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The AFLOW library of crystallographic prototypes: Part 4

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ABSTRACT

The AFLOW Library of Crystallographic Prototypes has been updated to include an additional 683 entries, which now reaches 1,783 prototypes. We have also made some changes to the presentation of the entries, including a more consistent definition of the AFLOW-prototype label and a better explanation of our choice of space group when the experimental data is ambiguous. A method is presented for users to submit new prototypes for the Encyclopedia. We also include a complete index linking to all the prototypes currently in the Library.

1. Introduction

There are a variety of available resources to find crystallographic information about the structure of materials. These include the *Pauling File Project* [1], the *American Mineralogist Crystal Structure Database* (AMCSD) [2], the Inorganic Crystal Structure Database (ICSD) [3], the Cambridge Structural Database (CSD) [4], and our own AFLOW (Automatic FLOW for Materials Discovery) [5]. This list is by no means complete. Most of these databases group similar crystal structures under one prototype, a specific compound that defines the entire class. These prototypes are usually labeled by the chemical formula of the prototype structure, which, while helpful, does not guarantee a unique definition. In fact, there is no agreed-upon method for designating prototypes, though many have been proposed and are in use [6].

Our approach is the AFLOW-prototype label [7], an alphanumeric string describing stoichiometry, unit cell Pearson symbol and space group, and occupied Wyckoff positions for each atomic species of a given structure. The label is the same for all structures in the prototype class and is independent of the choice of prototype compound, although we always make one choice to use as an example. All structures in a prototype class have the same AFLOW-prototype label. An example is the rock salt structure: NaCl — halite — and hundreds of binary compounds [8,9] all have the same prototype label, `AB_cF8_225_a_b`.

The AFLOW-prototype label is not unique in its basic form. As a trivial example, the label `AB_cF8_225_b_a` also describes the rock salt structure. The (4a) and (4b) Wyckoff positions of space group $Pm\bar{3}m$ #225 have the same symmetry, so swapping the positions of the A and B atoms does not change the structure. In orthorhombic space groups the Wyckoff positions of the structure, and hence the label, depend on the orientation of the crystal. In other cases, two structures with quite different atomic arrangements might have the same prototype label. The construction of a unique label therefore requires additional conditions to the naming convention that we explore in this article.

We use the AFLOW-prototype label to refer to structures in our Library of Crystallographic Prototypes. This database began with 298 structures [7] with later additions bringing the total to 1100 [6,10]. Here we report the addition of 683 new prototypes. Many of these were chosen by scanning the literature to find systems currently being explored by researchers. All have been included in the updated AFLOW-XtalFinder [11] and can be accessed directly from the `aflow++` software [12] and through the AFLOW.org web [5]. All the individual entries in the current library have been updated to include additional compounds that the same prototype can describe and to correct errors that unavoidably occur in a large project such as this. The library is now designed to be updated regularly, and we are accepting suggested prototypes from users.

This article describes the changes we made to the Library of Crystallographic Prototypes. The following section discusses the new structures added to the Library, changes in AFLOW-prototype labels and space groups, cross references with other databases, and extensions to the online version of the Library, the AFLOW Encyclopedia of Crystallographic Prototypes.

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2. Changes and updates to the library of crystallographic prototypes

The newest version of the Library includes several updates and changes in the way we index and present the prototypes. These are highlighted below.

2.1. New prototypes

We have added an additional 683 prototypes to the database, bringing the total number of entries to 1783 at the time of submission. Newly added systems include:

- Aurivillius phases [13] at the request of users;
- Ti_3Cu_4 [14] and others, based on recent mentioned in literature [15];
- ReB_2 [16] and others, to extend previous class of entries, in this case, the Re_xB_y system; and
- $U_2Co_3Si_5$ and other less-common structures [17], to provide more examples of structures in sparsely populated space groups.

All structures currently in the Encyclopedia are listed in the Appendix, with new structures highlighted by a filled bullet point (•). Links to the individual entries are provided there. Going forward from this point, we plan frequent updates to the entries in the online Encyclopedia of Crystallographic Prototypes [18], as well as more streamlined reports for archival literature.

While all prototypes are crystal structures, not all crystal structures are unique prototypes. Had we begun *ab initio*, we would define a prototype class using the misfit value ϵ defined by AFLOW-XtalFinder [11] and implemented by the `aflow++` software [12]. This defines all structures with the same AFLOW label and $\epsilon < 0.2$ as belonging to the same family. We would then designate the earliest structure identified in the literature to define the prototype.

Historical events make this neat identification impossible. As an example, FeAs (*Strukturbericht B*14) [21] and MnP (*Strukturbericht B*31) [22] both have the AFLOW label AB_oP8_62_c_c and a misfit score of only 0.045, so we should put them in the same class, with MnP as the prototype since it was described first [23]. This goes against the historical record, so we leave them as two different prototypes.

Conversely, the ICSD lists $TlCo_2S_2$ [24] under the $ThCr_2Si_2$ [25] prototype, even though there misfit score is quite large ("UNMATCHABLE" according to XtalFinder). In this case we made the somewhat arbitrary decision to classify structures with the label A2B2C_tI10_139_d_e_a as being in the $ThCr_2Si_2$ prototype if $c/a < 3$, and in the $TlCo_2S_2$ prototype if $c/a > 3$.

In the general case we will attempt to follow the prototype convention used by the ICSD or earlier sources. The prototype web pages note when we differ from this convention.

2.2. AFLOW labels

Any database of prototypes requires a unique method to catalog each entry. AFLOW and the Library of Crystallographic Prototypes are no exception. A unique label allows quick access to the Library's web pages and facilitates the generation of new structures within AFLOW. It would be helpful if there were a universally recognized method for labeling crystalline prototypes, but this goal has yet to be achieved.

The Library originated as a web page at the U.S. Naval Research Laboratory (NRL) [26]. There a prototype was usually referenced by its *Strukturbericht* designation [23,27–32], if one existed, or the chemical formula. These methods are not sustainable for large-scale databases: the practice of defining new *Strukturbericht* labels ceased early in the post World War II period. The seemingly obvious idea of using chemical formulas fails as many of these entities, e.g. WO_3, can be found in multiple phases even under ambient conditions, with many of the phases designated as the prototypes for their class. AFLOW circumvents this problem by introducing the prototype label [7] . The method is outlined in Fig. 1. Consider a chemical compound, here β-SeO_2 [33]. We have a complete description of this structure from the literature [34]. This includes the space group, the lattice constants, the Wyckoff positions occupied by each species, and the numerical values used to locate each atom associated with a given Wyckoff position. The prototype label is generated from this information, to wit:

- The chemical formula is written in alphabetical order: $SeO_2 \rightarrow O_2Se$. Assign the letter `A` to the first element and the letter `B` to the second. The stoichiometry of the compound is given by a number (if not 1) after the letter. Thus SeO_2 becomes `A2B`. This construction allows other compounds with the same structure to use this label.
- This compound has a primitive orthorhombic lattice with twelve atoms in the unit cell. The Pearson symbol [35] for this structure is then `oP12`.
- The compound is in space group $Pmc2_1$, which is #26 in the International Tables of Crystallography [20].
- The selenium atoms occupy (2a), (2b), and (4c) Wyckoff positions [36], while the oxygen atoms are on (2a) and (2b) sites. The numbers represent the number of atoms associated with each Wyckoff position, but they are redundant: the Wyckoff label (4c) and the Wyckoff letter `c` convey the same information.

The prototype label is constructed from these pieces: the abstract chemical formula, the Pearson symbol, the space group number, and the Wyckoff letters of each element, all separated by underscores. This gives us the prototype label `A2B_oP12_26_abc_ab`.

Now consider a slightly more complicated case, the Na_2PrO_3 structure [37]. This is a base-centered monoclinic structure, space group $C2/c$ #15. The sodium atoms are on (2a), (4e), and (8f) Wyckoff sites, praseodymium is found on two (4e) sites, and the oxygen atoms occupy three (8f) sites. When one atomic species occupies multiple Wyckoff positions with the same letter, we indicate this by placing the number of sites *before* the Wyckoff letter, so the prototype label is `A2B3C_mC48_15_aef_3f_2e`.

Once the label is constructed, and with knowledge of the atomic species and the numerical values of the positional parameters, AFLOW can generate the entire crystal structure. Using experimental data [34] for β-SeO_2, the AFLOW command:

```
aflow --proto=A2B_oP12_26_abc_ab:O:Se
--params=5.0722,0.88135,1.48474,0.746,0.672,
0.1219,0.3748,0.620,-0.039,0.2516,0.000,
0.247,0.152,0.841
```

generates the VASP POSCAR file for this structure. Adding the flag `--cif` to the command will instead produce a Crystallographic Information File (CIF) [38]. This process works even if the AFLOW-prototype label is not in the database.

The procedure outlined above is sufficient to generate a crystal structure for any periodic crystal. Once a prototype is incorporated into the database, however, problems can arise because we must produce unique labels. The first difficulty arises when two or more distinct crystal structures have the same label. For example, α-gallium (*Strukturbericht* designation *A*11), crystalline molecular iodine (*A*14), and black phosphorous (*A*17) all occupy a single (8f) Wyckoff position in space group *Cmca* #64, giving all of these structures the prototype label `A_oC8_64_f`. The crystals are very different, however, as seen in Fig. 2, which compares α-Ga and molecular I_2. While the structures have the same label, they cannot be said to have the same prototype. In the past, we distinguished these structures using arbitrary labels, in this case α-Ga [39], I [40], and P [41], but this is generally unwieldy. Our new method distinguishes these structures by adding a three-digit suffix to the label. This index number is determined by the order in which the structure was added to the AFLOW database [42]. In this case,

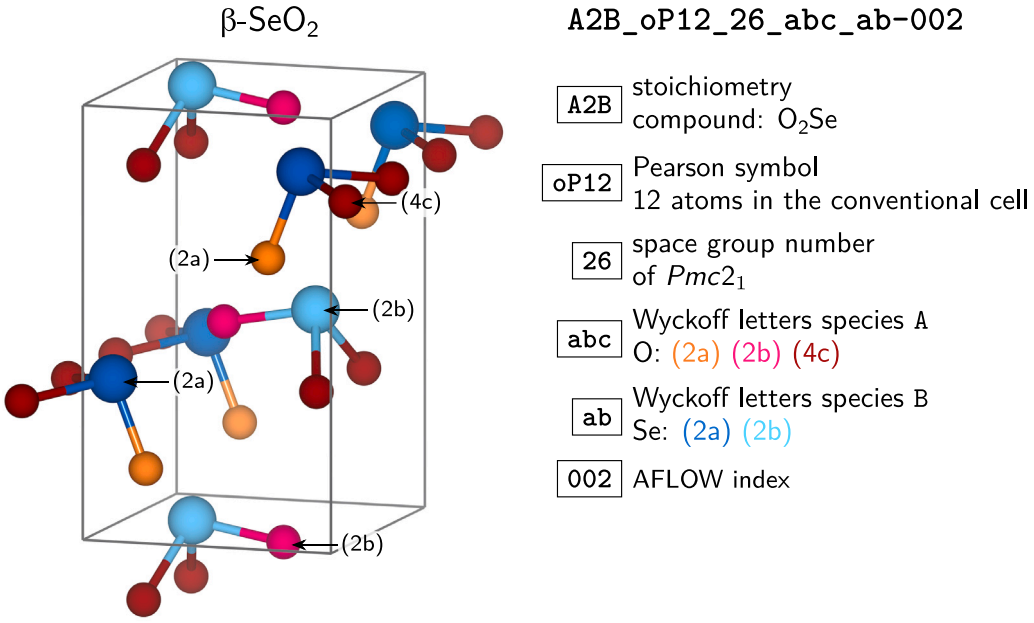

Fig. 1. Deconstruction of the AFLOW-prototype label, describing the atoms in the conventional unit cell of the system. On the left oxygen is drawn using VESTA [19] in shades of red, while blue is used for selenium. The different Wyckoff positions share the same colors and are labeled in the figure. The stoichiometry term is determined by listing the elements in the crystal in alphabetical order, calling the first element A, the second B, etc. The multiplicity of each element is indicated by the number after its letter. This is followed by the Pearson Symbol and the space group number assigned in the International Tables of Crystallography [20]. The Wyckoff letters are then listed for each atom. If there are multiple instances of the same Wyckoff positions for an atom, it is indicated by a number placed *before* the Wyckoff letter. Finally, the AFLOW index concludes the label. The `-002` here indicates that at least one other structure in the AFLOW database has the label `A2B_oP12_26_abc_ab`.

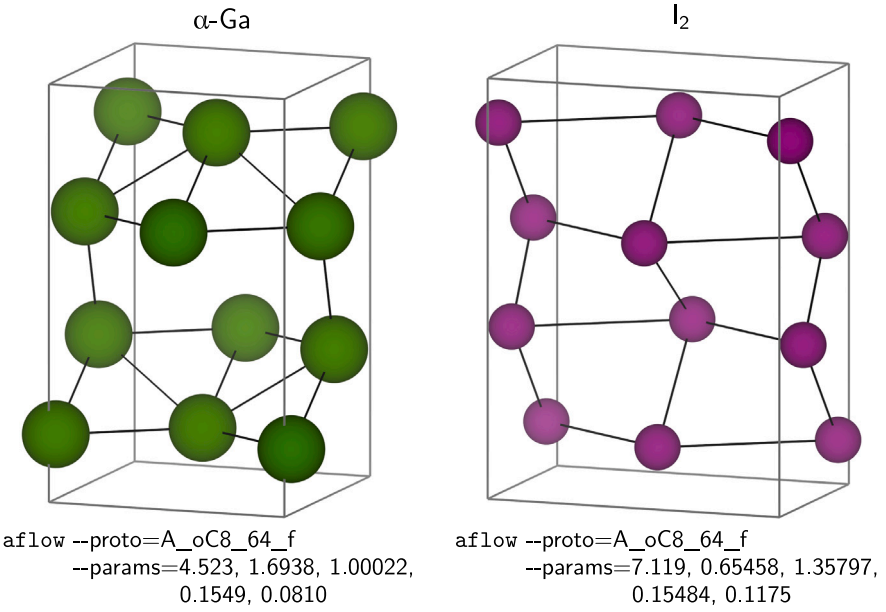

Fig. 2. Crystal structures of α-Ga (left) and molecular iodine (right), drawn using VESTA [19]. Both structures are in the same space group with a single (8f) occupied Wyckoff position, so they have the same AFLOW-prototype label, `A_oC8_64_f`. The boxes delineated the conventional unit cells for each structure, and black lines show the connection to the nearest neighbors, to guide the eye. The AFLOW command below each structure generates that structure.

- α-Ga is A_oC8_64_f-001,
- phosphorous is A_oC8_64_f-002, and
- molecular iodine is A_oC8_64_f-003.

As a further example, again consider β-SeO_2, AFLOW label A2B_oP12_26_abc_ab. This prototype label is the same for both β-SeO_2 and the high-pressure (70 GPa) H_2S structure [43]. In previous versions of the Library we distinguished between the two structures by placing the chemical formula after the label, e.g. A2B_oP12_26_abc_ab.H2S and A2B_oP12_26_abc_ab.SeO2, respectively. H_2S was added to our database before β-SeO_2, so the new labels become A2B_oP12_26_abc_ab-001 and A2B_oP12_26_abc_ab-002, respectively.

While we will always use the new labels in future work, the Library will maintain backward compatibility. In particular, this will allow links in our previously published reports to continue to function. Thus a reference to the label A2B_oP12_26_abc_ab.H2S will link to H_2S (A2B_oP12_26_abc_ab-001), while A2B_oP12_26_abc_ab.SeO2 will link to β-SeO_2 (A2B_oP12_26_abc_ab-002). Similarly both A_oC8_64_f.alpha-Ga and A_oC8_64_f-001 will resolve as *A*11 α-gallium.

One could hope that the above criteria would produce a unique label for every prototype. This turns out not to be the case, as many space groups permit several different choices of origin [44] and orientation [45] to describe the same structure. Each choice of origin and orientation will produce a different set of occupied Wyckoff positions.

For example, consider the compound UTe_2 [46], which has an orthorhombic structure in space group *Immm* #71. Hutanu et al. [47] describe this structure in an orientation with lattice constants $c > b > a$. Using this orientation, the crystal has the AFLOW-prototype label A2B_oI32_71_hj_i. Alternatively, since space group *Immm* allows us to make any permutation of the axes we wish to describe a structure, we could instead rotate the system so that $a > b > c$. In that case, the AFLOW-prototype label becomes A2B_oI32_71_eh_f. Other permutations give other possible labels. Still, more choices occur because the space group allows an origin shift of one-half of the lattice constant along any of the principle axes.

To avoid confusion, AFLOW versions beginning with 3.2.14 fix the origin and orientation of the unit cell by

- assigning a numerical score to each Wyckoff letter: $a = 1$, $b = 2$, etc., and take the sum over all Wyckoff positions. Only labels with the smallest sum will be considered.
- If there are still multiple permutations of Wyckoff positions with this sum, chose the one where the first atomic species has the smallest Wyckoff letter.

In our UTe_2 example, this gives us the label A2B_oI32_71_eh_f-001, the suffix signaling that this is the first structure we have found with this label. AFLOW will always report this as the label for UTe_2, even if it is generated using data from another orientation.

Combining AFLOW-prototype label plus suffix can generate unwieldy labels. We introduce a unique identifier (UID) for all published prototypes to alleviate this. This four-character UID is created using a similar approach to the AUID used for AFLOW database entries. The prototype label is hashed by utilizing a 64-bit variant of the cyclic redundancy check (CRC64) [48] with "Jones" coefficients. The resulting 64-bit integer is then represented as a string using a set of 34 characters (uppercase alphanumeric without the letters I and O to avoid confusion). As the number of anticipated prototypes is considerably smaller than the number of possible entries in the AFLOW database, just a fraction of the 64-bit long hash is utilized. With just the first four characters of the produced hash, over 1.3 million prototypes could be differentiated. While this is ample space to describe all foreseeable prototypes, the convenience of a smaller UID leads to a high risk of hash collisions. As creating a new label for a prototype depends on a database lookup to determine the suffix number, a collision can be avoided at this point by using the result of the first attempt as new input for the UID creation. This process can be repeated until a unique UID is found. The created UIDs are shown in the index in the Appendix and on the prototype index page. If the UID is known, the structure may be retrieved from the Library using the link http://aflow.org/p/UID, where UID is replaced by the four-character UID for the structure.

2.3. Assignment of the space group

By convention, a structure that could be described in multiple space groups is placed in the space group with the highest symmetry as determined by its index number in the International Tables. In practice, structures with relatively high symmetry are frequently reported as having lower symmetry [49–51]. This often happens when a reference places the structure in a low-symmetry space group, but assigns lattice and Wyckoff parameters consistent with a higher symmetry. An example is PtSn [52]. The original publication [53] placed this system in space group *Aea*2 (#41) with a primitive orthorhombic primitive cell. The platinum atoms occupy the (2a) site. The tin atoms occupy two (2b) Wyckoff sites, with $x_1 = y_2$, $x_2 = y_1$, and $z_2 = -z_1$. These relations make the atomic positions consistent with the higher symmetry space group *Ccce* (#68), with a base-centered orthorhombic primitive cell. In the former case, the two tin sites are nominally independent, but in the latter case, all tin atoms are on a single (16i) Wyckoff position.

Our approach to cases like this has varied. We usually place the problematic structure in the higher symmetry space group, especially if it was a structure highlighted by Cenzual et al. [49,50] or similar works. In the case of $PtSn_4$ (and a few other structures), we decided to emphasize the nature of the lower symmetry space group, *Aea*2, as there are relatively few structures in that group. We did this by slightly changing the lattice constants and/or atomic coordinates. In either case, the comments accompanying each entry discuss the situation: the published space group, the higher symmetry space group, and our choice of the space group to display.

Another problem arises when the experimentally reported structure is correctly placed in a low-symmetry space group. However, a small amount of uncertainty in the atomic positions or lattice parameters would make the structure consistent with a structure with a higher symmetry. In this case, electronic structure programs such as VASP assume that the structure will relax to the higher symmetry structure and so start calculations by making this assumption. By default AFLOW follows the same convention, but we felt it best to use the originally reported structure for our purposes. This requires us to change the default tolerance when calling AFLOW. One such case is α-FeSe [54]. This structure was reported in space group *Cmme* (#67) with a base-centered orthorhombic lattice [55], with the lattice constants *a* and *b* differing by less than 0.3%. As a result, the default tolerance set in AFLOW, as well as electronic structure programs such as VASP, place this in the higher symmetry tetragonal space grep *P*4/*nmm* (#129). Tightening the AFLOW tolerance eventually reveals the reported space group. In this type of case, we uniformly use the reported space group. However, we note the problem in the comment section for the prototype.

2.4. Cross reference with other databases

The Inorganic Crystal Structure Database (ICSD) [3] is perhaps the largest collection of published inorganic crystal structures. We currently provide the corresponding ICSD identification number for each structure in the Library, when available. If the structure is not in the ICSD, we then search through the Cambridge Crystallographic Data Centre (CCDC) [56] database, which also searches the Cambridge Structural Database (CSD) [4]. We include the CCDC identification number if the structure is found there. At the present time we have 1632 entries with ICSD or CCDC identifications. The remaining 151 structures are mostly hypothetical, computationally predicted, or obsolete structures not included in the ICSD or CCDC databases.

2.5. Extensions

We have made several improvements to the library and AFLOW. For example, AFLOW-XtalFinder [11] has been updated to include all of the structures currently in the library. When a user enters a structure, it is automatically compared to all existing prototype entries. If a matching entry is found, the relevant prototype information is returned (e.g., prototype label and parameters, *Strukturbericht* designation, symmetry descriptions, Inorganic Crystal Structure Database (ICSD) [3] or Cambridge Structural Database (CSD) [57] identifier, if available, and a weblink to the entry. If no matching entry is found – signaling a new prototype – users can report the structure by providing the following information in an online form:

i. Geometry file (in any standardized format),
ii. Reference(s) that reported the structure,
iii. Supplemental reference(s) used to find the structure (e.g., catalogs or online databases),
iv. The ICSD or CCDC entry number, if available.
v. Any useful comments about the prototype, such as its relationship to other entries in the database and
vi. The uploader's contact information (to credit the contributor on that structure's entry page, if desired).

Unique prototype suggestions will be collected for future enrichment of the encyclopedia. While previous library versions were only updated upon publication of a new article, we plan to switch to incremental updates. As new structures are added to the system, the online library will be directly expanded, with periodic reports such as this one focusing on additions and improvements to the library.

3. Conclusion

The AFLOW Library of Crystallographic Properties has been updated to provide users with complete crystallographic information for 1783 structures, with future expansion planned. This information can be used to construct input files for many electronic structure programs.

The updated Library changes the default definition of the AFLOW-prototype label to make it easier for users and programmers to construct a unique label for each prototype. Structures that can be placed in multiple space groups have been highlighted, and the comments for each structure outline why we have made that particular choice. Each entry now includes the ICSD or CCDC identification number, when available. Finally, we now provide an interface for users to suggest new structures to be added to the Library.

Code availability

The underlying software used in this study and its source code can be accessed via this link https://aflow.org/install-aflow/.

CRediT authorship contribution statement

Hagen Eckert: Writing – original draft, Visualization. **Simon Divilov:** Writing – original draft, Visualization. **Michael J. Mehl:** Writing – review & editing, Writing – original draft, Visualization, Formal analysis, Conceptualization. **David Hicks:** Software. **Adam C. Zettel:** Visualization, Software. **Marco Esters:** Software. **Xiomara Campilongo:** Writing – review & editing, Writing – original draft. **Stefano Curtarolo:** Writing – review & editing, Writing – original draft, Supervision, Software, Project administration, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

All of the crystallographic information and sources for the structures found in the Encyclopedia are available on the web page for each prototype. In addition, the structural information may be obtained from AFLOW using the command `aflow --proto=STRING` where STRING is the AFLOW label for that prototype.

