mp-571235	8068
ZrNCl	R3m	mp-568592	93740
ZrN	Fm $\bar{3}$ m	mp-1352	41934
ZrO ₂	P21/c	mp-2858	403484

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ZrS ₂	P $\bar{3}$ m1	mp-1186	604434
ZrSe ₂	P $\bar{3}$ m1	mp-2076	109291
ZrSiO ₄	I41/amd	mp-4820	96090

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