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Appendix. Index of prototypes ordered by space groups

This index lists all prototype structures in the current Encyclopedia of Crystallographic Prototypes. Entries headed by a filled bullet point (•) are new to this edition of the Encyclopedia, while previous entries are designated by an empty one (∘). Clicking on the UID or AFLOW-prototype label will open a web browser window showing the details of that structure. A PDF version of the page can be obtained by clicking the "PDF version" link on the web page.

P1 (**1**):		
∘	FeS_2 ($P1$):	
	AB2_aP12_1_4a_8a-001	RHYA
∘	$AsKSe_2$ ($P1$):	
	ABC2_aP16_1_4a_4a_8a-001	GZNE
∘	$NaC_5H_{11}O_8S$:	
	A5B11CD8E_aP26_1_5a_11a_a_8a_a-001	WTTR
P$\bar{1}$ (**2**):		
∘	Cf:	
	A_aP4_2_aci-001	G18C
∘	P_2I_4:	
	A2B_aP6_2_2i_i-001	V85G
∘	H_2S (90 GPa):	
	A2B_aP6_2_aei_i-001	Q769
•	Hexamethylbenzene II ($C_{12}H_{18}$):	
	A_aP12_2_6i-001	7LZP
•	γ-$CuZrF_6$:	
	AB12C_aP14_2_b_6i_c-001	5H3G
∘	TaTi (BCC SQS-16):	
	AB_aP16_2_4i_4i-001	BQ6Y
∘	$Co_2B_2O_5$:	
	A2B2C5_aP18_2_2i_2i_5i-001	RJNZ
•	Na_4SiO_4:	
	A4B4C_aP18_2_4i_4i_i-002	A8AW
•	$Cu_3(P_2O_6OH)_2$:	
	A3B12C2D4_aP21_2_ai_6i_i_2i-001	L1KQ
•	Low temperature "White" Phosphorous:	
	A_aP24_2_12i-001	YLP3
∘	Albite ($NaAlSi_3O_8$, $S6_8$):	
	ABC8D3_aP26_2_i_i_8i_3i-001	8BAG

- Boric Acid (H_3BO_3, $G5_1$):
  AB3C3_aP28_2_2i_6i_6i-001 H1GD
- Wollastonite ($CaSiO_3$):
  AB3C_aP30_2_3i_9i_3i-001 89U5
- Kyanite (Al_2SiO_5, $S0_1$):
  A2B5C_aP32_2_4i_10i_2i-001 4TPV
- δ-WO_3:
  A3B_aP32_2_12i_4i-001 9JTN
- $Co_3(SeO_3)_3{\cdot}H_2O$:
  A3B2C10D3_aP36_2_be2i_2i_10i_3i-001 0ZM1
- Chalcanthite ($CuSO_4{\cdot}5H_2O$, $H4_{10}$):
  AB10C9D_aP42_2_bc_10i_9i_i-001 NQQF
- α-$Ho_2Si_2O_7$:
  A2B7C2_aP44_2_4i_14i_4i-001 VN5Q
- $Ni(NO_3)(H_2O)_3$:
  A12B2CD12_aP54_2_12i_2i_i_12i-001 6GLF
- Pentacene ($C_{11}H_7$):
  A11B7_aP72_2_22i_14i-001 C9KZ

P2 (**3**):

- Predicted SiO_2 ($P2$):
  A2B_mP12_3_ab3e_2e-001 QAF3
- $Pb_3TeCo_3P_2O_{14}$:
  A3B14C2D3E_mP138_3_3c3d6e_42e_6e_3a3b6e_ 3a3b-001 TBT2

P2$_1$ (**4**):

- High-pressure Te:
  A_mP4_4_2a-001 H0F1
- α-BiPd:
  AB_mP16_4_4a_4a-001 QNKQ
- $Li_2SO_4{\cdot}H_2O$ ($H4_8$):
  A2B2C5D_mP20_4_2a_2a_5a_a-001 674K
- Ca_3UO_6:
  A3B6C_mP20_4_3a_6a_a-001 T9UP
- Monoclinic (I) Li_2FeSiO_4:
  AB2C4D_mP32_4_2a_4a_8a_2a-001 TK4X
- $W_2O_3(PO_4)_2$:
  A11B2C2_mP60_4_22a_4a_4a-001 Z0HK
- Monoclinic KH_2PO_4:
  A5B2C8D2_mP68_4_10a_4a_16a_4a-001 MD4G

C2 (**5**):

- $(Ba,Ca)CO_3$ ("$C2$"):
  ABC3_mC10_5_b_a_ac-001 6HGL
- $A19$ Po (*Obsolete*):
  A_mC12_5_3c-001 FECP
- $NbAs_2$:
  A2B_mC12_5_2c_c-001 0898
- $D0_{15}$ ($AlCl_3$) (*Obsolete*):
  AB3_mC16_5_c_3c-001 RSL8
- $CrPS_4$:
  ABC4_mC24_5_2a_c_4c-001 VB2Y
- $Rb_2CaCu_6(PO_4)_4O_2$:
  AB6C18D4E2_mC62_5_b_2a2c_9c_2c_c-001 74YK
- $Al_{17}Mo_4$:
  A17B4_mC84_5_ab16c_4c-001 QL9A
- Bassanite [$CaSO_4(H_2O)_{0.5}$, $H4_7$]:
  A2B2C9D2_mC90_5_ab2c_3c_a13c_3c-001 Q14S
- α-$Bi_4V_2O_{11}$:
  A3B9C2_mC112_5_6c_2a2b16c_4c-001 JBQX
- High temperature Monoclinic TlS:
  AB_mC256_5_2a2b30c_32c-001 J6WY

Pm (**6**):

- Tetrataenite (FeNi):
  AB_mP4_6_2a_2b-001 X3MC
- Mo_8P_5:
  A8B5_mP13_6_5a3b_2a3b-001 LEL6
- Ta_5Ti_{11} (BCC SQS-16):
  A5B11_mP16_6_2abc_2a3b3c-001 EUM5

Pc (**7**):

- H_2S IV:
  A2B_mP12_7_4a_2a-001 UVJS
- Calaverite ($AuTe_2$):
  AB2_mP12_7_2a_4a-001 G433
- ϵ-WO_3 (low-temperature):
  A3B_mP16_7_6a_2a-001 SUKZ
- $BaAs_2$:
  A2B_mP18_7_6a_3a-001 34FL
- Rh_2Ga_9:
  A9B2_mP22_7_9a_2a-001 2DRY
- Monoclinic $Bi_4Ti_3O_{12}$ $m = 3$ Aurivillius:
  A4B12C3_mP38_7_4a_12a_3a-001 S41T
- $Na_2Ca_6Si_4O_{15}$:
  A6B2C15D4_mP54_7_6a_2a_15a_4a-001 5V2T
- Low temperature Mo_8O_{23}:
  A8B23_mP124_7_16a_46a-001 5T76

Cm (**8**):

- $F5_{11}$ (KNO_2) (*Obsolete*):
  ABC2_mC8_8_a_a_b-001 X9AR
- Monoclinic PZT [$Pb(Zr_xTi_{1-x})O_3$]:
  A3BC_mC10_8_ab_a_a-001 XHKF
- Base-Centered Monoclinic La_2CuO_4:
  AB2C4_mC28_8_2a_4a_4a2b-001 T7TZ
- Al_4W:
  A4B_mC30_8_2a5b_ab-001 10PS
- $TaTi_3$-II (BCC SQS-16):
  AB3_mC32_8_4a_4a4b-001 P5PQ
- $TaTi_3$-I (BCC SQS-16):
  AB3_mC32_8_4a_12a-001 QVN8
- Monoclinic Co_4Al_{13}:
  A13B4_mC102_8_17a11b_8a2b-001 DU5A

Cc (**9**):

- H_3Cl (20 GPa):
  AB3_mC16_9_a_3a-001 QYSB
- Room temperature Ga_2Se_3:
  A2B3_mC20_9_2a_3a-001 4F67
- In_2Te_5 (I):
  A2B5_mC28_9_2a_5a-001 FD0C
- α-P_3N_5:
  A5B3_mC32_9_5a_3a-001 9173
- $CuInP_2S_6$:
  A2BC2D6_mC44_9_2a_a_2a_6a-001 G59D
- $GeCd_4S_6$:
  A4BC6_mC44_9_4a_a_6a-001 ZP3W
- Chrysotile [$Mg_3Si_2O_5(OH)_4$]:
  A3B5C4D2_mC56_9_3a_5a_4a_2a-001 BT10
- Nacrite [$Al_2Si_2O_5(OH)_4$, $S5_4$]:
  A2B4C9D2_mC68_9_2a_4a_9a_2a-001 SDY7
- Monoclinic (Cc) Low Tridymite (SiO_2):
  A2B_mC144_9_24a_12a-001 MK0W
- $Cs_6W_{11}O_{36}$:
  A6B36C11_mC212_9_6a_36a_11a-001 A3V8
- α-$LiZnPO_4$:
  AB4CD_mC224_9_8a_32a_8a_8a-001 L704

P2/m (**10**):

- δ-Pd_2Cl:
  A2B_mP6_10_mn_bc-001 ZWXH

- α-LiSn:
  AB_mP6_10_bn_cm-001 QVV1
- Muthmannite ($AuAgTe_2$):
  ABC2_mP8_10_ac_eh_mn-001 ALSR
- S-carbon:
  A_mP8_10_2m2n-001 XRQ1
- H_3Cl (400 GPa):
  AB3_mP16_10_mn_3m3n-001 1EYW
- Hulsite [$(Fe_{1.315}Mg_{0.56}Sn_{0.1})BO_5$]:
  A2B2C3D10E_mP18_10_m_ac_en_3m2n_g-001 8URQ

$P2_1/m$ (11):

- NiTi:
  AB_mP4_11_e_e-001 WBFX
- YO(OH):
  ABC_mP6_11_e_e_e-001 LNCX
- $CaSb_2$:
  AB2_mP6_11_e_2e-001 5Q2X
- $ZrSe_3$:
  A3B_mP8_11_3e_e-001 54KB
- $EuFeAs_2$:
  A2BC_mP8_11_2e_e_e-001 C60C
- $KClO_3$ ($G0_6$):
  ABC3_mP10_11_e_e_ef-001 RT35
- Mo_2S_3:
  A2B3_mP10_11_2e_3e-001 MUP5
- $SbAsO_2$:
  AB4C_mP12_11_e_2ef_e-001 C55J
- α-Pu:
  A_mP16_11_8e-001 2MX7
- β-$NbPt_3$:
  AB3_mP16_11_2e_2e2f-001 A6R9
- $K_2S_2O_5$ ($K0_1$):
  A2B5C2_mP18_11_2e_e2f_2e-001 YYGA
- Barytocalcite ($BaCa(CO_3)_2$):
  AB2CD6_mP20_11_e_2e_e_2e2f-001 YSME
- Squaric Acid ($H_2C_4O_4$):
  A2BC2_mP20_11_4e_2e_4e-001 0Y6Q
- Li_7Sn_3:
  A7B3_mP20_11_7e_3e-001 YDAL
- y-$Y_2Si_2O_7$:
  A7B2C2_mP22_11_3e2f_2e_ab-001 3RSG
- Pt_6Si_5:
  A6B5_mP22_11_6e_5e-001 H63U
- $NbSe_3$:
  AB3_mP24_11_3e_9e-001 4LKF
- Ho_2S_3:
  A2B3_mP30_11_6e_9e-001 TWS9

C2/m (12):

- α-O_2:
  A_mC4_12_i-001 M3W6
- Calaverite ($AuTe_2$, $C34$):
  AB2_mC6_12_a_i-001 1QX2
- Tolbachite ($CuCl_2$):
  A2B_mC6_12_i_a-001 PNDR
- NiO_2:
  AB2_mC6_12_a_i-003 DZY0
- α-HgO_2:
  AB2_mC6_12_a_i-004 RMCX
- CaC_2-III:
  A2B_mC12_12_2i_i-004 2JVM
- α-Bi_2Pd:
  A2B_mC12_12_2i_i-006 0NDQ
- $OsGe_2$:
  A2B_mC12_12_2i_i-007 RQLL
- RuU_2:
  AB2_mC12_12_i_aci-001 6TPG
- GdCBr:
  ABC_mC12_12_i_i_i-003 69PJ
- Au_5Mn_2:
  A5B2_mC14_12_a2i_i-001 9H7D
- δ-Ni_3Sn_4 ($D7_a$):
  A3B4_mC14_12_ai_2i-001 4WTF
- Brezinaite (Cr_3S_4):
  A3B4_mC14_12_ai_2i-002 17US
- $AlCl_3$:
  AB3_mC16_12_g_ij-001 2SQ0
- M-carbon:
  A_mC16_12_4i-001 MTF0
- Monoclinic $FeTlSe_2$:
  AB2C_mC16_12_g_2i_i-001 JGDH
- SrN:
  AB_mC16_12_2i_2i-001 ASFW
- β-BiI:
  AB_mC16_12_2i_2i-002 DA8J
- γ-BiI:
  AB_mC16_12_2i_2i-003 6RE9
- CoGe:
  AB_mC16_12_aci_2i-001 7BKU
- $K_2Ti_2O_5$:
  A2B5C2_mC18_12_i_a2i_i-001 JYHJ
- $NbTe_2$:
  AB2_mC18_12_ai_3i-002 FY6X
- Ta_2PdSe_6:
  AB6C2_mC18_12_a_3i_i-004 H8PR
- β-Ga_2O_3:
  A2B3_mC20_12_2i_3i-001 LKDZ
- $MnPS_3$:
  ABC3_mC20_12_g_i_ij-001 UPGR
- α-As_2Te_3:
  A2B3_mC20_12_2i_3i-003 8W6Z
- Au_2P_3:
  A2B3_mC20_12_eh_ij-001 PQQZ
- Mo_2As_3:
  A3B2_mC20_12_3i_2i-001 8QA4
- Gd_2Cl_3:
  A3B2_mC20_12_3i_2i-002 TUQ7
- Thortveitite ($[Sc,Y]_2Si_2O_7$, $S2_1$):
  A7B2C2_mC22_12_aij_h_i-001 0J1F
- Al_8Mo_3:
  A8B3_mC22_12_4i_ai-001 1Y1T
- LiOH·H_2O ($B36$):
  A3BC2_mC24_12_ij_g_hi-001 T76D
- $AlNbO_4$:
  ABC4_mC24_12_i_i_4i-001 HK1Y
- SiAs:
  AB_mC24_12_3i_3i-001 S6UY
- Li_2MnO_3:
  A2BC3_mC24_12_acg_h_ij-002 R3L4
- Nb_2Se:
  A2B_mC24_12_4i_2i-004 2691
- $Ag_3LiIr_2O_6$:
  A3B2CD6_mC24_12_ag_h_c_ij-001 ZSJ2
- $Li_3Zn_2SbO_6$:
  A3B6CD2_mC24_12_ag_ij_c_h-001 72ZM
- Y_5S_7:
  A7B5_mC24_12_a3i_c2i-001 G5Z0
- Pd_5As:
  AB5_mC24_12_i_g2ij-001 XSQ7

- Predicted ζ-$LiAlO_2$:
  ABC2_mC24_12_ah_cg_ij-001 JWKX
- V_5S_8:
  A8B5_mC26_12_2ij_ahi-001 ZQW6
- Hollandite ($BaMn_2O_4$):
  AB4C8_mC26_12_a_2i_4i-001 50AM
- $TlCr_5Se_8$:
  A5B8C_mC28_12_a2i_4i_c-001 AFXE
- $Au_{11}Mn_3$:
  A11B3_mC28_12_a5i_ci-001 J58A
- $CoZn_{13}$:
  AB13_mC28_12_a_c2i2j-001 6H3E
- $PuNi_4$:
  A4B_mC30_12_gi2j_ai-001 WBF9
- Cr_7Se_8:
  A7B8_mC30_12_aehi_2ij-001 H4M1
- Dolerophanite [$Cu_2O(SO_4)$]:
  A2B5C_mC32_12_ei_3ij_i-001 H100
- Sc_3RhC_4:
  A4BC3_mC32_12_2j_i_ghi-002 2TGL
- α-BiI:
  AB_mC32_12_4i_4i-001 DK3T
  - β-Pu:
    A_mC34_12_ah3i2j-001 VV4N
  - Os_4Al_{13}:
    A13B4_mC34_12_a6i_2i-001 XT4N
- Metastable PbV_2O_6:
  A6BC2_mC36_12_6i_i_2i-001 X6VQ
  - Sr_2NiTeO_6:
    AB6C2D_mC40_12_ac_gh4i_j_bd-001 79Y1
- $Pr_5Co_2Ge_4$:
  A2B3C5_mC40_12_2i_3i_5i-001 422U
  - Bischofite ($MgCl_2{\cdot}6H_2O$, $J1_7$):
    A2B12CD6_mC42_12_i_2i2j_a_ij-001 3SX5
- Nb_7P_4:
  A7B4_mC44_12_ac6i_4i-001 EWT8
  - $D2_2$ ($MgZn_5$?) (*Problematic*):
    AB5_mC48_12_2i_ac5i2j-001 5R9K
  - Sanidine ($KAlSi_3O_8$, $S6_7$):
    AB8C4_mC52_12_i_gi3j_2j-001 JF0M
- Radtkeite (Hg_3S_2ClI):
  AB3CD2_mC56_12_2i_eg2ij_2i_2j-001 4UG2
- NiBi:
  A16B17_mC66_12_4i2j_aeh4ij-001 V4P2
  - Tremolite ($Ca_2Mg_5Si_8O_{22}(OH)_2$ $S4_2$):
    A2B2C5D24E8_mC82_12_h_i_agh_2i5j_2j-001 BQ7Y
- Monoclinic $Nb_{12}O_{29}$:
  A12B29_mC82_12_6i_a14i-001 BPW1
  - Staurolite ($H_2Al_5Fe_2Si_2O_{12}$):
    A5B2C2D10E2_mC84_12_acghj_bdi_2i_5j_j-001 QHVX
  - $Al_{13}Fe_4$:
    A13B4_mC102_12_ah8i5j_4ij-001 U8YR
- $Al_{45}V_7$:
  A45B7_mC104_12_a8i7j_cij-001 4Z2U
  - Manganese-leonite [$K_2Mn(SO_4)_2{\cdot}4H_2O$, $H4_{23}$]:
    A8B2CD15E2_mC112_12_2i3j_j_ac_g4i5j_2i-001 KYS8
  - Chrysotile [$Mg_6O_{11}Si_4(H_2O)(OH)_6$, $S4_5$]:
    AB6C11D6E4_mC112_12_e_gi2j_i5j_2i2j_2j-001 CNLR

P2/c (13):

- Sylvanite ($AgAuTe_4$, $E1_b$):
  ABC4_mP12_13_e_a_2g-001 5BWB
  - H_2S (15 GPa):
    A2B_mP12_13_2g_ef-001 VYK4
  - Huanzalaite ($MgWO_4$, $H0_6$):
    AB4C_mP12_13_e_2g_f-003 2SHQ
- $AgCrP_2S_6$:
  ABC2D6_mP20_13_e_e_g_3g-001 NDG5
- $NaIn(WO_4)_2$:
  ABC8D2_mP24_13_e_f_4g_g-001 7246
- $Cu(PtS_2)_2$:
  AB2C4_mP28_13_g_efg_4g-001 HFY3
- Room temperature V_3O_5:
  A5B3_mP32_13_ef4g_ab2g-001 3J3M
- Rosickýite (γ-monoclinic Sulfur):
  A_mP32_13_8g-001 Y7J6
- Monoclinic (II) $Ba_3CoIr_2O_9$:
  A3BC2D9_mP60_13_ef2g_ab_2g_ef8g-001 2BLQ
  - Approximate High temperature Mo_8O_{23}:
    A8B23_mP62_13_4g_a11g-001 UWFW
  - Monoclinic (Hittorf's) Phosphorus:
    A_mP84_13_21g-001 SEQF

$P2_1/c$ (14):

- γ-$PdCl_2$:
  A2B_mP6_14_e_a-001 K9AG
- CdP_4:
  AB4_mP10_14_a_2e-001 L3ZV
  - Baddeleyite (ZrO_2, $C43$):
    A2B_mP12_14_2e_e-001 5CSN
  - Arsenopyrite (FeAsS, $E0_7$):
    ABC_mP12_14_e_e_e-002 RH3X
- Acanthite (Ag_2S):
  A2B_mP12_14_2e_e-011 0GFL
- $NdAs_2$:
  A2B_mP12_14_2e_e-012 5BM7
  - $HgCl_2{\cdot}2HgO$:
    A2B3C2_mP14_14_e_ae_e-001 AR8A
  - "$P2_1/c$"-B_2H_6:
    AB3_mP16_14_e_3e-002 3XCA
  - β-B_2H_6:
    AB3_mP16_14_e_3e-003 WZYX
  - KNO_2 III:
    ABC2_mP16_14_e_e_2e-003 JSKP
  - Manganite (γ-MnO(OH), $E0_6$):
    ABC2_mP16_14_e_e_2e-004 E23Q
  - Cu(OH)Cl:
    ABCD_mP16_14_e_e_e_e-001 CH4P
  - α-ICl:
    AB_mP16_14_2e_2e-001 HU5N
  - LiAs:
    AB_mP16_14_2e_2e-002 LRN3
- Luberoite (Pt_5Se_4):
  A5B4_mP18_14_a2e_2e-001 1FWE
- Phase I K_2SnCl_6:
  A6B2C_mP18_14_3e_e_a-001 C2DK
  - Orpiment (As_2S_3, $D5_f$):
    A2B3_mP20_14_2e_3e-002 4PSJ
  - Sanguite ($KCuCl_3$):
    A3BC_mP20_14_3e_e_e-001 M9HY
  - Sr_2MnTeO_6:
    AB6C2D_mP20_14_a_3e_e_b-001 QXEE
  - Cryolite (Na_3AlF_6, $J2_6$):
    AB6C3_mP20_14_a_3e_be-001 G2BV

- α-$SrRh_2As_2$:
  A2B2C_mP20_14_2e_2e_e-001 1XXN
- α-Bi_2O_3:
  A2B3_mP20_14_2e_3e-003 7G59
- Y_2OS_2:
  AB2C2_mP20_14_e_2e_2e-001 A73U
  - $Sb_4O_5Cl_2$:
    A2B5C4_mP22_14_e_a2e_2e-001 YL8Z
  - $K_2Ni(CN)_4$:
    A4B2C4D_mP22_14_2e_e_2e_a-001 RARL
  - Co_2Al_9 ($D8_d$):
    A9B2_mP22_14_a4e_e-001 T95J
- $Er_2Si_2O_7$:
  A2B7C2_mP22_14_e_a3e_e-001 WKQU
- Juangodoyite [$Na_2Cu(CO_3)_2$]:
  A2BC2D6_mP22_14_e_a_e_3e-001 DUCH
  - γ-$Y_2Si_2O_7$:
    A4BC_mP24_14_4e_e_e-001 3TA1
  - Anhydrous $KAuBr_4$:
    AB4C_mP24_14_ab_4e_e-001 2L05
  - Ammonium Persulfate [$(NH_4)SO_4$, $K4_1$]:
    AB4C_mP24_14_e_4e_e-001 1E0C
  - Monasite ($LaPO_4$):
    AB4C_mP24_14_e_4e_e-002 G325
  - $AgMnO_4$ ($H0_9$):
    ABC4_mP24_14_e_e_4e-001 8H0D
  - Nahcolite ($NaHCO_3$, $G0_{12}$):
    ABCD3_mP24_14_e_e_e_3e-001 KV55
  - ϵ-1,2,3,4,5,6-Hexachloro*cyclo*hexane (C_6Cl_6):
    AB_mP24_14_3e_3e-001 7TV0
- Monoclinic (black) ZnP_2:
  A2B_mP24_14_4e_2e-001 BW3Z
- β-Tl_2TeO_3:
  A3BC2_mP24_14_3e_e_2e-001 8M4S
- $AgTe_2Tl_3$:
  AB2C3_mP24_14_e_2e_3e-001 XDSH
- $CuTeO_4$:
  AB4C_mP24_14_ac_4e_e-001 LRGD
- $GaPS_4$:
  ABC4_mP24_14_e_e_4e-002 VQV1
  - Monoclinic Cu_2OSeO_3:
    A2B4C_mP28_14_abe_4e_e-001 D0DK
  - $KICl_4{\cdot}H_2O$ ($H0_{10}$):
    A4BCD_mP28_14_4e_e_e_e-001 YLSG
- Larnite (β-Ca_2SiO_4):
  A2B4C_mP28_14_2e_4e_e-001 QE0P
- Pyrostilpnite (Ag_3SbS_3):
  A3B3C_mP28_14_3e_3e_e-001 8N0K
- Tl_4S_3:
  A3B4_mP28_14_3e_4e-001 6ZEC
- Pd_6P:
  AB6_mP28_14_e_6e-001 VTUH
  - Azurite [$Cu_3(CO_3)_2(OH)_2$, $G7_4$]:
    A2B3C2D8_mP30_14_e_ae_e_4e-001 QANU
  - β-Se (A_l):
    A_mP32_14_8e-001 QMXV
  - Ca_2UO_5:
    A2B5C_mP32_14_2e_5e_ab-001 E7S8
  - Gd_2SiO_5 (RE_2SiO_5 X1):
    A2B5C_mP32_14_2e_5e_e-001 HBLG
  - γ-WO_3:
    A3B_mP32_14_6e_2e-001 S4UY
  - $KAuBr_4{\cdot}2H_2O$ ($H4_{19}$):
    AB4C2D_mP32_14_e_4e_2e_e-001 SAP5
  - Pararealgar (AsS):
    AB_mP32_14_4e_4e-001 WH80
  - Realgar (AsS, B_l):
    AB_mP32_14_4e_4e-002 R9YN
- Monoclinic (II) Li_2FeSiO_4:
  AB2C4D_mP32_14_e_2e_4e_e-001 U7VZ
- Lorándite ($TlAsS_2$):
  AB2C_mP32_14_2e_4e_2e-001 QZUF
- Monoclinic ClF_3:
  AB3_mP32_14_2e_6e-001 4D8B
- NaGe:
  AB_mP32_14_4e_4e-003 05NC
- NS:
  AB_mP32_14_4e_4e-004 YXLR
- α-monoclinic Selenium:
  A_mP32_14_8e-002 VEFR
- N-Hydroxyurea ($CH_4N_2O_2$):
  AB4C2D2_mP36_14_e_4e_2e_2e-001 XWQW
  - K_2NbF_7 ($K6_2$):
    A7B2C_mP40_14_7e_2e_e-001 TF3J
- α-$Ca_2P_2O_7$:
  A2B7C2_mP44_14_2e_7e_2e-001 9VRC
- α-$Na_2CuP_2O_7$:
  AB2C7D2_mP48_14_e_2e_7e_2e-001 8Z5C
- Clinometaborite (β-HBO_2, monoclinic):
  ABC2_mP48_14_3e_3e_6e-001 XNVP
- $Ce_7Pd_4Ge_2$:
  A7B2C4_mP52_14_7e_2e_4e-001 N56L
  - $K_2Pt(SCN)_6{\cdot}\ 2H_2O$:
    A6B4C2D6E2FG6_mP54_14_3e_2e_e_3e_e_a_3e-001 0UZV
  - $Cs_{11}O_3$:
    A11B3_mP56_14_11e_3e-001 2343
  - Parawollastonite ($CaSiO_3$, $S3_3$(II)):
    AB3C_mP60_14_3e_9e_3e-001 XADC
  - α-Se (A_k):
    A_mP64_14_16e-001 TBFR
- β-monoclinic Sulfur:
  A_mP64_14_16e-002 AYZW
- Monoclinic $Fe_2(SO_4)_3$:
  A2B12C3_mP68_14_2e_12e_3e-001 LK3Z
  - Tutton salt [$Cu(NH_4)_2(SO_4)_2{\cdot}H_2O$, $H4_4$]:
    AB20C2D14E2_mP78_14_a_10e_e_7e_e-001 KT73
  - Manganese-leonite 110K [$K_2Mn(SO_4)_2{\cdot}4H_2O$]:
    A8B2CD12E2_mP100_14_8e_2e_ab_12e_2e-001 V1SG
  - α-Toluene (C_7H_8):
    A7B8_mP120_14_14e_16e-001 NQ3P
- High temperature Bi_2MoO_6:
  A2BC6_mP144_14_8e_4e_24e-001 UYPX
- $Ag(tcm)(phz)_{1/2}$ ($AgC_{10}N_4H_4$):
  AB10C4D4_mP152_14_2e_20e_8e_8e-001 JN9W
- Monoclinic 2-4-6 Trinitrotoluene ($C_7H_5N_3O_6$):
  A7B5C3D6_mP168_14_14e_10e_6e_12e-001 MUZR
- [Zn_2(Benzoato)$_4$(Caffeine)$_2$]·2 Caffeine ($C_{30}H_{30}N_8O_8Zn$):
  A30B30C8D8E_mP308_14_30e_30e_8e_8e_e-001 6QN7

C2/c (15):

- β-Ga (*Obsolete*):
  A_mC4_15_e-001 BRYB
- Tenorite (CuO, $B26$):
  AB_mC8_15_a_e-001 HRJX
- CrS:
  AB_mC8_15_a_e-003 H6Z8
- ThC_2 (C_g):
  A2B_mC12_15_f_e-001 SKBR

- PdP_2:
  A2B_mC12_15_f_a-001 SPK1
- H_3Cl (50 GPa):
  AB3_mC16_15_e_af-001 T96Y
- $KFeS_2$ ($F5_a$):
  ABC2_mC16_15_e_e_f-004 G8C6
- Ag_2PbO_2:
  A2B2C_mC20_15_ac_f_e-001 8GWY
- CrP_4:
  AB4_mC20_15_e_2f-001 2S3X
- H-III (300 GPa):
  A_mC24_15_2e2f-001 MULK
- Clinocervantite (β-Sb_2O_4):
  A2B_mC24_15_2f_ae-001 YM7H
- Zabuyelite (Li_2CO_3):
  AB2C3_mC24_15_e_f_ef-001 JF5W
- B_2Pd_5:
  A2B5_mC28_15_f_e2f-001 CZ5K
- ζ-Nb_2O_5 (B-Nb_2O_5):
  A2B5_mC28_15_f_e2f-003 S3CP
- Monoclinic Ni_4B_3:
  A3B4_mC28_15_ef_2f-001 XJ9R
- Ta_2NiSe_5:
  AB5C2_mC32_15_e_e2f_f-001 YFLU
- Titanite ($CaTiSiO_5$, $S0_6$):
  AB5CD_mC32_15_e_e2f_e_a-001 EDTK
- Oxyvanite (V_3O_5):
  A5B3_mC32_15_e2f_af-003 C32G
- Miargyrite ($AgSbS_2$):
  AB2C_mC32_15_ae_2f_f-001 YUVG
- β'-$LiFeO_2$:
  ABC2_mC32_15_2e_2e_2f-002 VG40
- NSe:
  AB_mC32_15_2ef_2f-001 RDBP
- NaSi:
  AB_mC32_15_2f_2f-001 58NH
- $Rb_2C_2O_4{\cdot}H_2O$:
  A2BC4D2_mC36_15_f_e_2f_f-001 RBDM
- Foordite ($SnNb_2O_6$):
  A2B6C_mC36_15_f_3f_e-001 6QBH
- Esseneite ($CaFeSi_2O_6$):
  ABC6D2_mC40_15_e_e_3f_f-001 5WH8
- Diopside [$CaMg(SiO_3)_2$, $S4_1$]:
  ABC6D2_mC40_15_e_e_3f_f-002 J45L
- $Lu_2Co_3Si_5$:
  A3B2C5_mC40_15_ef_f_3ef-001 1Q2N
- VS_4:
  A4B_mC40_15_4f_f-001 6M9R
- $CoGeO_3$:
  ABC3_mC40_15_2e_f_3f-001 6YLQ
- α-$Zn_2V_2O_7$:
  A7B2C2_mC44_15_e3f_f_f-001 JMLC
- η'-Cu_6Sn_5:
  A6B5_mC44_15_ae2f_e2f-001 LPH7
- Coesite (SiO_2):
  A2B_mC48_15_ae3f_2f-001 QHEE
- Na_2PrO_3:
  A2B3C_mC48_15_aef_3f_2e-001 NFQU
- Gypsum ($CaSO_4{\cdot}2H_2O$, $H4_6$):
  AB4C6D_mC48_15_e_2f_3f_e-001 8924
- α-SnF_2:
  A2B_mC48_15_4f_2f-001 YKEJ
- β-$Na_2CuP_2O_7$:
  AB2C7D2_mC48_15_a_f_e3f_f-001 9DDX
- Wodginite ($LiFe(WO_4)_2$):
  ABC8D2_mC48_15_e_e_4f_f-001 013B
- $BaNi(CN)_4{\cdot}4H_2O$ ($H4_{22}$):
  AB4C4D4E_mC56_15_e_2f_2f_2f_a-001 QDTB
- Xanthoconite (Ag_3AsS_3):
  A3BC3_mC56_15_3f_f_3f-001 HRK9
- Ta_6S:
  AB6_mC56_15_f_6f-001 HXME
- Monoclinic (I) $Ba_3CoIr_2O_9$:
  A3BC2D9_mC60_15_ef_a_f_e4f-001 G3XE
- Monoclinic Pyrrhotite (Fe_7S_8):
  A7B8_mC60_15_e3f_4f-001 L5GZ
- Y_2SiO_5 (RE_2SiO_5 X2):
  A5BC2_mC64_15_5f_f_2f-001 G8V5
- Pyrophyllite [$AlSi_2O_5(OH)$, $S5_6$]:
  AB5CD2_mC72_15_f_5f_f_2f-001 J4ZX
- Rhodan Hydrate ($H_2C_2N_2S_2O$):
  A2B2C2DE2_mC72_15_2f_2f_2f_f_2f-001 UX1J
- Muscovite ($KH_2Al_3Si_3O_{12}$, $S5_1$):
  A2BC10D2E4_mC76_15_f_e_5f_f_2f-001 8J4A
- Alluaudite [$NaMnFe_2(PO_4)_3$]:
  A2BCD12E3_mC76_15_f_e_a_6f_ef-001 8ZWK
- In_2Te_5 (II):
  A2B5_mC84_15_3f_e7f-001 A3RY
- Smithite ($AgAsS_2$):
  ABC2_mC96_15_2e2f_3f_6f-001 69FP
- Clinochlore [$Mg_3(Mg_2Al)(Si_3Al)O_{10}(OH)_8$, $S5_5$]:
  A3B5C4D2_mC112_15_a3ef_5f_4f_2f-001 RDRH
- Eudidymite ($BeHNaO_8Si_3$):
  A2B4C2D17E6_mC124_15_f_2f_f_e8f_3f-001 AU9C
- MoP_3SiO_{11} (Monoclinic Model):
  AB11C3D_mC128_15_f_ae10f_3f_f-001 2HE4
- Catapleiite ($Na_2ZrSi_3O_9{\cdot}2H_2O$):
  A2B3C9D3E_mC144_15_2f_abcef_9f_3f_de-001 L4VZ
- Low temperature Cu_2Se:
  A2B_mC144_15_12f_6f-001 F9TK
- $Rb_2Cu2(MoO_4)_3$:
  A2B3C12D2_mC152_15_2f_3f_12f_aef-001 A42Z
- $(CdSO_4)_3{\cdot}8H_2O$ ($H4_{20}$):
  A3B16C20D3_mC168_15_ef_8f_10f_ef-001 VXAE
- Manganese-leonite 185K [$K_2Mn(SO_4)_2{\cdot}4H_2O$]:
  A8B2CD12E2_mC200_15_8f_2f_ae_2e11f_2f-001 5SVW

P222 (16):

- $AlPS_4$:
  ABC4_oP12_16_ae_bd_2u-001 8PL6

$P222_1$ (17):

- α-Naumannite (Ag_2Se):
  A2B_oP12_17_abe_e-001 G353
- $NaNbO_3$:
  ABC3_oP40_17_abcd_2e_abcd4e-001 D6BJ

$P2_12_12$ (18):

- γ-TeO_2 (*Erroneous*):
  A2B_oP12_18_2c_c-001 4QQ6
- BaS_3 (original $D0_{17}$):
  AB3_oP16_18_ab_3c-001 69TS
- Diamminetriamidodizinc Chloride ([$Zn_2(NH_3)_2(NH_2)_3$]Cl):
  AB12C5D2_oP40_18_a_6c_b2c_c-001 5HSN

$P2_12_12_1$ (19):

- Nauminnite (Ag_2Se II):
  A2B_oP12_19_2a_a-001 LU1L
- β-SnF_2:
  A2B_oP12_19_2a_a-002 RZ21
- H_3Cl (100 GPa):
  AB3_oP16_19_a_3a-001 WTE4
- NaP:
  AB_oP16_19_2a_2a-001 MEBJ
- Wülfingite (ϵ-$Zn(OH)_2$, C31):
  A2B2C_oP20_19_2a_2a_a-001 HY2J
- $NaAlCl_4$:
  AB4C_oP24_19_a_4a_a-001 43KD
- $Nd_2Si_2O_7$:
  A2B7C2_oP44_19_2a_7a_2a-001 TYGX
- Ferroelectric $(NH_4)H_2PO_4$:
  A6BC4D_oP48_19_6a_a_4a_a-001 P6ME
- β-Arabinose $(CO_2H)_{20}$:
  AB2C_oP80_19_5a_10a_5a-001 K9SN
- Ca-Malate-dihydrate ($CaC_4H_4O_5{\cdot}2H_2O$):
  A4BC8D7_oP80_19_4a_a_8a_7a-001 RRH1
- Morenosite ($NiSO_4{\cdot}7H_2O$, $H4_{12}$):
  A14BC11D_oP108_19_14a_a_11a_a-001 S9KY

$C222_1$ (20):

- $D0_7$ (CrO_3) (*Obsolete*):
  AB3_oC16_20_a_bc-001 KCMH
- Orthorhombic (High) Tridymite (SiO_2):
  A2B_oC24_20_abc_c-001 NDBQ
- $AlPO_4$ "low cristobalite type":
  AB4C_oC24_20_a_2c_b-001 HRBV
- $K3_3$ (Tl_2AlF_5):
  AB5C2_oC32_20_a_2abc_c-001 XBH3
- Na_2Tl:
  A2B_oC48_20_ab3c_2c-001 PRYE

C222 (21):

- Ta_2H:
  AB2_oC6_21_a_k-001 6XPU
- $HoSb_2$:
  AB2_oC6_21_a_k-002 DD5U
- Godlevskite (Ni_9S_8):
  A9B8_oC68_21_acehik2l_4l-001 L6M4

F222 (22):

- Low temperature FeS:
  AB_oF8_22_a_c-001 H691
- $CeRu_2B_2$:
  A2BC2_oF40_22_ej_ac_fi-001 PN0D
- Predicted Phase IV $Cd_2Re_2O_7$:
  A2B7C2_oF88_22_k_acefghij_k-001 71CA

I222 (23):

- BPS_4:
  ABC4_oI12_23_a_b_k-001 ZCCT
- $NaFeS_2$:
  ABC2_oI16_23_ac_e_k-001 J362
- H_3S (5 GPa):
  A3B_oI32_23_ef2k_k-001 4LGD
- Stannoidite ($Cu_8(Fe,Zn)_3Sn_2S_{12}$):
  A8B2C12D2E_oI50_23_acgk_e_3k_f_b-001 7NS2

$I2_12_12_1$ (24):

- Weberite (Na_2MgAlF_7):
  AB7CD2_oI44_24_a_c3d_b_ab-001 Q6TN

Pmm2 (25):

- High-pressure CdTe:
  AB_oP2_25_a_b-001 CPSQ

$Pmc2_1$ (26):

- H_2S 70 GPa:
  A2B_oP12_26_abc_ab-001 PC8F
- β-SeO_2:
  A2B_oP12_26_abc_ab-002 2MYY
- Metastable Au_5Zn_3:
  A5B3_oP16_26_a2c_a2b-001 PD7K
- TlP_5:
  A5B_oP24_26_3a3b2c_ab-001 AHE7
- γ-SeO_2:
  A2B_oP24_26_2a2b2c_2a2b-001 PVJF
- Low temperature $SmBaMn_2O_6$:
  AB2C6D_oP40_26_2a_2c_2a2b4c_2b-001 LDXU

Pcc2 (27):

- $Ca_4Al_6O_{16}S$:
  A6B4C16D_oP108_27_abcd4e_4e_16e_e-001 TBPX

Pma2 (28):

- Krennerite ($AuTe_2$):
  AB2_oP24_28_acd_2c3d-001 A9SX

$Pca2_1$ (29):

- ZrO_2:
  A2B_oP12_29_2a_a-001 UZKW
- Low temperature Pyrite (FeS_2):
  AB2_oP12_29_a_2a-001 09UM
- Cobaltite (CoAsS):
  ABC_oP12_29_a_a_a-001 8UWB
- Mercury (II) Azide $[Hg(N_3)_2]$:
  AB6_oP28_29_a_6a-001 KSW9
- Koechlinite (Room temperature Bi_2MoO_6):
  A2BC6_oP36_29_2a_a_6a-001 UQQ3
- Low temperature Bornite (Cu_5FeS_4):
  A5BC4_oP160_29_20a_4a_16a-001 H7LS
- Orthorhombic 2-4-6 Trinitrotoluene ($C_7H_5N_3O_6$):
  A7B5C3D6_oP168_29_14a_10a_6a_12a-001 EY4Y
- Low temperature $(NH_3CH_3)Al(SO_4)_2 \cdot 12H_2O$:
  ABC30DE20F2_oP220_29_a_a_30a_a_20a_2a-001 2B7C

Pnc2 (30):

- *Pnc*2 $CuBrSe_3$:
  ABC3_oP20_30_2a_c_3c-001 2SVA
- $Bi_5Nb_3O_{15}$:
  A5B3C15_oP46_30_a2c_bc_a7c-001 ABT7

$Pmn2_1$ (31):

- Guyanaite (β-CrOOH):
  ABC2_oP8_31_a_a_2a-001 TZ68
- WTe_2:
  A2B_oP12_31_4a_2a-001 ZLWB
- Shcherbinaite ($D8_7$, V_2O_5) (*Obsolete*):
  A5B2_oP14_31_a2b_b-001 T4NG
- Enargite ($AsCu_3S_4$, $H2_5$):
  AB3C4_oP16_31_a_ab_2ab-001 LOGQ
- β-Li_3PO_4:
  A3B4C_oP16_31_ab_2ab_a-002 0L2F
- B_4SrO_7:
  A4B7C_oP24_31_2b_a3b_a-001 DLX0
- Clinobarylite ($BaBe_2Si_2O_7$):
  AB2C7D2_oP24_31_a_b_a3b_b-001 WL10
- Seligmannite ($PbCuAsS_3$):
  ABCD3_oP24_31_2a_b_2a_2a2b-001 2RFK
- $Mg(ClO_4)_2{\cdot}6H_2O$ ($H4_{11}$):
  A2B6CD8_oP34_31_2a_2a2b_a_4a2b-001 ZN0T

- Orthorhombic Co_4Al_{13} (Approximate Quasicrystal):
  A13B4_oP102_31_17a11b_8a2b-001 DHFF

Pba2 (32):
- $Re_2O_5(SO_4)_2$:
  A13B2C2_oP34_32_a6c_c_c-001 16XX
- $Mo_{17}O_{47}$:
  A17B47_oP128_32_a8c_a23c-001 484W

$Pna2_1$ (33):
- Modderite (CoAs):
  AB_oP8_33_a_a-001 8Z7Q
- $LiGaO_2$:
  ABC2_oP16_33_a_a_2a-003 9S7L
- γ-$LiIO_3$:
  ABC3_oP20_33_a_a_3a-001 P3HQ
- Cervantite (α-Sb_2O_4):
  A2B_oP24_33_4a_2a-001 49UC
- β-$CuAlCl_4$:
  AB4C_oP24_33_a_4a_a-001 KHU7
- δ_1-$LiZnPO_4$:
  AB4CD_oP28_33_a_4a_a_a-001 FVBE
- AsK_3S_4:
  AB3C4_oP32_33_a_3a_4a-001 H422
- κ alumina (Al_2O_3):
  A2B3_oP40_33_4a_6a-001 SGA3
- $LiZnPO_4{\cdot}H_2O$:
  A2BC5DE_oP40_33_2a_a_5a_a_a-001 SJPR
- Possible δ-$Gd_2Si_2O_7$:
  A2B7C2_oP44_33_2a_7a_2a-001 9ZSV
- CsB_4O_6F:
  A4BCD6_oP48_33_4a_a_a_6a-001 ZOHT
- CaB_2O_4 (III):
  A2BC4_oP84_33_6a_3a_12a-001 S26L
- α'_L-Ca_2SiO_4:
  A2B4C_oP84_33_6a_12a_3a-001 2RUZ

Pnn2 (34):
- $FeSb_2$:
  AB2_oP6_34_a_c-001 5KTQ
- $MnF_{1-x}(OH)_x$:
  A2BC2_oP10_34_c_a_c-001 5413
- $TiAl_2Br_8$:
  A2B8C_oP22_34_c_4c_a-001 7UTD
- K_2AgSbS_4:
  AB2C4D_oP32_34_ab_abc_4c_c-001 Z6KJ

Cmm2 (35):
- V_2MoO_8:
  AB8C2_oC22_35_a_ab3d_d-002 8B57

$Cmc2_1$ (36):
- Low temperature HCl:
  AB_oC8_36_a_a-001 SAL5
- $HgBr_2$ ($C24$):
  A2B_oC12_36_2a_a-001 FWL2
- MoP_2:
  AB2_oC12_36_a_2a-002 JTSA
- Si_2N_2O:
  A2BC2_oC20_36_b_a_b-001 8BR1
- K_2S_3:
  A2B3_oC20_36_2a_ab-001 36FH
- Orthorhombic B_2O_3:
  A2B3_oC20_36_b_ab-001 KLS9
- $BaZnF_4$:
  AB4C_oC24_36_a_4a_a-002 F77P
- Bi_2GeO_5:
  A2BC5_oC32_36_b_a_a2b-001 ZATP
- β-BiPd:
  AB_oC32_36_2ab_2ab-001 6W3L
- α-NiI_4:
  A4B_oC40_36_4a2b_b-001 MTWW
- $Ca_3Ti_2O_7$:
  A3B7C2_oC48_36_ab_a3b_b-001 FD1H
- Bertrandite ($Be_4Si_2O_7(OH)_2$, $S4_6$):
  A4B7C2D2_oC60_36_2b_a3b_2a_b-001 NZ59
- Ni_3Si_2:
  A3B2_oC80_36_4a4b_2a3b-001 5H38
- α-Potassium Nitrate (KNO_3) II:
  ABC3_oC80_36_2ab_2ab_2a5b-001 3YA6
- Low temperature $BaBi_4Ti_4O_{15}$:
  AB4C15D4_oC96_36_a_2b_a7b_2b-001 8N75

Ccc2 (37):
- $Li_2Si_2O_5$:
  A2B5C2_oC36_37_d_c2d_d-001 JE1T
- $Bi_2Sr_2Ca_2Cu_3O_{10+x}$ (Bi-2223):
  A2B2C3D10E2_oC76_37_d_d_cd_5d_d-001 ZBUL

Amm2 (38):
- C_2CeNi:
  A2BC_oC8_38_d_b_a-001 37DH
- Orthorhombic $BaTiO_3$:
  AB3C_oC10_38_a_ae_b-002 8STH
- Au_2V:
  A2B_oC12_38_de_ab-001 PCHF
- $GdSn_3$:
  AB3_oC16_38_ab_3a3b-001 L5S8
- Ta_3Ti_5 (BCC SQS-16):
  A3B5_oC32_38_abcd_abcef-001 0NF7
- Ta_3Ti_{13} (BCC SQS-16):
  A3B13_oC32_38_ac_a2bcdef-001 A2U8
- $NaNb_6O_{15}F$:
  ABC6D15_oC46_38_b_b_2a2d_2ab4d2e-001 MYRE

Aem2 (39):
- Ta_3S_2:
  A2B3_oC40_39_2d_2c2d-001 4YG0
- $VPCl_9$:
  A9BC_oC44_39_3c3d_a_c-001 5ZH7

Ama2 (40):
- K_2CdPb:
  AB2C_oC16_40_a_2b_b-001 K8N1
- $CeTe_3$:
  AB3_oC16_40_b_3b-001 WA7J
- Orthorhombic CrO_3:
  AB3_oC16_40_b_a2b-002 8E60
- $Rb_2Mo_2O_7$:
  A2B7C2_oC88_40_abc_2b6c_a3b-001 CBWE

Aea2 (41):
- $PtSn_4$ ($D1_c$):
  AB4_oC20_41_a_2b-001 MALE

- $PdSn_2$ (C_c):
  AB2_oC24_41_2a_2b-001 BVS7
- Orthorhombic $Bi_4Ti_3O_{12}$ $m = 3$ Aurivillius (*Obsolete*):
  A4B12C3_oC76_41_2b_6b_ab-001 5TXE
- Santite ($KB_5O_8{\cdot}4H_2O$, $K3_5$):
  A5B8CD12_oC104_41_a2b_4b_a_6b-001 C7EQ

Fmm2 (**42**):

- BN (High-pressure, high-temperature):
  AB_oF8_42_a_a-001 0Q2T
- W_3O_{10} ($WO_3 \cdot \frac{1}{3}H_2O$):
  A10B3_oF52_42_2abce_ab-001 TH7F
- $Bi_7(Fe,Ti)_6O_{21}$ $m = 6$ Aurivillius:
  A7B6C21_oF136_42_a3c_3c_ab3c3e-001 M0MD

Fdd2 (**43**):

- Cs_2Se:
  A2B_oF24_43_b_a-001 DUC7
- Ag_2O_3:
  A2B3_oF40_43_b_ab-001 X02L
- Zr_2Al_3:
  A3B2_oF40_43_ab_b-001 7D48
- Archerite (KH_2PO_4):
  A2BC4D_oF64_43_b_a_2b_a-001 DS2R
- GeS_2 ($C44$):
  AB2_oF72_43_ab_3b-001 4KUZ
- Blossite (α-$Cu_2V_2O_7$):
  A2B7C2_oF88_43_b_a3b_b-001 D9YZ
- Natrolite ($Na_2Al_2Si_3O_{10}{\cdot}2H_2O$, $S6_{10}$):
  A2B4C2D12E3_oF184_43_b_2b_b_6b_ab-001 FT02
- $Al_{22}Mo_5$:
  A22B5_oF216_43_11b_a2b-001 15LF

Imm2 (**44**):

- High-pressure GaAs:
  AB_oI4_44_a_b-001 JZUV
- Ferroelectric $NaNO_2$ ($F5_5$):
  ABC2_oI8_44_a_a_c-001 JZVB
- $AgNO_2$ ($F5_{12}$):
  ABC2_oI8_44_a_a_c-002 VTNW
- Hemimorphite ($Zn_4Si_2O_7(OH)_2{\cdot}H_2O$, $S2_2$):
  A2B5CD2_oI40_44_2c_abcde_d_e-001 W7BE
- $B30$ (MgZn?) (*Problematic*):
  AB_oI48_44_6c_abc2de-001 WDVJ

Iba2 (**45**):

- $MnGa_2Sb_2$:
  A2BC2_oI20_45_c_a_c-001 LNLG
- $Ca_{11}InSb_9$:
  A11BC9_oI84_45_a5c_a_b4c-001 DZ16

Ima2 (**46**):

- Room temperature AgC_4N_3:
  AB4C3_oI32_46_b_2bc_bc-001 77VH
- Low temperature AgC_4N_3:
  AB4C3_oI32_46_b_2bc_bc-002 AS99
- TiFeSi:
  ABC_oI36_46_ac_bc_3b-001 7FJR
- $Nb_2Zr_6O_{17}$:
  A2B17C6_oI100_46_ab_b8c_3c-001 DKTF

Pmmm (**47**):

- AuMn:
  AB_oP2_47_a_h-001 JM3Q
- 1212C [$YBa_2Cu_3O_{7-x}$] High-T_c:
  A2B3C7D_oP13_47_k_cj_aijl_f-001 MZYC

Pnnn (**48**):

- α-$RbPr[MoO_4]_2$:
  A2B8CD_oP24_48_h_2m_a_b-001 7YK7

Pccm (**49**):

- β-Ta_2O_5:
  A5B2_oP14_49_cehq_ab-001 XVUH
- δ-V_4D_3:
  A3B4_oP14_49_ej_2q-001 6B3F
- $CsPr(MoO_4)_2$:
  AB2C8D_oP24_49_e_q_2qr_f-001 M8U7

Pban (**50**):

- Orthorhombic La_2NiO_4:
  A2BC4_oP28_50_gh_ac_ghm-001 69JP
- α-Tl_2TeO_3:
  A3BC2_oP48_50_3m_m_2m-001 06EV

Pmma (**51**):

- β'-AuCd ($B19$):
  AB_oP4_51_e_f-001 WLS6
- Parkerite ($Ni_3Bi_2S_4$):
  AB2C_oP8_51_e_be_f-001 LY1V
- α-UB_2C:
  A2BC_oP8_51_i_a_f-001 DRSV
- TaRh:
  AB_oP12_51_ei_fj-001 1M54
- Kenhsuite (γ-$Hg_3S_2Cl_2$):
  AB2C_oP16_51_2e_bfi_j-001 LQ5X
- α-$BiPd_3$:
  AB3_oP16_51_af_behk-001 9W5L
- $LiNb_6O_{15}F$:
  ABC6D15_oP46_51_f_b_2e2i_cef4i2j-001 0JVV

Pnna (**52**):

- Sr_2Bi_3:
  A3B2_oP20_52_de_cd-001 12L3
- High-pressure $GaCl_2$:
  A2B_oP24_52_2e_cd-001 PL6D
- Carnallite [$Mg(H_2O)_6KCl_3$]:
  A3B12CDE6_oP276_52_d4e_18e_ce_de_2d8e-001 40W9

Pmna (**53**):

- $TaNiTe_2$:
  ABC2_oP16_53_h_e_gh-001 AVNP
- NH_4HF_2 ($F5_8$):
  A2BC_oP16_53_eh_ab_g-001 DCYY
- Eriochalcite ($CuCl_2{\cdot}2H_2O$, $C45$):
  A2BC4D2_oP18_53_h_a_i_e-001 UFSK
- *Pmna* $CuBrSe_3$:
  ABC3_oP20_53_e_g_hi-001 SET9

Pcca (**54**):

- $AgClO_2$:
  ABC2_oP16_54_c_c_f-001 RAQG
- $BiGaO_3$:
  ABC3_oP20_54_e_d_cf-001 WWU9

Pbam (**55**):

- Rh_5Ge_3:
  A3B5_oP16_55_ah_cgh-001 WXAV
- R-carbon:
  A_oP16_55_2g2h-001 QPSD
- ScB_2C_2:
  A2B2C_oP20_55_2g_2g_h-001 93YX
- $GeAs_2$:
  A2B_oP24_55_2g2h_gh-001 X52Z
- $YCrB_4$:
  A4BC_oP24_55_4g_h_h-001 67TW
- $Nb_2Pd_3Se_8$:
  A2B3C8_oP26_55_h_ag_2g2h-001 X0K9
- $Ca_5Ga_2As_6$:
  A6B5C2_oP26_55_g2h_a2g_h-001 JZ3U

- Ambient pressure $Bi_2Fe_4O_9$:
  A2B4C9_oP30_55_h_fg_aghi-001 7EHM
- $K_2HgCl_4{\cdot}H_2O$ ($E3_4$):
  A4BCD2_oP32_55_ghi_e_f_gh-001 07TT
- $HoMn_2O_5$:
  AB2C5_oP32_55_g_eh_fghi-001 KF2N
- Ta_4SiTe_4:
  AB4C4_oP36_55_e_2g2h_2g2h-001 UXGR
- Ludwigite (Mg_2FeBO_5):
  ABC2D5_oP36_55_g_g_adh_3g2h-001 A5YT
- $Ru_{11}B_8$:
  A8B11_oP38_55_3gh_b2g3h-001 6FNW
- Nb_8P_5:
  A17B10_oP54_55_a3g5h_3g2h-001 BWRM
- Orthorhombic $Sr_4Ru_3O_{10}$:
  A10B3C4_oP68_55_2e2fgh2i_adef_2e2f-001 PEKW

Pccn (**56**):

- Valentinite (Sb_2O_3, $D5_{11}$):
  A3B2_oP20_56_ce_e-001 HKUU
- Calciborite (CaB_2O_4 II):
  A2BC4_oP56_56_2e_e_4e-001 ZD64

Pbcm (**57**):

- TlF-II:
  AB_oP8_57_d_d-001 E914
- KNCS ($F5_9$):
  ABCD_oP16_57_d_c_d_d-001 K4A8
- $D0_{10}$ (WO_3) (*Obsolete*):
  A3B_oP16_57_a2d_d-001 5B3E
- DyAl:
  AB_oP16_57_cd_2d-001 GHY9
- $SrUO_4$:
  A4BC_oP24_57_cde_d_a-001 JM5X
- Ca_4Al_3Mg:
  A3B4C_oP32_57_c2d_4d_a-001 6529
- Ta_2S:
  AB2_oP36_57_ce_2d2e-001 4L1U
- Lueshite ($NaNbO_3$):
  ABC3_oP40_57_cd_e_cd2e-001 1JM3
- Hg_7Hg_5:
  A7B5_oP48_57_c3e_5d-001 9PR5

Pnnm (**58**):

- Hydrophilite ($CaCl_2$, $C35$):
  AB2_oP6_58_a_g-001 YTPF
- η-Fe_2C:
  AB2_oP6_58_a_g-002 FF5Q
- Marcasite (FeS_2, $C18$):
  AB2_oP6_58_a_g-003 USY5
- α-$PdCl_2$ ($C50$):
  A2B_oP6_58_g_a-001 HU31
- InS:
  AB_oP8_58_g_g-001 A7M6
- Kotoite ($Mg_3(BO_3)_2$):
  A2B3C6_oP22_58_g_af_gh-001 59YW
- γ-Alane (AlH_3):
  AB3_oP24_58_ag_c2gh-001 WUSJ
- S_{12} Sulfur:
  A_oP24_58_eg2h-001 7TXG
- In_4Se_3:
  A4B3_oP28_58_4g_3g-001 B01P
- Andalusite (Al_2SiO_5, $S0_2$):
  A2B5C_oP32_58_eg_3gh_g-001 V93J
- Adamite [$Zn_2(AsO_4)(OH)$, $H2_7$]:
  ABC5D2_oP36_58_g_g_3gh_eg-001 YE34
- Ta_2P:
  AB2_oP36_58_3g_6g-001 9JBK
- Protoanthophyllite ($H_2Mg_7Si_8O_{24}$):
  A2B7C24D8_oP82_58_g_ae2f_2g5h_2h-001 APMF

Pmmn (**59**):

- Vulcanite (CuTe):
  AB_oP4_59_a_b-001 9JE2
- CNCl:
  ABC_oP6_59_a_a_a-001 Z1TY
- FeOCl ($E0_5$):
  ABC_oP6_59_a_b_a-001 DN69
- RuB_2:
  A2B_oP6_59_e_a-001 BRW1
- β-$TiCu_3$ ($D0_a$):
  A3B_oP8_59_ae_b-001 CJHD
- Orthorhombic $LiFeO_2$ (o-$LiFeO_2$):
  ABC2_oP8_59_a_a_2b-004 WEQC
- Shcherbinaite (V_2O_5) (*Revised*):
  A5B2_oP14_59_a2e_e-001 KZMB
- NH_4NO_3 IV ($G0_{11}$):
  A4B2C3_oP18_59_ef_ab_ae-001 NABB
- β-$NbPd_3$:
  AB3_oP24_59_ae_befg-001 5BSF
- $RbAlF_4$ III:
  AB4C_oP24_59_c_efg_ab-001 Q57Q

Pbcn (**60**):

- ζ-Fe_2N:
  A2B_oP12_60_d_c-001 5GP6
- α-PbO_2:
  A2B_oP12_60_d_c-003 9BKR
- Rh_2O_3:
  A2B3_oP20_60_d_cd-001 WEMD
- $E3_2$ (CaB_2O_4 I):
  A2BC4_oP28_60_d_c_2d-001 44A7
- β-WO_3:
  A3B_oP32_60_3d_d-001 S00Q
- Columbite ($FeNb_2O_4$, $E5_1$):
  AB2C6_oP36_60_c_d_3d-001 ZB5U
- Ru_2Ge_3 Nowotny Chimney-Ladder:
  A3B2_oP40_60_3d_2cd-001 EU3H
- Cr_5O_{12}:
  A5B12_oP68_60_c2d_6d-001 NF0B
- Na_2FeSbO_5:
  AB2C5D_oP72_60_d_2cd_5d_2c-001 2H6S
- β-Toluene:
  A7B8_oP120_60_7d_8d-001 7NVJ

Pbca (**61**):

- β-HgO_2:
  AB2_oP12_61_a_c-001 JQ93
- AgF_2:
  AB2_oP12_61_a_c-002 F3J5
- $PdSe_2$:
  AB2_oP12_61_a_c-003 WV1J
- CdSb (B_e):
  AB_oP16_61_c_c-001 RL87
- Cyanogen [$(CN)_2$]:
  AB_oP16_61_c_c-002 NEGW
- Brookite (TiO_2, $C21$):
  A2B_oP24_61_2c_c-001 ZJ0C
- Tellurite (β-TeO_2, $C52$):
  A2B_oP24_61_2c_c-002 GK2A
- COCl:
  ABC_oP24_61_c_c_c-001 EHTG
- Pararammelsbergite (α-$NiAs_2$):
  A2B_oP24_61_2c_c-003 ZBG0

- $AuSn_2$:
  AB2_oP24_61_c_2c-001 FZA4
  - Ca_2RuO_4:
    A2B4C_oP28_61_c_2c_a-001 NDWA
- ReP_4:
  A4B_oP40_61_4c_c-001 3PB1
  - Benzene:
    AB_oP48_61_3c_3c-001 PWJE
- Tl_3AsS_3:
  AB3C3_oP56_61_c_3c_3c-001 233Q
  - Hambergite [$Be_2BO_3(OH)$ ($G7_2$)]:
    AB2CD4_oP64_61_c_2c_c_4c-001 PKYK
- $Ca_4Ti_3O_{10}$:
  A4B10C3_oP68_61_2c_5c_ac-001 R6BH
- O-Carbamoylhydroxylamine ($CH_4N_2O_2$):
  AB4C2D2_oP72_61_c_4c_2c_2c-001 K3UE
  - ($TiCl_4{\cdot}POCl_3)_2$:
    A7BCD_oP80_61_7c_c_c_c-001 Q18C
  - Enstatite ($MgSiO_3$, $S4_3$):
    AB3C_oP80_61_2c_6c_2c-001 N16Y
- $CuMo_3I_7$:
  AB7C3_oP88_61_c_7c_3c-001 WLBF
- $SrZn(VO)(PO_4)_2$:
  A9B2CDE_oP112_61_9c_2c_c_c_c-001 VHVW
- Room temperature Bornite (Cu_5FeS_4):
  A5BC4_oP160_61_10c_2c_8c-001 L8SE

Pnma (**62**):

- GeS ($B16$):
  AB_oP8_62_c_c-001 Y0CA
  - MnP ($B31$):
    AB_oP8_62_c_c-002 36ZK
  - FeB ($B27$):
    AB_oP8_62_c_c-003 GH4J
  - α-SnS ($B29$):
    AB_oP8_62_c_c-004 QZKW
  - α-Np (A_c):
    A_oP8_62_2c-001 L3MB
  - Westerveldite (FeAs, $B14$):
    AB_oP8_62_c_c-005 P0GV
  - η-NiSi (B_d):
    AB_oP8_62_c_c-010 4N6D
- High-pressure oP8 Sodium:
  A_oP8_62_2c-002 3BFR
  - Co_2Si ($C37$):
    A2B_oP12_62_2c_c-001 6EYJ
  - $HgCl_2$ ($C25$):
    A2B_oP12_62_2c_c-002 DNGY
  - Cotunnite ($PbCl_2$, $C23$):
    A2B_oP12_62_2c_c-003 GSD1
  - SrH_2 ($C29$):
    A2B_oP12_62_2c_c-004 4GNV
  - $C53$ ($SrBr_2$) (*Obsolete*):
    A2B_oP12_62_2c_c-010 NJ0X
  - MnCuP:
    ABC_oP12_62_c_c_c-003 BN2H
- Lautite (CuAsS):
  ABC_oP12_62_c_c_c-017 DUB2
  - Chalcostibite ($CuSbS_2$, $F5_6$):
    AB2C_oP16_62_c_2c_c-001 H6D5
  - Cementite (Fe_3C, $D0_{11}$):
    AB3_oP16_62_c_cd-001 KYLC
  - ϵ-Al_3Ni ($D0_{20}$):
    A3B_oP16_62_cd_c-001 TJ6A
  - Molybdite (MoO_3, $D0_8$):
    AB3_oP16_62_c_3c-001 2C2N
  - NH_4I_3 ($D0_{16}$):
    A3B_oP16_62_3c_c-002 DE18
  - Diaspore ($AlOOH$, $E0_2$):
    ABC2_oP16_62_c_c_2c-002 XPSY
  - NH_4ClBrI ($F5_{14}$):
    ABCD_oP16_62_c_c_c_c-001 N0R6
- $UMoC_2$:
  A2BC_oP16_62_2c_c_c-003 69FA
- $NiBi_3$:
  A3B_oP16_62_3c_c-003 J16T
- Orthorhombic ClF_3:
  AB3_oP16_62_c_cd-005 AZN3
- $CaMnSb_2$:
  ABC2_oP16_62_c_c_2c-003 JHY5
- ThNi:
  AB_oP16_62_2c_2c-002 QLCJ
  - Stibnite (Sb_2S_3, $D5_8$):
    A3B2_oP20_62_3c_2c-001 1WMN
  - MgB_4:
    A4B_oP20_62_2cd_c-001 8U8B
  - $CaTiO_3$ Pnma Perovskite:
    AB3C_oP20_62_c_cd_a-001 2KF1
  - Tongbaite (Cr_3C_2, $D5_{10}$):
    A2B3_oP20_62_2c_3c-001 KS86
  - $(NH_4)CdCl_3$ ($E2_4$):
    AB3C_oP20_62_c_3c_c-001 Z6H8
  - α-Potassium Nitrate (KNO_3) I:
    ABC3_oP20_62_c_c_cd-001 3DEN
  - NH_4NO_3 III ($G0_{10}$):
    ABC3_oP20_62_c_c_cd-002 8RDG
  - Aragonite ($G0_2$, $CaCO_3$):
    ABC3_oP20_62_c_c_cd-003 7S19
- K_2Te_3:
  A2B3_oP20_62_d_3c-001 GCVK
- Pt_2Ge_3:
  A3B2_oP20_62_3c_2c-002 GDA9
- Ottemannite (Sn_2S_3):
  A3B2_oP20_62_3c_2c-003 1ZQE
- Au_4Zr:
  A4B_oP20_62_4c_c-001 KLZ3
- $CuTaS_3$:
  AB3C_oP20_62_c_3c_c-002 S2FJ
- Monoclinic Vaterite ($CaCO_3$):
  ABC3_oP20_62_c_a_cd-001 RGRE
  - Cubanite ($CuFe_2S_3$, $E9_e$):
    AB2C3_oP24_62_c_d_cd-001 7QNH
  - Barite ($BaSO_4$, $H0_2$):
    AB4C_oP24_62_c_2cd_c-001 CXQX
  - Cs_2Sb:
    A2B_oP24_62_4c_2c-001 9L36
  - Chalcocyanite ($CuSO_4$):
    AB4C_oP24_62_a_2cd_c-001 QVKJ
- $SrAu_3Al_2$:
  A2B3C_oP24_62_d_3c_c-001 DAG0
- K_2CuCl_3:
  A3BC2_oP24_62_3c_c_2c-001 WK7H
- $IrSe_2$:
  AB2_oP24_62_2c_4c-001 UH0Z
- $SrCuYSe_3$ (Eu_2CuS_3):
  AB3CD_oP24_62_c_3c_c_c-001 SFSU
- $SrZn_5$:
  AB5_oP24_62_c_3cd-001 BRA8

- Forsterite (Mg_2SiO_4, $S1_2$):
  A2B4C_oP28_62_ac_2cd_c-001 V88M
- Arcanite (K_2SO_4, $H1_6$):
  A2B4C_oP28_62_2c_2cd_c-001 HEYH
- $VOSO_4$:
  A5BC_oP28_62_3cd_c_c-001 3N5K
- Berthierite ($FeSb_2S_4$, $E3_3$):
  AB4C2_oP28_62_c_4c_2c-001 CAYJ
- Copper (II) Azide [$Cu(N_3)_2$]:
  AB6_oP28_62_c_6c-001 VP85
- Galenobismutite ($PbBi_2S_4$):
  A2BC4_oP28_62_2c_c_4c-001 PUZH
- Orthorhombic Ni_4B_3:
  A3B4_oP28_62_3c_4c-001 49QQ
- Rh_4P_3:
  A3B4_oP28_62_3c_4c-002 71TB
- Monticellite ($CaMgSiO_4$):
  ABC4D_oP28_62_c_a_2cd_c-001 TYTV
- Warwickite ($FeCoBO_4$):
  ABCD4_oP28_62_c_c_c_4c-001 G1FS
- Sillimanite (Al_2SiO_5, $S0_3$):
  A2B5C_oP32_62_ac_3cd_c-001 XCRT
- Original β-WO_3 (*Obsolete*):
  A3B_oP32_62_ab4c_2c-001 KPH8
- $E3_5$ ($K_2SnCl_4{\cdot}H_2O$):
  A4BC2D_oP32_62_2cd_a_2c_b-001 EVKH
- $K_2SnCl_4{\cdot}H_2O$:
  A4BC2D_oP32_62_2cd_c_d_c-001 ZADN
- Li_2CdSiO_4:
  AB2C4D_oP32_62_c_d_2cd_c-001 J1AT
- Empressite (AgTe):
  AB_oP32_62_2cd_2cd-001 JH5H
- Topaz ($Al_2SiO_4F_2$, $S0_5$):
  A2B2C4D_oP36_62_d_d_2cd_c-001 7RBD
- Atacamite ($Cu_2(OH)_3Cl$):
  AB2C3D3_oP36_62_c_ac_cd_cd-001 4QUY
- Rynersonite (Orthorhombic $CaTa_2O_6$):
  AB6C2_oP36_62_c_2c2d_d-001 07R8
- PbV_2O_6:
  A6BC2_oP36_62_6c_c_2c-001 XXTA
- $BaCuSm_2O_5$:
  ABC5D2_oP36_62_c_c_c2d_2c-001 W9F8
- C_3Cr_7 ($D10_1$):
  A3B7_oP40_62_cd_3c2d-001 9Z5M
- Norbergite [$Mg(F,OH)_2{\cdot}\ Mg_2SiO_6$, $S0_7$]:
  A2B3C4D_oP40_62_d_cd_2cd_c-001 J7L1
- $Ta_2Ni_3Te_5$:
  A3B2C5_oP40_62_3c_2c_5c-001 72A0
- $K_2SnCl_4{\cdot}H_2O$:
  A4B2C2DE_oP40_62_2cd_2c_d_c_c-001 AZ89
- $K_2S_3O_6$ ($K5_1$):
  A2B6C3_oP44_62_2c_2c2d_3c-001 PD3R
- Possible δ-$Y_2Si_2O_7$:
  A7B2C2_oP44_62_3c2d_2c_d-001 Y82X
- $SbCl_5{\cdot}POCl_3$:
  A8BCD_oP44_62_4c2d_c_c_c-001 XAT4
- α-HBO_2 (orthorhombic):
  ABC2_oP48_62_3c_3c_6c-001 XYXT
- Danburite ($CaB_2Si_2O_8$, $S6_3$):
  A2BC8D2_oP52_62_d_c_2c3d_d-001 APE4
- α'_H-Ca_2SiO_4:
  A4B8C_oP52_62_2d_4d_c-001 1R45
- Mo_4P_3:
  A4B3_oP56_62_8c_6c-001 S9HM
- High pressure $Bi_2Fe_4O_9$:
  A2B4C9_oP60_62_d_2cd_3c3d-001 BYQL
- Approximate $Cu_3(TeO_4)(SO_4){\cdot}H_2O$:
  A3B2C9DE_oP64_62_cd_2c_5c2d_c_c-001 WLK8
- $CdSnP_{14}$ ($HgPbP_{14}$):
  AB14C_oP64_62_c_4c5d_c-001 LZG8
- Ag(tcm)(pyz) [$AgC_8N_5H_4$]:
  AB8C4D5_oP72_62_c_4c2d_2d_3cd-001 L9Y6
- $Ba_5AlIr_2O_{11}$:
  AB5C2D11_oP76_62_c_5c_2c_5c3d-001 CZW8
- Room temperature $SmBaMn_2O_6$:
  AB2C6D_oP80_62_2c_2d_2c5d_d-001 8TUC
- $RhCl_2(NH_3)_5Cl$ ($J1_8$):
  A3B15C5D_oP96_62_cd_3c6d_3cd_c-001 3AAY
- $K_4[Mo(CN)_8]{\cdot}\ 2H_2O$ ($F2_1$):
  A8B4C4DE8F2_oP108_62_4c2d_2d_2cd_c_4c2d_d-001 BH4W
- P_4Se_3:
  A4B3_oP112_62_8c4d_4c4d-001 DMDS
- Epididymite ($BeHNaO_8Si_3$, $S4_7$):
  ABCD8E3_oP112_62_d_2c_d_4c6d_3d-001 QQ21
- Anthophyllite ($Mg_5Fe_2Si_8O_{22}(OH)_2$, $S4_4$):
  A2B5C22D2E8_oP156_62_d_c2d_2c10d_2c_4d-001 P9BG
- Al_3Mn:
  A9B4_oP156_62_5c11d_6c3d-001 WUDY
- Autunite $Ca[(UO_2)(PO_4)]_2(H_2O)_{11}$:
  AB22C23D2E2_oP200_62_c_11d_3c10d_d_d-001 PYMC

Cmcm (63):

- α-U ($A20$):
  A_oC4_63_c-001 AFG5
- CrB ($B33$):
  AB_oC8_63_c_c-001 QWV1
- β-SnS:
  AB_oC8_63_c_c-004 8MTK
- $ZrSi_2$ ($C49$):
  A2B_oC12_63_2c_c-001 HPCM
- UBC:
  ABC_oC12_63_c_c_c-004 NQGP
- MoAlB:
  ABC_oC12_63_c_c_c-005 XSM0
- $SrCuO_2$:
  AB2C_oC16_63_c_2c_c-001 WL5U
- $MgCuAl_2$ ($E1_a$):
  A2BC_oC16_63_f_c_c-002 ECJE
- Mn_3As ($D0_d$):
  AB3_oC16_63_c_3c-001 DPFG
- Re_3B:
  AB3_oC16_63_c_cf-001 EW0Y
- NaHg:
  AB_oC16_63_g_2c-001 BVCU
- Post-perovskite ($MgSiO_3$):
  AB3C_oC20_63_c_cf_a-001 BCSA
- Lepidocrocite [γ-FeO(OH), $E0_4$]:
  AB2C2_oC20_63_c_f_2c-001 WBGV
- $ThFe_2SiC$:
  AB2CD_oC20_63_a_f_c_c-001 UF5S
- V_3AsC:
  ABC3_oC20_63_c_a_cf-003 2T8B
- $SrPdGa_3$:
  A3BC_oC20_63_ce_c_c-001 2P2W
- Rasvumite (KFe_2S_3):
  A2BC3_oC24_63_e_c_cg-001 88NB
- Anhydrite ($CaSO_4$, $H0_1$):
  AB4C_oC24_63_c_fg_c-001 EHW6

- $MgSO_4$:
  ABC4_oC24_63_c_a_fg-001 FNXT
- $ZrTe_5$:
  A5B_oC24_63_c2f_c-001 EE51
- Si_{24} Clathrate:
  A_oC24_63_3f-001 TPXT
- URe_2:
  A2B_oC24_63_acg_f-001 RKF7
- $YNiAl_4$:
  A4BC_oC24_63_acf_c_c-002 ULYP
- η-Fe_2Al_5:
  A5B_oC24_63_afg_c-001 US2Q
- $BaZn_5$:
  AB5_oC24_63_c_ceg-001 BGG4
- $KCuZrS_3$:
  ABC3D_oC24_63_c_c_cf_a-001 3902
- $MnAl_6$ ($D2_h$):
  A6B_oC28_63_efg_c-001 386R
- Na_2CrO_4 ($H1_8$):
  AB2C4_oC28_63_c_ac_fg-001 A786
- $NbNiTe_5$:
  ABC5_oC28_63_c_a_c2f-001 BN2Z
- Pseudobrookite (Fe_2TiO_5, $E4_1$):
  A2B5C_oC32_63_f_c2f_c-001 NJWX
- Pd_5Pu_3:
  A5B3_oC32_63_cfg_ce-001 9AGN
- Ta_2NiS_5:
  AB5C2_oC32_63_c_c2f_f-004 FETU
- Refined Tl_2AlF_5:
  AB5C2_oC32_63_a_cef_g-001 KA1Q
- Ag_7Ca_2:
  A7B2_oC36_63_cgh_f-001 PMU3
- $CaFe_3O_5$:
  AB3C5_oC36_63_c_af_c2f-001 8XTL
- Pinalite ($Pb_3WO_5Cl_2$):
  A2B5C3D_oC44_63_ac_ch_cf_c-001 S4ZE
- $CaFe_4O_6$:
  AB4C6_oC44_63_c_2f_ac2f-001 8HU9
- β-AlF_3:
  AB3_oC48_63_ad_cfgh-001 W7TS
- $Cu_2Pb(SeO_3)_2Br_2$:
  A2B2C6DE2_oC52_63_g_e_fh_c_f-001 RZ26
- $CaFe_5O_7$:
  AB5C7_oC52_63_c_a2f_c3f-001 KAT1
- Nb_4As_3:
  A3B4_oC56_63_2c2f_ac3f-001 J9UY
- $Y_2Ga_9Co_3$:
  A3B9C2_oC56_63_ae_cfgh_g-001 1YQJ
- α-Ni_7S_6:
  A9B5_oC56_63_c4f_c2f-001 T4VC
- $S0_4$ (Staurolite, $Fe(OH)_2Al_4SiO_{10}$) (*Obsolete*):
  A4BC12D2_oC76_63_eg_c_f3gh_g-001 CXFF
- β-$Bi_4V_2O_{11}$:
  A4B12C3_oC76_63_eg_fg2h_cf-001 AB76
- Orthorhombic $Nb_{12}O_{29}$:
  A12B29_oC164_63_6f_3c13f-001 V0KX
- $La_{43}Ni_{17}Mg_5$:
  A43B5C17_oC260_63_c8fg6h_cfg_ce3f2h-001 Z34R

Cmce (64):

- α-Ga ($A11$):
  A_oC8_64_f-001 JS9R
- Black Phosphorus ($A17$):
  A_oC8_64_f-002 7VYH
- Molecular Iodine ($A14$):
  A_oC8_64_f-003 234K
- KO:
  AB_oC16_64_e_f-002 HZUD
- La_2Ni_3:
  A2B3_oC20_64_f_ae-001 4LJZ
- H_2S (170 GPa):
  A2B_oC24_64_2f_f-001 7FZR
- $SmSb_2$:
  A2B_oC24_64_ef_f-001 370K
- $CoGe_2$:
  AB2_oC24_64_d_ef-002 QB3A
- Gd_2CuO_4:
  AB2C4_oC28_64_a_d_ef-001 UBCB
- Base-Centered Orthorhombic La_2CuO_4:
  AB2C4_oC28_64_a_f_ef-003 Y6BX
- R_2 Au_3Zn:
  A3B_oC32_64_def_d-001 GVGD
- $PdSn_3$:
  AB3_oC32_64_d_fg-001 J38S
- Low temperature $FeSi_2$:
  AB2_oC48_64_df_2g-001 MR28
- Experimental Li_3AlP_2:
  AB3C2_oC48_64_d_dg_ef-001 94E5
- Base-centered Orthorhombic $Sr_4Ru_3O_{10}$:
  A10B3C4_oC68_64_2dfg_ad_2d-001 XC67
- $Cs_4Mg_3F_{10}$:
  A4B10C3_oC68_64_2f_e2fg_af-001 B9LX
- Zr_7Ni_{10}:
  A10B7_oC68_64_f2g_adef-001 7BKZ
- MgB_2C_2:
  A2B2C_oC80_64_efg_efg_df-001 BJ3W
- $Na_2Mo_2O_7$:
  A2B2C7_oC88_64_ef_df_3f2g-001 0H5D
- Zektzerite ($NaLiZrSi_6O_{15}$):
  ABC15D6E_oC192_64_d_e_3f6g_3g_e-001 MZR4

Cmmm (65):

- $CdPt_3$ ("New" $L1_3$):
  AB3_oC8_65_a_bf-001 JBK1
- α-IrV:
  AB_oC8_65_g_j-001 S2CY
- Mn_2AlB_2:
  AB2C2_oC10_65_a_g_h-001 XPEY
- Li_2PrO_3:
  A2B3C_oC12_65_h_ah_b-001 2B54
- Ga_2Zr:
  A2B_oC12_65_acg_h-001 V3JJ
- Ag_3Te_2Tl:
  A3B2C_oC12_65_ah_g_c-001 35VG
- Ga_3Pt_5:
  A3B5_oC16_65_ah_bej-001 36DL
- Nb_3O_7F:
  A3B8_oC22_65_bg_ac2gh-001 YUGM
- Cr_4AlB_6:
  AB6C4_oC22_65_a_3g_2h-001 6ZPS
- $ThMoB_4$:
  A4BC_oC24_65_gip_h_j-001 B95F
- $Mg(NH_3)_2Cl_2$ ($E1_3$):
  A2B8CD2_oC26_65_h_r_a_i-001 5BTF
- Tb_3Sn_7:
  A11B3_oC28_65_c4gh_ah-001 2ATW
- "124 Superconductor" ($YBa_2Cu_4O_8$):
  A2B4C8D_oC30_65_h_2g_3gh_c-001 2EBJ
- Li_7Ge_2:
  A2B7_oC36_65_gj_achipq-001 3WXK
- High temperature $SmBaMn_2O_6$:
  AB2C6D_oC40_65_g_n_ijklm_h-001 VMAN

- "247 Superconductor" ($Y_2Ba_4Cu_7O_{15}$):
  A4B7C16D2_oC58_65_2h_b3g_ac5g2h_h-001 TTW9

Cccm (**66**):
- NbD:
  AB_oC8_66_a_e-001 087H
- $SrAl_2Se_4$:
  A2B4C_oC28_66_l_kl_a-001 QSR1
- H_3S (60 GPa):
  A3B_oC64_66_gi2lm_2l-001 DQEU
- β-ThI_3:
  A3B_oC64_66_kl2m_acl-001 7JBJ
- γ-Li_2IrO_3:
  AB2C3_oC96_66_ik_cdj2k_gl2m-001 9VYY

Cmme (**67**):
- α-FeSe:
  AB_oC8_67_a_g-001 JFD1
- α-PbO:
  AB_oC8_67_a_g-002 TSNN
- Al_2CuIr:
  A2BC_oC16_67_ag_b_g-001 08UR
- $HoCuP_2$:
  ABC2_oC16_67_a_g_bg-001 BX6K
- $NH_4H_2PO_2$ ($F5_7$):
  A2BC2D_oC24_67_m_a_n_g-001 ZLA7
- $RbPaF_6$ (V):
  A6BC_oC32_67_no_c_g-001 PLRV

Ccce (**68**):
- $PdSn_4$:
  AB4_oC20_68_a_i-001 LGPW

Fmmm (**69**):
- TlF ($B24$) (*Obsolete*):
  AB_oF8_69_a_b-001 XT4M
- β-$SrRh_2As_2$:
  A2B2C_oF20_69_g_f_a-001 DY16
- Face-Centered Orthorhombic La_2CuO_4:
  AB2C4_oF28_69_a_g_cg-001 LB5P
- Rb_2P_3:
  A3B2_oF40_69_hm_fg-001 QBNS
- Orthorhombic Bi_3NbTiO_9 $m = 2$ Aurivillius:
  A3B2C9_oF56_69_ag_g_bfgl-001 FSA1
- Orthorhombic $Bi_4Ti_3O_{12}$ $m = 3$ Aurivillius:
  A4B12C3_oF76_69_2g_cf2gl_ag-001 Y2ES

Fddd (**70**):
- γ-Pu:
  A_oF8_70_a-001 7VYN
- $TiSi_2$ ($C54$) Nowotony Chimney-Ladder:
  A2B_oF24_70_e_a-001 KN7L
- Mn_2B ($D1_f$):
  AB2_oF48_70_e_ef-001 RZ74
- Mg_2Cu (C_b):
  AB2_oF48_70_e_ef-002 S336
- Thenardite [Na_2SO_4 (V), $H1_7$]:
  A2B4C_oF56_70_e_h_a-001 8CBQ
- $RbVSe_2$:
  AB2C_oF64_70_e_h_ab-001 1RMB
- Sc_2S_3:
  A3B2_oF80_70_fh_2e-001 HQ18
- β-Na_2PtO_3:
  A2B3C_oF96_70_2e_fh_e-001 7WUP
- α-S ($A16$):
  A_oF128_70_4h-001 MYP4

Immm (**71**):
- $MoPt_2$:
  AB2_oI6_71_a_e-001 EKX0
- $ReSi_2$:
  AB2_oI6_71_a_e-002 9FBX
- CsO:
  AB_oI8_71_e_g-001 2UZJ
- NbPS:
  ABC_oI12_71_e_h_f-001 B529
- UTe_2:
  A2B_oI12_71_eh_f-001 7HXW
- Ta_3B_4 ($D7_b$):
  A4B3_oI14_71_ef_af-001 3XYE
- $CsFeS_2$ (100K):
  ABC2_oI16_71_e_g_fi-001 R5TH
- Sc_3CoC_4:
  A4BC3_oI16_71_m_a_bf-001 KR8A
- High-Temperature Cryolite (Na_3AlF_6):
  AB6C3_oI20_71_a_el_bf-001 6BL9
- La_3Al_{11}:
  A11B3_oI28_71_bf2m_ai-001 TNYL
- Nb_6Sn_5:
  A6B5_oI44_71_egkl_fghl-001 Q45R
- Orthorhombic Fullerene (Cs_3C_{60}):
  A15B_oI128_71_lmn6o_eg-001 88NV

Ibam (**72**):
- SiS_2 ($C42$):
  A2B_oI12_72_j_a-001 PYBC
- Ga_2Mg_5 ($D8_g$):
  A2B5_oI28_72_j_afj-001 AB10
- $U_2Co_3Si_5$:
  A3B5C2_oI40_72_aj_bfj_j-001 LD1K

Ibca (**73**):
- $KAg[CO_3]$:
  ABCD3_oI48_73_d_c_c_cf-001 H0D0
- Predicted Li_3AlP_2:
  AB3C2_oI96_73_f_3f_acde-001 QKN5

Imma (**74**):
- KHg_2:
  A2B_oI12_74_h_e-001 TWQQ
- $CeCu_2$:
  AB2_oI12_74_e_h-001 237T
- $GdSi_2$:
  AB2_oI12_74_e_2e-001 EQ3C
- Al_4U ($D1_b$):
  A4B_oI20_74_aeh_e-001 FNF2
- $LiCuVO_4$:
  ABC4D_oI28_74_a_c_hi_e-001 50N0
- $Zn(NH_3)_2Cl_2$ ($E1_2$):
  A2B6C2D_oI44_74_i_hj_h_e-001 XWSU
- $Hg_3S_2I_2$:
  A3B2C2_oI56_74_fhi_2ei_j-001 EXRV
- $MgAlB_{14}$:
  AB14C2_oI68_74_a_3i2j_h-001 U35P
- Moskvinite ($Na_2KYSi_6O_{15}$):
  AB2C15D6E_oI100_74_e_g_e2hi2j_hj_a-001 F0JR

P4 (**75**):
- Hexagonal Hollandite ($BaRu_4Cr_2O_{12}$):
  AB2C12D4_tP76_75_2a2b_2d_12d_4d-001 MXLF

$P4_1$ (**76**):
- $LaRhC_2$:
  A2BC_tP16_76_2a_a_a-001 5CQR
- Cs_3P_7:
  A3B7_tP40_76_3a_7a-001 DCAK
- β-$Ca_2P_2O_7$:
  A2B7C2_tP88_76_4a_14a_4a-001 BAJJ

$P4_2$ (77):
- H_2S III:
  A2B_tP48_77_8d_4d-001 GRWY
- Pinnoite ($MgB_2O[OH]_6$):
  A2B6CD7_tP64_77_2d_6d_d_ab6d-001 Z918
- Gwihabaite (NH_4NO_3 V):
  A4B2C3_tP72_77_8d_ab2c2d_6d-001 JS41

$P4_3$ (78):
- $Sr_2As_2O_7$:
  A2B7C2_tP88_78_4a_14a_4a-001 SCRS

I4 (79):
- $TlZn_2Sb_2$:
  A2BC2_tI20_79_c_2a_c-001 T892

$I4_1$ (80):
- β-NbO_2:
  AB2_tI48_80_2b_4b-001 2XGR

$P\bar{4}$ (81):
- $GeSe_2$ (High pressure):
  AB2_tP12_81_adg_2h-001 1L9R

$I\bar{4}$ (82):
- BPO_4 ($H0_7$):
  AB4C_tI12_82_c_g_a-001 C601
- $InPS_4$:
  ABC4_tI12_82_a_c_g-001 SUXC
- $CdAl_2S_4$ ($E3$):
  A2BC4_tI14_82_bc_a_g-001 S1AD
- Kesterite [$Cu_2(Zn,Fe)SnS_4$]:
  A2B4CD_tI16_82_ac_g_b_d-001 92JU
- Ni_3P ($D0_e$):
  A3B_tI32_82_3g_g-001 WHNY

P4/m (83):
- Ti_2Ga_3:
  A3B2_tP10_83_adj_k-001 FCWX
- $Au_{31}Mn_9$:
  A31B9_tP40_83_ae3j4k_cjk-001 FCR5

$P4_2/m$ (84):
- Vysotskite (PdS, $B34$):
  AB_tP16_84_cej_k-001 KXWJ
- Cu_4Pd:
  A4B_tP20_84_afjk_j-001 L3AR

P4/n (85):
- $MoPO_5$:
  AB5C_tP14_85_c_cg_a-001 N6T3
- α-$SrBr_2$:
  A2B_tP30_85_ab2g_cg-001 G8GD
- Bromocarnallite ($E2_6$, $KMg(H_2O)_6(Cl,Br)_3$):
  A3B6CD_tP44_85_acg_3g_bc_d-001 PV6C
- Provisional δ-Alane (AlH_3):
  AB3_tP64_85_2ceg_2cf5g-001 U4T0
- $BaRu_6O_{12}$:
  AB12C6_tP76_85_2c_6g_3g-001 QUVT

$P4_2/n$ (86):
- Ti_3P:
  AB3_tP32_86_g_3g-001 ENA6
- $PNCl_2$ ($E1_4$):
  A2BC_tP32_86_2g_g_g-001 QLZ6
- $NaSb(OH)_6$ ($J1_{11}$):
  AB6C_tP32_86_c_3g_d-001 NR43
- β-$LiIO_3$:
  ABC3_tP40_86_g_g_3g-001 9SQG
- "Double-Double" Perovskite $CaMnCrSbO_6$:
  ABCD6E_tP40_86_e_c_ab_3g_d-001 UT10
- $Nd_4Re_2O_{11}$:
  A4B11C2_tP68_86_2g_ab5g_g-001 8MQB

I4/m (87):
- Ni_4Mo ($D1_a$):
  AB4_tI10_87_a_h-001 VMNQ
- Ga_2Te_5:
  A2B5_tI14_87_d_ah-001 4RP0
- Ti_5Te_4:
  A4B5_tI18_87_h_ah-001 E7DL
- Sr_2NiWO_6:
  AB6C2D_tI20_87_a_eh_d_b-001 QP36
- High temperature Metastable VO_2:
  A2B_tI24_87_2h_h-001 MHEM
- $Ni_{12}P_5$:
  A12B5_tI34_87_hi_ah-001 13WH
- $Ba_5Yb_8Ni_4O_{21}$:
  A5B4C21D8_tI76_87_ah_h_bh2i_2h-001 M4UL
- Marialite Scapolite [$Na_4Cl(AlSi_3)_3O_{24}$, $S6_4$]:
  AB4C24D12_tI82_87_a_h_2h2i_hi-001 8NAD

$I4_1/a$ (88):
- α-$ThCl_4$:
  A4B_tI20_88_f_a-001 5VT7
- Scheelite ($CaWO_4$, $H0_4$):
  AB4C_tI24_88_a_f_b-003 Y9T0
- Copper (I) Azide (CuN_3):
  AB3_tI32_88_c_df-001 L0WX
- α-NbO_2:
  AB2_tI96_88_2f_4f-001 BLKR
- $Na_4Ge_9O_{20}$:
  A9B4C20_tI132_88_a2f_f_5f-001 JMG5

P422 (89):
- $(CH)_{17}FeO_4Pt$ (Original Page):
  A17BC4D_tP184_89_17p_p_4p_il-001 EK6P
- $(CH)_{17}FeO_4Pt$ (*Revised*):
  A17BC17D4E_tP320_89_17p_p_17p_4p_il-001 HZJM

$P42_12$ (90):
- $G7_5$ ($PbCO_3{\cdot}PbCl_2$, Phosgenite) (*Obsolete*):
  AB2C3D2_tP16_90_c_f_ce_e-001 ZUNT
- $Na_4Ti_2Si_8O_{22}[H_2O]_4$:
  A4B2C13D4E_tP48_90_g_d_cef2g_g_c-001 9JHP
- $BaCu_4[VO][PO_4]_4$:
  AB4C17D4E_tP54_90_a_g_c4g_g_c-001 61ZR

$P4_122$ (91):
- ThBC:
  ABC_tP24_91_d_d_d-001 S6UF

$P4_12_12$ (92):
- α-Cristobalite (SiO_2, low, $C30$):
  A2B_tP12_92_b_a-001 VHRN
- Paratellurite (αTeO_2):
  A2B_tP12_92_b_a-002 6BKE
- γ-$LiAlO_2$:
  ABC2_tP16_92_a_a_b-001 TYEK
- Tetragonal (red) ZnP_2:
  A2B_tP24_92_2b_b-001 WWPP
- Zr_5Si_4:
  A4B5_tP36_92_2b_a2b-001 C3GS
- Intermediate temperature Tetragonal TlS:
  AB_tP64_92_2a3b_4b-001 X71C
- Maucherite ($Ni_{11}As_8$):
  A8B11_tP76_92_2a3b_a5b-001 CBJ0
- Y_3Ni_2:
  A2B3_tP80_92_4b_2a5b-001 J821
- Retgersite (α-$NiSO_4{\cdot}6H_2O$, $H4_5$):
  A12BC10D_tP96_92_6b_a_5b_a-001 JAKV

$P4_22$ (93):
- $AsPh_4CeS_8P_4Me_8$:
  AB32CD4E8_tP184_93_i_16p_af_2p_4p-001 PSUB

$P4_22_12$ (94):
- Li_2MoF_6:
  A6B2C_tP18_94_eg_c_a-001 1ZGT
- $Na_5Fe_3F_{14}$:
  A14B3C5_tP44_94_c3g_ad_bg-001 CH2B

$P4_322$ (95):
- ThBC:
  ABC_tP24_95_d_d_d-001 8RZF

$P4_32_12$ (96):
- "ST12" of Si:
  A_tP12_96_ab-001 YUU3
- Keatite (SiO_2):
  A2B_tP36_96_3b_ab-001 J0BF
- α-AlB_{12}:
  A5B22_tP216_96_5b_2a21b-001 ZF6C

I422 (97):
- $NaGdCu_2F_8$:
  A2B8CD_tI24_97_d_k_a_b-001 FH59
- Ta_2Se_8I:
  AB8C2_tI44_97_e_2k_cd-001 4HFE

$I4_122$ (98):
- $CdAs_2$:
  A2B_tI12_98_f_a-001 G4QQ
- Phase III $Cd_2Re_2O_7$:
  A2B7C2_tI44_98_f_acde_f-001 XLYF

P4mm (99):
- Tetragonal PZT [$Pb(Zr_xTi_{1-x})O_3$]:
  A3BC_tP5_99_ac_b_a-002 Z2SB
- Room temperature Tetragonal $BaTiO_3$:
  AB3C_tP5_99_b_ac_a-001 3BZX

P4bm (100):
- $F5_4$ (NH_4ClO_2) (*Obsolete*):
  ABC2_tP8_100_b_a_c-001 YZB2
- NH_4NO_3 II ($G0_9$):
  ABC3_tP10_100_b_a_bc-001 80PK
- Fresnoite ($Ba_2TiSi_2O_8$):
  A2B8C2D_tP26_100_c_abcd_c_a-001 QC0E
- $Ce_3Si_6N_{11}$:
  A3B11C6_tP40_100_ac_bc2d_cd-001 LZ7C

$P4_2cm$ (101):
- Y-MgNiSn:
  A7B7C2_tP32_101_ade_bde_d-001 LR8K

$P4_2nm$ (102):
- Gd_3Al_2:
  A2B3_tP20_102_2c_b2c-001 AY9W

P4cc (103):
- High temperature $NbTe_4$:
  AB4_tP10_103_a_d-001 MRXL
- VSe_2O_6:
  A6B2C_tP72_103_abc5d_2d_abc-001 9ZX1

P4nc (104):
- Tl_4HgI_6:
  AB6C4_tP22_104_a_2ac_c-001 Z85J
- $Ba_5In_4Bi_5$:
  A5B5C4_tP28_104_ac_ac_c-001 GFEJ

$P4_2mc$ (105):
- $BaGe_2As_2$:
  A2BC2_tP20_105_f_bc_2d-001 W96U

$P4_2bc$ (106):
- $NaZn[OH]_3$:
  A3BC3D_tP64_106_3c_c_3c_c-001 SP8Q

I4mm (107):
- GeP (High-pressure, superconducting):
  AB_tI4_107_a_a-001 B4LQ
- $BaNiSn_3$:
  ABC3_tI10_107_a_a_ab-001 N3SR
- Co_5Ge_7:
  A5B7_tI24_107_ac_abd-001 Y7TL
- UP_2:
  A2B_tI24_107_2abc_2ab-001 3JHK

I4cm (108):
- Sr_5Si_3 (*Obsolete*):
  A3B5_tI32_108_ac_a2c-001 BY2X

$I4_1md$ (109):
- NbAs:
  AB_tI8_109_a_a-001 M2PT
- LaPtSi:
  ABC_tI12_109_a_a_a-001 RTEY

$I4_1cd$ (110):
- $Be[BH_4]_2$:
  A2BC8_tI176_110_2b_b_8b-001 29CG

$P\bar{4}2_1m$ (111):
- $E3_1$ (β-Ag_2HgI_4):
  A2BC4_tP7_111_e_b_n-001 34W5
- VN (Low-temperature):
  AB_tP8_111_n_n-001 GUN1
- MnF_2:
  A2B_tP12_111_2n_bce-001 YKCX
- Mooihoekite ($Cu_9Fe_9S_{16}$):
  A9B9C16_tP34_111_ajn_bcdek_2no-001 2KD6

$P\bar{4}2c$ (112):
- α-$CuAlCl_4$:
  AB4C_tP12_112_b_n_e-001 FV74

$P\bar{4}2_1m$ (113):
- BaS_3 ($D0_{17}$):
  AB3_tP8_113_a_ce-001 0A77
- Ammonium Chlorite (NH_4ClO_2):
  AB4CD2_tP16_113_c_f_a_e-001 RYUC
- Akermanite ($Ca_2MgSi_2O_7$, $S5_3$):
  A2BC7D2_tP24_113_e_a_cef_e-001 QV01

$P\bar{4}2_1c$ (114):
- Pd_4Se:
  A4B_tP10_114_e_a-001 C2PK
- SeO_3:
  A3B_tP32_114_3e_e-001 U620
- $Ag_2SO_4{\cdot}4NH_3$ ($H4_{17}$):
  A2B12C4D4E_tP46_114_d_3e_e_e_a-001 PABV
- $C_{19}Sc_{15}$:
  A19B15_tP68_114_ac4e_bc3e-001 PVAV

$P\bar{4}m2$ (115):
- $F6_1$ Chalcopyrite ($CuFeS_2$) (*Obsolete*):
  ABC2_tP4_115_a_c_g-001 88N3
- Rh_3P_2:
  A2B3_tP5_115_g_ag-001 EXDQ
- Zr_2CuSb_3:
  AB3C2_tP6_115_a_bg_g-001 NQAB
- Orange (averaged) HgI_2:
  AB2_tP12_115_j_egi-001 RJ86
- Deltalumite (δ-alumina, Al_2O_3):
  A3B4_tP84_115_acef3g3j3k_6j6k-001 YL8L

$P\bar{4}c2$ (116):
- Ru_2Sn_3:
  A2B3_tP20_116_adi_ej-001 RJFD
- Mn_4Ge_7 Nowotny Chimney-Ladder:
  A4B7_tP44_116_ach2i_e3j-001 2NXF

- $Rh_{10}Ga_{17}$:
  A17B10_tP108_116_e8j_ad2g2h5i-001 D8JE

$P\bar{4}b2$ (117):
- β-Bi_2O_3 ($D5_{12}$):
  A2B3_tP20_117_i_adgh-001 B48H

$P\bar{4}n2$ (118):
- $RuIn_3$:
  A3B_tP16_118_ei_f-001 0ZUR
- Ir_3Ga_5:
  A5B3_tP32_118_f2i_aceh-001 DCPJ

$I\bar{4}m2$ (119):
- GaSb (II):
  AB_tI4_119_c_a-001 K2V9
- Tetragonal $TlFeS_2$:
  AB2C_tI8_119_c_e_a-001 J41Y
- Mn_2RhSn Tetragonal Heusler:
  A2BC_tI8_119_ac_b_d-001 4BRY
- $RbGa_3$:
  A3B_tI24_119_a2i_bf-001 6TQK
- Phase II $Cd_2Re_2O_7$:
  A2B7C2_tI44_119_i_acefgh_i-001 AZDB

$I\bar{4}c2$ (120):
- KAu_4Sn_2:
  A4BC2_tI28_120_i_a_h-001 KAKD
- $BeSO_4{\cdot}4H_2O$ ($H4_3$):
  AB8C8D_tI72_120_b_2i_2i_c-001 KR2S

$I\bar{4}2m$ (121):
- C17 (Fe_2B) (*Obsolete*):
  AB2_tI12_121_ab_i-001 1BSH
- Stannite (Cu_2FeS_4Sn, $H2_6$):
  A2BC4D_tI16_121_d_a_i_b-001 JRUG
- Luzonite (Cu_3AsS_4):
  AB3C4_tI16_121_a_bd_i-001 3FZ9
- $Tl_2CdGeTe_4$:
  ABC4D2_tI16_121_a_b_i_c-001 RB89
- K_3CrO_8:
  AB3C8_tI24_121_a_bd_2i-001 FR9M
- α-V_3S:
  AB3_tI32_121_f_g2i-001 QHX2
- $SrCu_2(BO_3)_2$:
  A2B2C6D_tI44_121_i_i_ij_c-001 USSD

$I\bar{4}2d$ (122):
- Chalcopyrite ($CuFeS_2$, $E1_1$):
  ABC2_tI16_122_a_b_d-001 XWJF
- $Mn_{1.4}PtSn$:
  A3B2C2_tI28_122_ad_c_d-001 1YSS
- Mercury Cyanide [$Hg(CN)_2$, $F1_1$]:
  A2BC2_tI40_122_e_d_e-001 05M4
- KH_2PO_4 ($H2_2$):
  A4BC4D_tI40_122_e_b_e_a-001 TLFW
- NaS_2:
  AB2_tI48_122_cd_2e-001 Q5KE
- $NH_4H_2PO_4$:
  A8BC4D_tI56_122_2e_b_e_a-001 PGWH
- $Ba_{19}Li_{44}$:
  A19B44_tI252_122_ac4e_2d10e-001 HB2V

P4/mmm (123):
- CuAu(I) ($L1_0$):
  AB_tP2_123_a_d-001 9JUZ
- δ-CuTi ($L2_a$):
  AB_tP2_123_a_d-002 C9G2
- Linzhiite (High temperature $FeSi_2$):
  AB2_tP3_123_a_h-001 N538
- FeNNi:
  ABC_tP3_123_c_a_b-001 C14E
- $CuTi_3$ ($L6_0$):
  AB3_tP4_123_a_ce-001 B4JD
- $CaCuO_2$:
  ABC2_tP4_123_a_d_e-001 ACQJ
- NH_4HgCl_3 ($E2_5$):
  A3BC_tP5_123_ah_c_b-001 5MRT
- Mn_2Co_2C:
  AB2C2_tP5_123_b_e_ac-001 8ZWP
- $TlAlF_4$ ($H0_8$):
  AB4C_tP6_123_b_eg_c-001 416G
- $CeCr_2Si_2C$:
  ABC2D2_tP6_123_b_a_e_h-001 G8WV
- $HoCoGa_5$:
  AB5C_tP7_123_b_ci_a-001 SBCX
- K_2PtCl_4 ($H1_5$):
  A4B2C_tP7_123_j_e_a-001 3SRH
- $CePdGa_6$:
  AB6C_tP8_123_a_hi_b-001 1ALT
- $CaRbFe_4As_4$ (Superconducting):
  A4BC4D_tP10_123_gh_a_i_d-001 X7PG
- $E6_1$ [$Sr(OH)_2(H_2O)_8$] (*Obsolete*):
  A8B2C_tP11_123_r_e_b-001 QEVQ
- $E6_2$ [$SrO_2(H_2O)_8$] (Possibly Obsolete):
  A8B2C_tP11_123_r_h_a-001 E0G5
- $YBaCuFeO_5$:
  AB2C2D5E_tP11_123_a_h_h_ci_b-001 K0VP
- Ho_2CoGa_8:
  AB8C2_tP11_123_a_ehi_g-003 G7WP
- $AuMn_3$:
  AB3_tP12_123_ae_cghi-001 U1FT
- $HgBa_2CaCu_2O_{6+\delta}$:
  A2BC2DE7_tP13_123_g_b_h_c_ahi-001 BESE
- Ce_3PdIn_{11}:
  A3B11C_tP15_123_ag_ch2i_b-001 7DQQ
- $Ce_5Pd_2In_{19}$:
  A5B19C2_tP26_123_a2g_ce2h3i_g-001 RR9W

P4/mcc (124):
- Room temperature $NbTe_4$:
  AB4_tP10_124_a_m-001 XFHX
- Nb_4CoSi:
  AB4C_tP12_124_a_m_c-001 LAN3
- $CaO_2(H_2O)_8$:
  AB8C2_tP22_124_a_n_h-001 QCQG

P4/nbm (125):
- $PtPb_4$ ($D1_d$):
  A4B_tP10_125_m_a-001 0BXW
- $KCeSe_4$:
  ABC4_tP12_125_a_b_m-001 575A
- $PuGa_6$:
  A6B_tP14_125_gm_c-001 PCUV
- $SrFe_2S_4$:
  AB2C4D_tP16_125_a_cd_m_b-001 DV64
- Sm_2NiGa_{12}:
  A12BC2_tP30_125_2g2m_c_h-001 UYGN

P4/nnc (126):
- $BiAl_2S_4$:
  A2BC4_tP28_126_cd_e_k-001 4WPC
- $Ag[Co(NH_3)_2(NO_2)_4]$ ($J1_9$):
  ABC4D2E8_tP32_126_a_b_h_e_k-001 EW36
- Vesuvianite ($Ca_{10}Al_4(Mg,Fe)_2Si_9O_{34}(OH)_4$, $S2_3$):
  A4B10C2D34E4F9_tP252_126_k_ce2k_f_h8k_k_d2k-001 QSJ3

P4/mbm (127):
- Si_2U_3 ($D5_a$):
  A2B3_tP10_127_g_ah-001 6QGS
- Mo_2FeB_2:
  A2BC2_tP10_127_g_a_h-002 5SWM
- $RbAlF_4$ II:
  AB4C_tP12_127_a_eg_c-001 QJN8
- Mn_2Hg_5:
  A5B2_tP14_127_cj_g-001 BAHM
- $Pd(NH_3)_4Cl_2{\cdot}H_2O$ ($H4_9$):
  A2BC4D_tP16_127_g_c_j_b-001 Y171
- ThB_4 ($D1_e$):
  A4B_tP20_127_ehj_g-001 GQBH
- Phosgenite [$Pb_2Cl_2(CO_3)$]:
  AB2C3D2_tP32_127_g_eh_gk_k-001 URTV
- κ-AlF_3:
  AB3_tP40_127_di_cg2ij-001 46QF
- Tetragonal Potassium Bronze ($K_3W_5O_{15}$):
  A3B15C5_tP46_127_bh_cg2ij_di-001 LCR4

P4/mnc (128):
- Phase II K_2SnCl_6:
  A6B2C_tP18_128_eh_d_a-001 AD9M
- $FeCu_2Al_7$ ($E9_a$):
  A7B2C_tP40_128_egi_h_e-001 YX16
- $U_2Mn_3Si_5$:
  A3B5C2_tP40_128_dh_egh_h-001 P4UA
- Chiolite ($Na_5Al_3F_{14}$, $K7_5$):
  A3B14C5_tP44_128_ac_ehi_bg-001 GFQ6
- Apophyllite ($KCa_4Si_8O_{20}F{\cdot}8H_2O$, $S5_2$):
  A4BC16DE28F8_tP116_128_h_a_2i_b_g3i_i-001 DPWF

P4/nmm (129):
- Litharge (tetragonal PbO, $B10$):
  AB_tP4_129_a_c-001 CWTN
- γ-CuTi ($B11$):
  AB_tP4_129_c_c-001 EKF2
- β-Np (A_d):
  A_tP4_129_ac-001 UNPK
- Cu_2Sb ($C38$):
  A2B_tP6_129_ac_c-001 YG4M
- Matlockite ($E0_1$, PbFCl):
  ABC_tP6_129_c_a_c-001 0VRY
- LaOF:
  ABC_tP6_129_a_c_b-001 JX34
- AsCuSiZr:
  ABCD_tP8_129_c_b_a_c-001 1T51
- LaOAgS:
  ABCD_tP8_129_b_c_a_c-001 VCTW
- $UCoC_2$:
  A2BC_tP8_129_2c_a_c-002 K32Y
- $HfCuSi_2$:
  ABC2_tP8_129_a_c_bc-002 3Z42
- $CaBe_2Ge_2$:
  A2BC2_tP10_129_ac_c_bc-001 HOMM
- Ti_2Cu_3:
  A3B2_tP10_129_3c_2c-001 T7XE
- $SrPt_3P$:
  AB3C_tP10_129_c_ce_a-001 YXBN
- NH_4Br ($B25$):
  AB4C_tP12_129_c_i_a-001 G1GD
- $CsFeF_4$ II:
  AB4C_tP24_129_bc_ij_d-001 K69U
- Meta-autunite (I) [$Ca(UO_2)_2(PO_4)_2{\cdot}6H_2O$, $H5_{10}$]:
  AB4C6DE_tP26_129_c_j_2ci_a_c-001 VQBJ
- θ-AlF_3:
  AB3_tP64_129_2cdi_2cfhijk-001 HQ3Z

P4/ncc (130):
- α-WO_3:
  A3B_tP16_130_cf_c-001 HPJW
- $CuBi_2O_4$:
  A2BC4_tP28_130_f_c_g-001 N4MV
- Ba_5Si_3:
  A5B3_tP32_130_cg_cf-001 0VYM
- Room temperature Metastable VO_2:
  A2B_tP48_130_2g_g-001 P5YW
- $Sr(OH)_2(H_2O)_8$:
  A18B10C_tP116_130_2c4g_2c2g_a-001 JDN7

$P4_2$/mmc (131):
- Cooperite (PtS, $B17$):
  AB_tP4_131_c_e-001 8GEP
- LaB_2C_2:
  A2B2C_tP10_131_j_l_f-001 XLRT

$P4_2$/mcm (132):
- $AgUF_6$:
  AB6C_tP16_132_b_io_c-001 U3ZM
- $Rb_2TiCu_2S_4$:
  A2B2C4D_tP18_132_e_i_o_b-001 BD46

$P4_2$/nbc (133):
- β-V_3S:
  AB3_tP32_133_h_i2j-001 2PY4
- Zr_3PD_3:
  A4BC3_tP64_133_2k_h_i2j-001 XBGP

$P4_2$/nnm (134):
- T-50 B (A_g):
  A_tP50_134_a2m2n-001 R7N6

$P4_2$/mbc (135):
- Downeyite (α-SeO_2, $C47$):
  A2B_tP24_135_gh_h-001 YNQK
- $ZnSb_2O_4$:
  A4B2C_tP28_135_gh_h_d-001 20MM
- $Bi_4Fe_5O_{13}F$:
  A4B4C5D14_tP108_135_i_i_dfh_egh2i-001 55HD

$P4_2$/mnm (136):
- γ-N:
  A_tP4_136_f-001 VJ5B
- Rutile (TiO_2, $C4$):
  A2B_tP6_136_f_a-001 D4ZH
- β-BeO:
  AB_tP8_136_f_g-001 FJT4
- α-Li_3BN_2:
  AB3C2_tP12_136_a_bd_f-001 2PDY
- $ZrFe_4Si_2$:
  A4B2C_tP14_136_i_f_a-001 U6YK
- $IrIn_3$:
  A3B_tP16_136_cj_f-001 YFFG
- Ordoñezite ($ZnSb_2O_6$):
  A6B2C_tP18_136_fj_e_a-001 8DHD
- α'-V_8O:
  AB8_tP18_136_a_2fi-001 WVZU
- Zr_3Al_2:
  A2B3_tP20_136_j_dfg-001 QSNP
- Na_3Hg_2:
  A2B3_tP20_136_j_cfg-001 T3N4
- $K_2CuCl_4 \cdot 2H_2O$ ($H4_1$):
  A4BC4D2E2_tP26_136_fg_a_j_d_e-001 40BA
- σ-CrFe ($D8_b$):
  A4B4C4DE2_tP30_136_i_j_i_a_f-001 6EHC
- β-U (A_b):
  A_tP30_136_af2ij-001 5T44
- $Nd_2Fe_{14}B$:
  AB14C2_tP68_136_f_ce2j2k_fg-001 FUR0

$P4_2/nmc$ (137):
- ZrO_2 (High-temperature):
  A2B_tP6_137_d_a-001 T9FR
- Coccinite (Red HgI_2, $C13$):
  AB2_tP6_137_a_d-001 2F93
- Low temperature KBD_4:
  AB4C_tP12_137_a_g_b-001 Q06Z
- $CeCo_4B_4$:
  A4BC4_tP18_137_g_a_g-001 EUHG
- Li_6CoO_4:
  AB6C4_tP22_137_a_df_g-001 ZQRP
- Orange (II) HgI_2:
  AB2_tP24_137_g_cdf-001 L566
- Zn_3P_2 ($D5_9$):
  A2B3_tP40_137_cdf_3g-001 68SX

$P4_2/ncm$ (138):
- C (T12 Group IV):
  A_tP12_138_bi-001 HZJ9
- Cl ($A18$) (*Obsolete*):
  A_tP16_138_j-001 ZBJR
- Tetragonal La_2NiO_4:
  A2BC4_tP28_138_i_c_aei-001 J1M9

$I4/mmm$ (139):
- In ($A6$):
  A_tI2_139_a-001 F5BG
- Pa (A_a):
  A_tI2_139_a-002 YF8N
- Hypothetical BCT5 Si:
  A_tI4_139_e-001 ZSDQ
- "Martensite Type" FeC_x ($x < 0.06$) ($L'2_0$):
  AB_tI4_139_a_b-002 ZN4Y
- β-$LiFeO_2$:
  AB_tI4_139_a_b-003 G0K3
- ThH_2 ($L'2_b$):
  A2B_tI6_139_d_a-001 R0C0
- $MoSi_2$ ($C11_b$):
  AB2_tI6_139_a_e-001 NG7F
- CaC_2-I ($C11_a$):
  A2B_tI6_139_e_a-001 RDQF
- Al_3Ti ($D0_{22}$):
  A3B_tI8_139_ad_b-001 7W3W
- Hypothetical Tetrahedrally Bonded Carbon with 4-Member Rings:
  A_tI8_139_h-001 TE0L
- Calomel (Hg_2Cl_2, $D3_1$):
  AB_tI8_139_e_e-001 T1KN
- $D1_3$ ($BaAl_4$):
  A4B_tI10_139_de_a-001 676C
- $TlCo_2S_2$:
  A2B2C_tI10_139_d_e_a-002 D85X
- $ThCr_2Si_2$:
  A2B2C_tI10_139_d_e_a-003 LS62
- Au_2Nb_3:
  A2B3_tI10_139_e_ae-001 5STC
- Li_2CN_2:
  AB2C2_tI10_139_a_d_e-002 5K3T
- $H5_9$ [Autunite $Ca(UO_2)_2(PO_4)_2 \cdot 10\frac{1}{2}H_2O$] (*Obsolete*):
  AB2C2_tI10_139_a_d_e-003 SC3Z
- Na_2HgO_2:
  AB2C2_tI10_139_a_e_e-001 6LGV
- $LuNi_2B_2C$:
  A2BCD2_tI12_139_e_a_b_d-001 4LX6
- 0201 [$(La,Ba)_2CuO_4$] High-T_c:
  AB2C4_tI14_139_a_e_ce-001 V35A
- K_2NiF_4:
  A4B2C_tI14_139_ce_e_a-001 SENW
- $Sr_2CuO_2Cl_2$:
  A2BC2D2_tI14_139_e_a_c_e-001 0HCF
- Ti_3Cu_4:
  A4B3_tI14_139_2e_ae-001 N44F
- (T′) Nd_2CuO_4:
  AB2C4_tI14_139_a_e_cd-003 1V8W
- Al_3Zr ($D0_{23}$):
  A3B_tI16_139_cde_e-001 CSTH
- $BaZnSb_2$:
  AB2C_tI16_139_e_ce_d-003 00JM
- V_4Zn_5:
  A4B5_tI18_139_i_ah-001 84H6
- Pt_8Ti:
  A8B_tI18_139_hi_a-001 XTZU
- $K_2OsO_2Cl_4$ ($J1_5$):
  A4B2C2D_tI18_139_h_d_e_a-001 1KN8
- Fe_8N ($D2_g$):
  A8B_tI18_139_deh_a-001 6VR8
- $Sr_2Mn_3As_2O_2$:
  A2B3C2D2_tI18_139_e_ad_c_e-001 JBSJ
- $AuCsCl_3$ ($K7_6$):
  AB3C_tI20_139_ab_eh_d-001 QC4Q
- $CePt_2In_7$:
  AB7C2_tI20_139_a_bdg_e-001 P6JF
- $Ba_2Ti_2Fe_2As_4O$:
  A4B2C2DE2_tI22_139_2e_e_d_a_c-001 8C3Q
- $Sr_3Ti_2O_7$:
  A7B3C2_tI24_139_aeg_be_e-001 PDHZ
- $Mn_{12}Th$ ($D2_b$):
  A12B_tI26_139_fij_a-001 AJGV
- $KCa_2Fe_4As_4F_2$ (12442-type superconductor):
  A4B2C2D4E_tI26_139_2e_e_d_g_a-001 YU5Q
- $Bi_2Sr_2CaCu_2O_8$ (BSCCO):
  A2BC2D8E2_tI30_139_e_a_e_2eg_e-001 BZRA
- $Nd_4Ni_3O_8$:
  A4B3C8_tI30_139_2e_ae_cdg-002 W8GW
- $Sr_4Ti_3O_{10}$:
  A10B4C3_tI34_139_c2eg_2e_ae-001 TJ17
- High temperature $BaBi_4Ti_4O_{15}$ $m = 4$ Aurivillius:
  AB4C15D4_tI48_139_a_2e_bd2e2g_2e-001 Y186
- γ-$Bi_4V_2O_{11}$:
  A5B9C2_tI64_139_em_d2n_h-001 0N6E
- $Ho_{11}Ge_{10}$:
  A10B11_tI84_139_dehim_eh2n-001 HN10
- $K_3TlCl_6{\cdot}2H_2O$ ($J3_1$):
  A6B2C3D_tI168_139_egikl2m_ejn_bh2n_acf-001 8AAX

$I4/mcm$ (140):
- Khatyrkite (Al_2Cu, $C16$):
  A2B_tI12_140_h_a-001 PARL
- α-SiU_3 ($D0_c$):
  AB3_tI16_140_b_ah-001 6CWC
- β-SeTl ($B37$):
  AB_tI16_140_ab_h-001 BFE0
- KHF_2 ($F5_2$):
  A2BC_tI16_140_h_d_a-001 B7FR
- $PdGa_5$:
  A5B_tI24_140_cl_a-001 528Z
- V_4SiSb_2:
  A2BC4_tI28_140_h_a_k-001 VENL
- U_6Mn ($D2_c$):
  AB6_tI28_140_a_hk-001 1Q6T
- W_5Si_3 ($D8_m$):
  A3B5_tI32_140_ah_bk-001 4K4U
- Cr_5B_3 ($D8_l$):
  A3B5_tI32_140_ah_cl-001 AK18

- ○ $(NH_4)Pb_2Br_5$ ($K3_4$) (*Erroneous*):
  A5BC2_tI32_140_bl_a_h-001 HL9W
- • $(NH_4)Pb_2Br_5$ ($K3_4$) (*Revised*):
  A5BC2_tI32_140_cl_a_h-001 REV7
- ○ Cs_3CoCl_5 ($K3_1$):
  A5BC3_tI36_140_cl_b_ah-001 GHEH
- • $BaLa_2ZnO_5$:
  AB2C5D_tI36_140_a_h_cl_b-001 4VUW
- ○ $Pu_{31}Rh_{20}$:
  A31B20_tI204_140_b2gh3m_ac2fh3l-001 TBHL

$I4_1/amd$ (141):

- ○ β-Sn ($A5$):
  A_tI4_141_a-001 2BUF
- ○ NbP ("40"):
  AB_tI8_141_a_b-001 R06D
- ○ Anatase (TiO_2, $C5$):
  A2B_tI12_141_e_a-001 1TUW
- ○ α-$ThSi_2$ (C_c):
  A2B_tI12_141_e_a-002 NF8F
- ○ MoB (B_g):
  AB_tI16_141_e_e-001 B9A8
- • γ-$LiFeO_2$:
  ABC2_tI16_141_a_b_e-003 XJE5
- • β-$ThCl_4$:
  A4B_tI20_141_h_a-001 NG21
- ○ Ga_2Hf:
  A2B_tI24_141_2e_e-001 DBUS
- ○ Zircon ($ZrSiO_4$, $S1_1$):
  A4BC_tI24_141_h_a_b-001 0FQT
- • β-LiSn:
  AB_tI24_141_ae_be-001 1GTY
- ○ Haussmannite (Mn_3O_4):
  A3B4_tI28_141_ad_h-001 KP7A
- • $CuCr_2O_4$:
  A2BC4_tI28_141_c_b_h-001 763J
- • Paramelaconite (Cu_4O_3):
  A4B3_tI28_141_cd_ae-002 P57T
- ○ $BaCd_{11}$:
  AB11_tI48_141_b_aci-001 EV03
- • Orange (I) HgI_2:
  AB2_tI48_141_h_2eg-001 Q9V3
- ○ β-In_2S_3:
  A2B3_tI80_141_ceh_3h-001 PJGC
- • $V_{13}O_{16}$:
  A16B13_tI116_141_2hi_a2fh-001 NCQA

$I4_1/acd$ (142):

- ○ S-III:
  A_tI16_142_f-001 GC8R
- • α-$PdSn_2$:
  AB2_tI48_142_d_ef-001 FUUU
- • Sr_2IrO_4:
  AB4C2_tI56_142_a_df_d-001 EHYC
- • R_1 Au_3Zn:
  A3B_tI64_142_def_d-001 Q6FW
- • NaPb:
  AB_tI64_142_ef_g-001 X6RS
- ○ $PPrS_4$:
  ABC4_tI96_142_e_ab_2g-001 B2Y6
- • $BaCo_2V_2O_8$:
  AB2C8D2_tI104_142_a_f_2g_e-001 BMKB
- ○ Cd_3As_2:
  A2B3_tI160_142_deg_3g-001 1P80
- • Tetragonal Be_3P_2:
  A3B2_tI160_142_3g_abcef-001 4A1E
- ○ Analcime ($NaAlSi_2O_6{\cdot}H_2O$, $S6_1$):
  A2B2C3D12E4_tI184_142_f_f_be_3g_g-001 PFBA
- • $Er_5Rh_6Sn_{18}$:
  A5B6C18_tI232_142_bg_dg_e2f3g-001 21TS

P3 (143):

- ○ $ScRh_6P_4$:
  A4B6C_hP11_143_ad_2d_b-001 HTHS
- ○ Trigonal MoS_2:
  AB2_hP12_143_ad_bc2d-001 1G0H
- ○ Simpsonite ($Ta_3Al_4O_{13}[OH]$):
  A4B14C3_hP21_143_ad_bc4d_d-001 TY99
- ○ $P3$ La_3BWO_9:
  AB3C9D_hP28_143_2a_2d_6d_bc-001 0XN3
- • Trigonal (h′) Al_5Mo:
  A5B_hP60_143_7a7b6c10d_3a3b4c-001 TWK7

$P3_1$ (144):

- ○ ZnTe (high-pressure):
  AB_hP6_144_a_a-001 LX4R
- ○ $IrGe_4$:
  A4B_hP15_144_4a_a-001 0VM9
- ○ $RbNO_3$ (IV):
  AB3C_hP45_144_3a_9a_3a-001 UV9A

$P3_2$ (145):

- ○ Sheldrickite ($NaCa_3[CO_3]_2F_3[H_2O]$):
  A2B3C3DE7_hP48_145_2a_3a_3a_a_7a-001 3V4Q

R3 (146):

- ○ γ-Ag_3SI (Low-Temperature):
  A3BC_hR5_146_b_a_a-001 YGSU
- ○ $FePSe_3$:
  ABC3_hR10_146_2a_2a_2b-001 EARG
- • Li_2ZrTeO_6:
  A2B6CD_hR10_146_2a_2b_a_a-001 T7PA
- • Pd_7P_3:
  A3B7_hR20_146_2b_2a4b-001 35AG
- • Carlinite (Tl_2S):
  AB2_hR27_146_3a2b_6b-001 X2PG
- • Rhombohedral $LiZnPO_4$:
  AB4CD_hR42_146_2b_8b_2b_2b-001 BGS4

$R\bar{3}$ (147):

- ○ γ-AgZn (B_b):
  A2B_hP9_147_g_ad-001 RQCB
- • $PtBi_2$:
  A2B_hP9_147_g_ad-002 0RUP
- ○ Na_2SO_3 ($G3_2$):
  A2B3C_hP12_147_abd_g_d-001 H9Z3
- • $Na_2BaNi(PO_4)_2$:
  AB2CD8E2_hP14_147_a_d_b_dg_d-001 B64B
- • URu_3B_2:
  A2B3C_hP48_147_2d2g_4g_abef-001 B1DH

$R\bar{3}$ (148):

- • S_6 (ρ-S) Sulfur:
  A_hR6_148_f-001 XW0B
- ○ BiI_3 ($D0_5$):
  AB3_hR8_148_c_f-001 TZC0
- • β-$CuZrF_6$:
  AB6C_hR8_148_a_f_b-001 7RW9
- ○ Ilmenite ($FeTiO_3$, $E2_2$):
  AB3C_hR10_148_c_f_c-001 4YUA
- ○ Dolomite [$MgCa(CO_3)_2$, $G1_1$:]
  A2BCD6_hR10_148_c_a_b_f-001 WCJU
- • Rhombohedral Cr_2S_3:
  A2B3_hR10_148_abc_f-001 CVKE
- • $FePSe_3$:
  ABC3_hR10_148_c_c_f-001 CFP9

- $BaNi_2As_2O_8$:
  A2BC2D8_hR13_148_c_a_c_cf-001 VJPX
  - $Ni(H_2O)_6SnCl_6$ ($I6_1$):
    A6B6CD_hR14_148_f_f_a_b-001 5954
  - $K_2Sn(OH)_6$ ($H6_2$):
    A6B2C6D_hR15_148_f_c_f_a-001 FKGA
  - Li_7TaO_6:
    A8B6C_hR15_148_cf_f_a-001 L1GH
- $BaMo_6S_8$:
  AB6C8_hR15_148_a_f_cf-001 CY1Y
  - Solid Cubane (C_8H_8):
    AB_hR16_148_cf_cf-001 8Z24
- $Pd_{15}P_2$:
  A2B15_hR17_148_c_ac2f-001 Z055
  - β-$PdCl_2$:
    A2B_hR18_148_2f_f-001 8GMP
- Mg_3TeO_6:
  A3B6C_hR20_148_f_2f_ab-001 K70X
- $SrMn_7O_{12}$:
  A7B12C_hR20_148_ade_2f_b-001 5YFD
- Trechmannite ($AgAsS_2$):
  ABC2_hR24_148_f_f_2f-001 3VWQ
  - PdAl:
    AB_hR26_148_a2f_b2f-001 5EQ4
- Mikasaite (Rhombohedral $Fe_2(SO_4)_3$):
  A2B12C3_hR34_148_2c_4f_f-001 GHH0
  - Phenakite (Be_2SiO_4, $S1_3$):
    A2B4C_hR42_148_2f_4f_f-001 BQNX
- Dioptase [$Cu_6(Si_6O_{18})\cdot 6H_2O$]:
  AB2C4D_hR48_148_f_2f_4f_f-001 4C7V
- $Mg_{23}Al_{30}$:
  A30B23_hR53_148_5f_a2c3f-001 DB0A
- $Y_3Cu_9(OH)_{19}Cl_8$:
  A8B9C24D19E3_hR63_148_cf_df_4f_a3f_bc-001 GGPS

P312 (**149**):

- $PbMnTeO_6$:
  AB6CD_hP9_149_a_l_d_e-001 63FP
  - Ti_3O (Room-Temperature):
    AB3_hP24_149_acgi_3l-001 9DMX

P321 (**150**):

- Original Fe_2P ($C22$):
  A2B_hP9_150_ef_ad-001 6CGG
- β-Na_2ThF_6:
  A6B2C_hP9_150_ef_d_a-001 R3Z7
  - Steklite [$KAl(SO_4)_2$, $H3_2$]:
    ABC8D2_hP12_150_a_b_dg_d-001 SDL2
  - $Cs_3As_2Cl_9$ ($K7_3$):
    A2B9C3_hP14_150_d_eg_ad-001 4FK1
  - $SrCl_2\cdot(H_2O)_6$:
    A2B12C6D_hP21_150_d_2g_ef_a-001 FX47
- Dugganite ($Pb_3Zn_3TeAs_2O_{14}$):
  A2B14C3DE3_hP23_150_d_d2g_e_a_f-001 8A06
  - Paralstonite ($BaCa(CO_3)_2$):
    AB2CD6_hP30_150_e_c2d_f_3g-001 FL2F
  - KSO_3 ($K1_1$):
    AB3C_hP30_150_ef_3g_c2d-001 YVPA

$P3_112$ (**151**):

- $CrCl_3$ ($D0_4$):
  A3B_hP24_151_3c_2a-001 5EPG
- V_6C_5:
  A5B6_hP33_151_3a2b_3c-001 V1KT

$P3_121$ (**152**):

- γ-Se ($A8$):
  A_hP3_152_a-001 SM1V
  - α-Quartz (low Quartz):
    A2B_hP9_152_c_a-001 P53L
- Trigonal B_2O_3:
  A2B3_hP15_152_c_ac-001 MKFS
- Alarsite ($AlAsO_4$):
  ABC4_hP18_152_a_b_2c-001 P55Q
- $Ni_{13}Ga_3Ge_6$:
  A3B6C13_hP66_152_ac_3c_a2b5c-001 A5TG

$P3_{212}$ (**153**):

- $CrCl_3$:
  A3B_hP24_153_3c_2a-001 Z0S9

$P3_{221}$ (**154**):

- Cinnabar (HgS, $B9$):
  AB_hP6_154_a_b-001 A3TK
  - S-II:
    A_hP9_154_ac-001 GAZQ
- $EuIr_2P_2$:
  AB2C2_hP15_154_a_ab_c-001 3CT8
- $RbAg_2SbS_4$:
  A2BC4D_hP24_154_c_a_2c_b-001 8R3H

R32 (**155**):

- Hazelwoodite (Ni_3S_2, $D5_e$):
  A3B2_hR5_155_e_c-001 WQGS
  - AlF_3 ($D0_{14}$):
    AB3_hR8_155_c_de-001 QG2U
  - $KBe_2BO_3F_2$:
    AB2C2DE3_hR9_155_a_c_c_b_d-001 Q3TB
- Huntite [$CaMg_3(CO_3)_4$]:
  A4BC3D12_hR20_155_ad_b_e_2df-001 1B5F
- $ErNi_3Al_9$:
  A9BC3_hR26_155_3cdef_c_f-001 9G5F
- Low temperature $GdBO_3$:
  ABC3_hR30_155_de_f_de2f-001 5YKD

P3m1 (**156**):

- β-CuI (Sakuma):
  AB_hP4_156_ab_ab-001 1M22
  - CdI_2 (Polytype $6H_1$):
    AB2_hP9_156_2ab_a2b3c-001 0FK1
  - β-CuI (Kurdyumova):
    AB_hP12_156_3a2bc_3a2bc-001 ZMXD
- $KNaSO_4$:
  ABC4D_hP14_156_ac_bc_ab2d_ab-001 Z1Y1

P31m (**157**):

- $Ag_5Pb_2O_6$:
  A5B6C2_hP13_157_2ac_2c_b-001 1YM0

P3c1 (**158**):

- β-$RuCl_3$:
  A3B_hP8_158_d_a-001 KC70

P31c (**159**):

- HP-Bi_2O_3:
  A2B3_hP20_159_bc_2c-001 XT2J
  - $YbBaCo_4O_7$:
    AB4C7D_hP26_159_b_ac_a2c_b-001 ZUBF
  - Nierite (α-Si_3N_4):
    A4B3_hP28_159_ab2c_2c-001 9UA2

R3m (**160**):

- GeTe:
  AB_hR2_160_a_a-002 8379
  - Carbonyl Sulphide (COS, $F0_2$):
    ABC_hR3_160_a_a_a-001 V77F
- Rhombohedral MoS_2:
  AB2_hR3_160_a_2a-001 EW06
  - H_3S (130 GPa):
    A3B_hR4_160_b_a-001 P2LA

- Grimaldiite (α-CrOOH):
  ABC2_hR4_160_a_a_2a-002 LP35
- $CrCuS_2$:
  ABC2_hR4_160_a_a_2a-003 BC9T
- γ-GaSe:
  AB_hR4_160_2a_2a-001 M3V5
  - $KBrO_3$ ($G0_7$):
    ABC3_hR5_160_a_a_b-001 0ZSQ
  - γ-Potassium Nitrate (KNO_3):
    ABC3_hR5_160_a_a_b-002 V4KY
- Rhombohedral $BaTiO_3$:
  AB3C_hR5_160_a_b_a-001 X85U
  - Moissanite 9R (CSi):
    AB_hR6_160_3a_3a-001 T8Y7
  - Millerite (NiS, $B13$):
    AB_hR6_160_b_b-001 MV4U
  - Cronstedtite $Fe(Fe,Si)[(OH)_2O]O_3OH$, $S5_7$:
    AB3C2D_hR7_160_a_b_2a_a-001 H9NP
- Sn_4As_3:
  A3B4_hR7_160_3a_4a-001 RN9C
- $Fe_{5-\delta}GeTe_2$:
  A5BC2_hR8_160_5a_a_2a-001 6V4S
  - Moissanite-15R (SiC, $B7$):
    AB_hR10_160_5a_5a-001 KX5G
  - Fe_3PO_7:
    A3B7C_hR11_160_b_a2b_a-001 JN4A
  - Low temperature $GaMo_4S_8$:
    AB4C8_hR13_160_a_ab_2a2b-001 5V5H
- γ-$Na_2Ti_3Cl_8$:
  A8B2C3_hR13_160_2a2b_2a_b-001 L333
  - Cr_5Al_8 ($D8_{10}$):
    A8B5_hR26_160_a3bc_a3b-001 X9QA
  - SbI_3S_{24}:
    A3B24C_hR28_160_b_2b3c_a-001 8TMQ

R3c (**161**):

- Ferroelectric $LiNbO_3$:
  ABC3_hR10_161_a_a_b-001 FZF0
- Proustite (Ag_3AsS_3):
  A3BC3_hR14_161_b_a_b-001 TXGA
  - α-BaB_2O_4 (Low temperature):
    A2BC4_hR42_161_2b_b_4b-001 UFMT
- Stepanovite ($NaMgFe(C_2O_4)_3{\cdot}9H_2O$):
  A6BC18DEF21_hR96_161_2b_a_6b_a_a_7b-001 KKZD

P$\bar{3}$1m (**162**):

- β-V_2N ($L'3_2$):
  AB2_hP9_162_ad_k-001 RBZR
  - $I1_3$ $[SrCl_2{\cdot}(H_2O)_6]$ (*Obsolete*):
    A2B6C_hP9_162_c_k_b-001 WZ1P
  - Rosiaite ($PbSb_2O_6$):
    A6BC2_hP9_162_k_a_d-001 8OKE
- Trigonal $Au_7P_{10}I$:
  A7BC10_hP18_162_ceg_a_hk-001 RQ68

P$\bar{3}$1c (**163**):

- $NaSbF_4(OH)_2$ ($J1_{12}$):
  A6BC_hP16_163_i_b_c-001 KLNT
  - Colquiriite ($LiCaAlF_6$):
    ABC6D_hP18_163_c_b_i_d-001 8D1V
- β-Na_2GeTeO_6:
  AB2C6D_hP20_163_c_f_i_a-001 UZBW
- $Mn_3Si_2Te_6$:
  A3B2C6_hP22_163_cf_e_i-001 ELB0
- Trigonal Cr_5S_6:
  A5B6_hP22_163_abcf_i-001 Z6CB
  - $KAg(CN)_2$ ($F5_{10}$):
    AB2CD2_hP36_163_h_i_bf_i-001 JLGL
- Si_2Te_3:
  A7B3_hP40_163_e2i_i-001 MVBJ

P$\bar{3}$m1 (**164**):

- ω Phase (CdI_2, $C6$):
  AB2_hP3_164_a_d-001 32EZ
  - Zlatogorite ($CuNiSb_2$):
    ABC2_hP4_164_a_b_d-001 PUFU
  - $D0_{13}$ ($AlCl_3$) (*Obsolete*):
    AB3_hP4_164_a_bd-001 K2MJ
  - Al_3Ni_2 ($D5_{13}$):
    A3B2_hP5_164_ad_d-001 EUFT
  - La_2O_3 ($D5_2$):
    A2B3_hP5_164_d_ad-001 D3QE
  - Ce_2O_2S:
    A2B2C_hP5_164_d_d_a-002 FG79
  - Brucite $[Mg(OH)_2]$:
    A2BC2_hP5_164_d_a_d-001 N2MR
- β-CuI (Keen-Hull):
  A2B_hP6_164_2d_d-001 TVVQ
- Nukundamite $[(Cu_{1-x}Fe_x)_4S_4]$:
  ABC2_hP8_164_d_d_cd-001 CG4B
  - δ_H^{II}-NW_2:
    AB2_hP9_164_ad_c2d-001 Z07R
  - $K_2Pt(SCN)_6$ ($H6_3$):
    A2BC6_hP9_164_d_a_i-001 F3SY
  - Bararite [Trigonal $(NH_4)_2SiF_6$, $J1_6$]:
    A6B2C_hP9_164_i_d_a-001 4BR9
  - K_2GeF_6 ($J1_{13}$):
    A6BC2_hP9_164_i_a_d-001 2HX1
- Li_7Pb_2:
  A7B2_hP9_164_ac2d_d-001 FCSA
- K_2Hg_7:
  A7B2_hP9_164_ai_d-001 QCMW
  - Jacutingaite (Pt_2HgSe_3):
    AB2C3_hP12_164_d_ae_i-001 DCW7
  - Nevskite (BiSe):
    AB_hP12_164_c2d_c2d-001 UEMM
- Kapellasite ($Cu_3Zn(OH)_6Cl_2$):
  A2B3C6D_hP12_164_d_e_i_a-001 K216
- $MnBi_4Te_7$:
  A4BC7_hP12_164_2d_a_bc2d-001 SPWJ
- $AgBiSe_2$:
  ABC2_hP12_164_ad_bd_c2d-001 1TV2
- Trigonal α-Ca_2SiO_4:
  A2B4C_hP14_164_abd_di_d-001 DBUP
- Aphthitalite/Glaserite $[K_3Na(SO_4)_2]$:
  A3BC8D2_hP14_164_ad_b_di_d-001 9RQB
- $Ba_3SrTa_2O_9$:
  A3B9CD2_hP15_164_ad_ei_b_d-001 4LGS
- $Li_{13}Sn_5$:
  A13B5_hP18_164_a2c4d_b2d-001 G8A6
  - Predicted Li_2MgH_{16} 300 GPa:
    A16B2C_hP19_164_2d2i_d_a-001 LLDQ
- $YCu_3(OH)_6Cl_3$:
  ABC2D2E_hP21_164_bd_e_i_i_ac-001 1PRT

P$\bar{3}$c1 (**165**):

- H_3Ho:
  A3B_hP24_165_adg_f-001 V86P
  - Cu_3P ($D0_{21}$):
    A3B_hP24_165_bdg_f-001 Z2X0
- $Nb_2Mn_4O_9$:
  A4B2C9_hP30_165_2d_c_fg-001 GPQH

- $Li_9Al_3(P_2O_7)_3(PO_4)_2$:
  A3B9C29D8_hP98_165_f_bdg_df4g_dg-001 JRX6

R$\bar{3}$m (166):

- β-Po (A_i):
  A_hR1_166_a-001 RUSN
- α-Hg (A10):
  A_hR1_166_a-002 8ZQP
- Rhombohedral CuPt ($L1_1$):
  AB_hR2_166_a_b-001 3A9R
- α-As ($A7$):
  A_hR2_166_c-001 F2V5
- Rhombohedral Graphite:
  A_hR2_166_c-002 NXUA
- β-O_2:
  A_hR2_166_c-003 KTH0
- KSH ($B22$):
  AB_hR2_166_a_b-003 HA1H
- α-Sm ($C19$):
  A_hR3_166_ac-001 MPB6
- $CdCl_2$:
  AB2_hR3_166_a_c-004 TKCJ
- Caswellsilverite ($CrNaS_2$, $F5_1$):
  ABC2_hR4_166_a_b_c-001 J6ND
- Rhombohedral Delafossite ($CuFeO_2$):
  ABC2_hR4_166_a_b_c-004 Y8C3
- α-$NaFeO_2$:
  ABC2_hR4_166_a_b_c-009 5FG5
- Bi_2Te_3 ($C33$):
  A2B3_hR5_166_c_ac-001 NGV5
- SmSI:
  ABC_hR6_166_c_c_c-001 YTD1
- $CaSi_2$ ($C12$):
  AB2_hR6_166_c_2c-002 85MW
- $CaUO_4$:
  AB4C_hR6_166_a_2c_b-001 MMVG
- YOF:
  ABC_hR6_166_c_c_c-002 DGDK
- Mo_2B_5 ($D8_i$):
  A5B2_hR7_166_a2c_c-001 WZKM
- CaC_6:
  A6B_hR7_166_f_b-001 N45M
- Al_4C_3 ($D7_1$):
  A4B3_hR7_166_2c_ac-001 YAHB
- $MnBi_2Te_4$:
  A2BC4_hR7_166_c_a_2c-002 MU2V
- Shandite ($Ni_3Pb_2S_2$):
  A3B2C2_hR7_166_d_ab_c-001 SD1B
- $CaCu_4P_2$:
  AB4C2_hR7_166_a_2c_c-001 SFS1
- $YbFe_2O_4$:
  A2B4C_hR7_166_c_2c_a-001 EVRK
- In_3Se_4:
  A3B4_hR7_166_ac_2c-001 DJRQ
- Bi_4Te_3:
  A4B3_hR7_166_2c_ac-002 MVZB
- $GeSb_2Te_4$:
  AB2C4_hR7_166_a_c_2c-002 5J2E
- β-Potassium Nitrate (KNO_3):
  ABC6_hR8_166_a_b_h-001 XD6C
- SnP_3:
  A3B_hR8_166_h_c-001 JF25
- Fe_3Sn_2:
  A3B2_hR10_166_h_2c-001 KQQW
- $Al_6C_3N_2$:
  A6B3C2_hR11_166_3c_ac_c-001 T8T4
- Li_8Pb_2:
  A8B3_hR11_166_4c_ac-001 758U
- α-B (R-12):
  A_hR12_166_2h-001 1Y2H
- ThB_2C:
  A2BC_hR12_166_g_d_ac-001 AFH9
- $NbBe_3$:
  A3B_hR12_166_ach_bc-001 3QUZ
- $BaPb_3$:
  AB3_hR12_166_ac_eh-001 NHXQ
- Fe_7W_6 ($D8_5$) μ-phase:
  A7B6_hR13_166_ah_3c-001 MXB3
- $Ba_3Cr_2O_8$:
  A3B2C8_hR13_166_ac_c_ch-002 7UDV
- $Na_2Mn_3Cl_8$:
  A8B3C2_hR13_166_ch_e_c-001 799E
- $B_{13}C_2$ "B_4C" ($D1_g$):
  A13B2_hR15_166_a2h_c-001 PZDF
- $Al_8C_3N_4$:
  A8B3C4_hR15_166_4c_ac_2c-001 HGYT
- $TaTi_7$ (BCC SQS-16):
  AB7_hR16_166_c_c2h-001 56NK
- $MnBi_6Te_{10}$:
  A6BC10_hR17_166_3c_a_5c-001 LD13
- Er_2Co_7:
  A7B2_hR18_166_a2cdh_2c-001 VGKE
- Th_2Zn_{17}:
  A2B17_hR19_166_c_cdfh-001 PZ2T
- Nb_2Be_{17}:
  A17B2_hR19_166_cegh_c-001 3JAE
- $Ba_4NbRu_3O_{12}$:
  A4BC12D3_hR20_166_2c_a_2h_bc-001 9CFG
- High temperature K_2LiAlF_6:
  AB6C2D_hR20_166_ab_2h_2c_c-001 KTF5
- $Mn_2La_3Sb_3O_{14}$:
  A3B2C14D3_hR22_166_d_ab_c2h_e-001 6NJM
- Rhombohedral $CuTi_2S_4$:
  AB4C2_hR28_166_2c_2c2h_abh-001 8BYU
- Chabazite ($Ca_{1.4}Sr_{0.3}Al_{3.8}Si_{8.3}O_{24}{\cdot}13H_2O$, $S3_4$ (I)):
  A5B21C24D12_hR62_166_a2c_ehi_fg2h_i-001 2K92
- β-B (R-105):
  A_hR105_166_ac9h4i-001 Y6TF

R$\bar{3}$c (167):

- FeF_3 ($D0_{12}$):
  A3B_hR8_167_e_b-001 GPY3
- Corundum (α-alumina, Al_2O_3, $D5_1$):
  A2B3_hR10_167_c_e-001 CBQY
- Paraelectric $LiNbO_3$:
  ABC3_hR10_167_a_b_e-001 TXPE
- Calcite ($CaCO_3$, $G0_1$):
  ABC3_hR10_167_a_b_e-002 UVUF
- $PrNiO_3$:
  AB3C_hR10_167_b_e_a-001 XMCY
- Rhombohedral Al_5Mo:
  A5B_hR12_167_ce_b-001 584Z
- $CrCl_3(H_2O)_6$ ($J2_2$):
  A3BC6_hR20_167_e_b_f-001 YFN8
- $AgRuO_3$:
  AB3C_hR20_167_c_f_c-001 QQE1
- Rinneite ($K_3NaFeCl_6$):
  A6BC3D_hR22_167_f_b_e_a-001 PYAM
- $ScRh_3Si_7$:
  A3BC7_hR22_167_e_b_af-001 NS5K
- KBO_2 ($F5_{13}$):
  ABC2_hR24_167_e_e_2e-001 L33F

◦ $Cs_3Tl_2Cl_9$ ($K7_2$):	
A9B3C2_hR28_167_ef_e_c-001	7M03
◦ β-BaB_2O_4 (High temperature):	
A2BC4_hR42_167_f_ac_2f-001	RYPV
• MoP_3SiO_{11} (Rhombohedral model):	
AB11C3D_hR64_167_c_be3f_f_c-001	A76C
◦ $Zr_{21}Re_{25}$:	
A25B21_hR92_167_b2e3f_e3f-001	1BVC
P6 (168):	
◦ $K_2Ta_4O_9F_4$:	
A2B13C4_hP57_168_d_c6d_2d-001	6140
◦ $Al[PO_4]$:	
AB4C_hP72_168_2d_8d_2d-001	5X6W
$P6_1$ (169):	
◦ Al_2S_3:	
A2B3_hP30_169_2a_3a-001	0WYL
$P6_5$ (170):	
◦ Al_2S_3:	
A2B3_hP30_170_2a_3a-001	G6GN
$P6_2$ (171):	
◦ $Sr[S_2O_6][H_2O]_4$:	
A10B2C_hP39_171_5c_c_a-001	WCPM
$P6_4$ (172):	
◦ $Sr[S_2O_6][H_2O]_4$:	
A10B2C_hP39_172_5c_c_a-001	XXQ8
$P6_3$ (173):	
◦ PI_3:	
A3B_hP8_173_c_b-001	RB2M
◦ α-$LiIO_3$:	
ABC3_hP10_173_b_a_c-001	DF6Y
◦ β-Si_3N_4:	
A4B3_hP14_173_bc_c-001	Y4EE
◦ $LiKSO_4$ ($H1_4$):	
ABC4D_hP14_173_a_b_bc_b-001	F86C
◦ La_3CuSiS_7:	
AB3C7D_hP24_173_a_c_b2c_b-001	H1TU
◦ $P6_3$ La_3BWO_9:	
AB3C9D_hP28_173_a_c_3c_b-001	DVKH
◦ Crancrinite ($Na_6Ca_2Al_6Si_6O_{24}(CO_3)_2$, $S3_3$(I)):	
A3BCD3E15F3_hP52_173_c_b_b_c_5c_c-001	7U5Z
$P\bar{6}$ (174):	
◦ GdSI:	
ABC_hP12_174_aj_dk_ej-001	4BHM
◦ $Fe_{12}Zr_2P_7$:	
A12B7C2_hP21_174_2j2k_ajk_cf-001	EE97
• $Tl_3Ga_9S_{13}O_2$:	
A9B2C13D3_hP27_174_jl_i_ajkl_bcd-001	Q3WS
• Stützite ($Ag_{5-x}Te_3$):	
A12B7_hP57_174_2j2k4l_ghi3j2k-001	T2R2
P6/m (175):	
◦ $Nb_7Ru_6B_8$:	
A8B7C6_hP21_175_ck_aj_k-001	F86A
◦ Mg[NH]:	
ABC_hP36_175_jk_jk_jk-001	12DH
• Na_4Ge_{13}:	
A19B10_hP58_175_e2j2kl_djl-001	XPLN
• $Ag_{51}Gd_{14}$:	
A27B7_hP68_175_chjk3l_ejk-001	V9AH
$P6_3/m$ (176):	
◦ UCl_3:	
A3B_hP8_176_h_c-001	CZNF
◦ Er_3Ru_2:	
A3B2_hP10_176_h_bc-001	1QZH
• $LaRu_3Si_2$:	
AB3C2_hP12_176_b_h_f-001	JSY8
◦ $TlFe_3Te_3$:	
A3B3C_hP14_176_h_h_c-001	BQR4
◦ β-Si_3N_4:	
A4B3_hP14_176_ch_h-001	YEJK
• Nb_3Te_4:	
A3B4_hP14_176_h_ch-002	FUM3
◦ Th_7S_{12} ($D8_k$):	
A3B2_hP20_176_2h_ah-001	X9DF
• ζ-$Cu_{10}Sn_3$:	
A10B3_hP26_176_bcfi_h-001	YGNT
• $Cu_{10}Sb_3$:	
A10B3_hP26_176_c3h_h-001	4QXQ
◦ $K_3W_2Cl_9$ ($K7_1$):	
A9B3C2_hP28_176_hi_af_f-001	XV4Y
◦ $Rh_{20}Si_{13}$:	
A10B7_hP34_176_c3h_b2h-001	L6DT
◦ $Fe_2(CO)_9$ ($F4_1$):	
A9B2C9_hP40_176_hi_f_hi-001	858V
◦ Fluorapatite [$Ca_5F(PO_4)_3$, $H5_7$]:	
A5BC12D3_hP42_176_fh_a_2hi_h-001	KHCK
• Lead Apatite [$Pb_{10}(PO_4)_6O$]:	
A14B3C5_hP44_176_e2hi_h_fh-001	4302
• $YBa_3B_9O_{18}$:	
A9B3C18D_hP62_176_hi_af_2h2i_b-001	PC4V
• $Na_5Co_{15.5}Te_6O_{36}$ (NCTO):	
A7B5C18D3_hP66_176_ci_bef_2h2i_h-001	KL15
• $Nb_7Rh_6B_8$:	
A8B7C6_hP126_176_2h3i_acd6h_3i-001	01SA
P622 (177):	
◦ Hypothetical hexagonal SiO_2:	
A2B_hP36_177_j2lm_n-001	XNAH
• $[Fe(OMe)_2(proline)]_{12}[ClO_4]_{12}$:	
A7BCD15EF12_hP444_177_7n_n_jl_15n_n_12n-001	TXX6
$P6_122$ (178):	
◦ Sc-V (High-pressure):	
A_hP6_178_a-001	Z993
◦ AuF_3:	
AB3_hP24_178_b_ac-001	UBNE
• $CsCuCl_3$:	
A3BC_hP30_178_bc_b_a-001	8791
• Zr_5Ir_3:	
A3B5_hP48_178_ac_a2bc-001	15N7
$P6_522$ (179):	
◦ AuF_3:	
AB3_hP24_179_b_ac-001	45S0
• $Sc(H_2O)_2[BP_2O_8]\cdot H_2O$:	
AB4C12D2E_hP120_179_b_2c_6c_c_b-001	1CPH
$P6_222$ (180):	
◦ β-SiO_2 ($C8$):	
A2B_hP9_180_i_d-001	MK1H
◦ $CrSi_2$ ($C40$):	
AB2_hP9_180_c_i-001	3K6M
◦ Mg_2Ni (C_a):	
A2B_hP18_180_fj_ac-001	TDY8
◦ Hg_2O_2NaI:	
A2BCD2_hP18_180_f_c_b_i-001	TQ0B
• Rhadophane ($CePO_4$):	
AB4C_hP18_180_c_k_d-001	QL18
• CsC_8:	
A8B_hP27_180_2ik_d-001	T338

$P6_422$ (181):
- β-SiO_2 ($C8$):
  A2B_hP9_181_i_d-001 VH37
- $Co[Au(CN)_2]_2$:
  A2B4CD4_hP66_181_k_2k_f_2k-001 R3D2
- β-Eucryptite ($LiAlSiO_4$):
  ABC4D_hP84_181_gi_bcf_4k_hj-001 N1MQ

$P6_322$ (182):
- Bainite (Fe_3C):
  AB3_hP8_182_c_g-001 JRHU
- $E2_3$ ($LiIO_3$) (*Obsolete*):
  ABC3_hP10_182_c_b_g-001 6B26
- WAl_5:
  A5B_hP12_182_bcg_d-001 BQ6N
- $BaAl_2O_4$ ($H2_8$):
  A2BC6_hP18_182_f_b_gh-001 6VW9
- $CoNb_3S_6$:
  AB3C6_hP20_182_c_af_i-001 A0VJ
- $Na_2Co_2TeO_6$:
  A2B13C6D_hP44_182_bc_a2i_i_d-001 1XST

P6mm (183):
- AuCN:
  ABC_hP3_183_a_a_a-001 Q8EL
- $CrFe_3NiSn_5$:
  AB_hP6_183_c_ab-001 C57U
- $Ta_{21}Te_{13}$:
  A21B13_hP136_183_abc3d6e2f_2ab3d5e-001 7BEE

P6cc (184):
- Al[PO_4] (Framework type AFI):
  AB4C_hP72_184_d_4d_d-001 72JS
- $NaTi_2(PS_4)_3$:
  A13B6C24D4_hP188_184_2a4d_2d_8d_bd-001 7PRY

$P6_3cm$ (185):
- β-$RuCl_3$:
  A3B_hP8_185_c_a-001 5RVU
- Cu_3P:
  A3B_hP24_185_ab2c_c-001 L8U5
- Na_3As:
  AB3_hP24_185_c_ab2c-001 3ERL
- $KNiCl_3$:
  A3BC_hP30_185_cd_c_ab-001 PKFR
- $LuMnO_3$:
  ABC3_hP30_185_ab_c_ab2c-001 YGS5
- Stibiopalladinite (Pd_5Sb_2):
  A5B2_hP42_185_ab4c_abc-001 04LT
- $Sr_8Os_{6.3}O_{24}$:
  A36B11C12_hP118_185_4c4d_a2b2c_ab3c-001 AL94

$P6_3mc$ (186):
- Original BN ($B12$) (*Obsolete*):
  AB_hP4_186_b_a-001 QUDC
- Wurtzite (ZnS, $B4$):
  AB_hP4_186_b_b-001 6CGK
- Buckled Graphite:
  A_hP4_186_ab-001 F6SX
- C27 (CdI_2) (*Questionable*):
  AB2_hP6_186_b_ab-001 G4EJ
- LiGaGe Crystal:
  ABC_hP6_186_b_b_a-003 ZZ7U
- Moissanite-4H SiC ($B5$):
  AB_hP8_186_ab_ab-001 FSH2
- Cd(OH)Cl ($E0_3$):
  ABCD_hP8_186_b_b_a_a-001 R9CA
- O2-$LiCoO_2$:
  ABC2_hP8_186_b_b_ab-001 5BYD
- Moissanite-6H SiC ($B6$):
  AB_hP12_186_a2b_a2b-001 NYRK
- O4-$LiCoO_2$:
  ABC2_hP16_186_ab_ab_a3b-001 3DYH
- δ-GaSe:
  AB_hP16_186_2a2b_2a2b-001 W6UW
- Al_5C_3N ($E9_4$):
  A5B3C_hP18_186_2a3b_2ab_b-001 KHLK
- Fe_3Th_7 ($D10_2$):
  A3B7_hP20_186_c_b2c-001 VGVG
- HPC-Bi_2O_3:
  A2B3_hP20_186_bc_2c-001 14M3
- $Ti_3Al_2N_2$:
  A2B4C5_hP22_186_ab_4b_a4b-001 7JMK
- $Zn_2Mo_3O_8$:
  A3B8C2_hP26_186_c_ab2c_2b-001 DG1Q
- Swedenborgite ($NaBe_4SbO_7$, $E9_2$):
  A4BC7D_hP26_186_ac_b_a2c_b-001 QF4S
- $Al_7C_3N_3$:
  A7B3C3_hP26_186_3a4b_2ab_a2b-001 JALT
- $LiClO_4{\cdot}3H_2O$ ($H4_{18}$):
  AB6CD7_hP30_186_b_d_a_b2c-001 TXNW
- $Nd(BrO_3)_3{\cdot}9H_2O$ ($G2_2$):
  A3B9CD9_hP44_186_c_3c_b_cd-001 776H
- Ca_5Pb_3:
  A5B3_hP48_186_3cd_3c-001 XPM6
- $Ce_{24}Co_{11}$:
  A24B11_hP70_186_2ab7c_ab3c-001 D6S6

$P\bar{6}m2$ (187):
- Tungsten Carbide (WC, B_h):
  AB_hP2_187_a_d-001 X4K0
- BaPtSb:
  ABC_hP3_187_b_c_e-001 NKMF
- Re_3N:
  AB3_hP4_187_a_bh-001 6BD5
- ZrTaNO:
  ABCD_hP4_187_c_b_a_f-001 84DL
- Ti_2InB_2:
  A2BC2_hP5_187_ac_b_i-001 AJFU
- β-CuI (Bührer-Hälg):
  A2B_hP6_187_gi_ad-001 P31P
- ϵ-GaSe:
  AB_hP8_187_gh_gh-001 M3JC
- $LiCo_6P_4$:
  A6BC4_hP11_187_jk_a_ck-001 NFL9
- Cr-233 Quasi-One-Dimensional Superconductor($K_2Cr_3As_3$):
  A3B3C2_hP16_187_jk_jk_ak-001 XP6Z
- Cs_7O:
  A7B_hP24_187_ah2j2kn_j-001 BZC9

$P\bar{6}c2$ (188):
- $LiScI_3$:
  A3BC_hP10_188_k_a_c-001 BL96
- $Sr_2Be_2B_2O_7$:
  A2B2C7D2_hP26_188_i_h_cl_ab-001 FFAL
- $BaSi_4O_9$ ($S3_2$):
  AB9C4_hP28_188_a_kl_ck-001 2DJ4

$P\bar{6}2m$ (189):
- Th_3Pd_5:
  A5B3_hP8_189_cf_g-001 K8CX
- Barringerite (Revised Fe_2P, $C22$) Crystal:
  A2B_hP9_189_fg_ad-001 6UK2
- ZrNiAl:
  ABC_hP9_189_f_bc_g-003 0T4U

- β_1-K_2UF_6:
  A6B2C_hP9_189_fg_c_b-001 XTDJ
- NaO:
  AB_hP12_189_fg_eh-001 PQWK
  - π-$FeMg_3Al_8Si_6$ ($E9_b$):
    A8BC3D6_hP18_189_agh_b_f_i-001 WS3B
  - π-$FeMg_3Al_9Si_5$:
    A9BC3D5_hP18_189_fi_a_g_bh-001 0WD7
- Hexagonal $Au_7P_{10}I$:
  A7BC10_hP18_189_ceg_a_hi-001 16HD
- $CsCrF_4$:
  ABC4_hP18_189_f_g_fgj-001 6BNK
- $Ca_5Ir_3O_{12}$:
  A5B3C12_hP20_189_dg_f_2gj-001 8TFL

$\bar{P}62c$ (190):

- α-Sm_3Ge_5 (High-temperature):
  A5B3_hP16_190_bch_g-001 PJF4
- Li_2Sb:
  A2B_hP18_190_gh_bf-001 DA98
- $CsSO_3$ ($K1_2$):
  AB3C_hP20_190_ac_i_f-001 XJYL
- Troilite (FeS):
  AB_hP24_190_i_afh-001 6ZXP
- Bastnäsite [$CeF(CO_3)$, $G7_1$]:
  ABCD3_hP36_190_h_g_af_hi-001 XFRG

P6/mmm (191):

- Simple Hexagonal ($HgSn_{6-10}$ A_f):
  A_hP1_191_a-001 3V7H
- Hexagonal ω ($C32$):
  AB2_hP3_191_a_d-001 75K4
- Li_3N:
  A3B_hP4_191_bc_a-001 RYZL
- Cu_2Te (C_h):
  A2B_hP6_191_h_e-001 X9YK
- AlB_4Mg:
  AB4C_hP6_191_a_h_b-001 PDN7
- $CaCu_5$ ($D2_d$):
  AB5_hP6_191_a_cg-001 F7Y6
- CoSn ($B35$):
  AB_hP6_191_f_ad-001 Z7YH
- Zr_4Al_3:
  A3B4_hP7_191_f_de-001 AMP4
- KV_3Sb_5:
  AB5C3_hP9_191_b_ah_f-001 F3TR
- Hexagonal WO_3:
  A3B_hP12_191_gl_f-001 SQAX
- Lucabindiite (KAs_4O_6Cl):
  A4BCD6_hP12_191_h_a_b_i-001 4NVE
- $BaFe_2Al_9$:
  A9BC2_hP12_191_fm_a_c-001 CSJ8
- $D2_a$ (approximate $TiBe_{12}$):
  A12B_hP13_191_cdei_a-001 FEUM
- $HfFe_6Ge_6$:
  A6B6C_hP13_191_i_cde_a-002 4E59

P6/mcc (192):

- Beryl ($Be_3Al_2Si_6O_{18}$, $S3_1$):
  A2B3C18D6_hP58_192_c_f_lm_l-001 52T5
- $AlPO_4$:
  AB2_hP72_192_m_j2kl-001 M1VB
- Osumilite ($KMg_2Al_3Si_{12}O_{30}$):
  A3BC2D30E12_hP96_192_f_a_c_l2m_m-001 FPN8

$P6_3/mcm$ (193):

- Mavlyanovite (Mn_5Si_3, $D8_8$):
  A5B3_hP16_193_dg_g-001 AQ0J
- Ti_5Ga_4:
  A4B5_hP18_193_bg_dg-001 443S
- $D0_6$ (Tysonite, LaF_3) (*Obsolete*):
  A3B_hP24_193_ack_g-001 JJ07
- Ordered $TmBO_3$:
  AB3C_hP30_193_g_gk_bd-001 AE3Q

$P6_3/mmc$ (194):

- Hexagonal close packed (Mg, $A3$, hcp):
  A_hP2_194_c-001 LZW5
- Nickeline (NiAs, $B8_1$):
  AB_hP4_194_c_a-001 Y3TN
- BN (B_k):
  AB_hP4_194_c_d-001 SHYT
- α-La ($A3'$):
  A_hP4_194_ac-001 9631
- Hexagonal Graphite ($A9$):
  A_hP4_194_bc-001 W4SC
- Lonsdaleite (Hexagonal Diamond):
  A_hP4_194_f-001 4AMD
- $LiZn_2$ (C_k):
  AB_hP4_194_a_c-003 CY59
- $L'3_0$ (approximate Fe_2N):
  AB_hP4_194_c_a-003 Q425
- $CaIn_2$:
  AB2_hP6_194_b_f-001 21YK
- $InNi_2$ ($B8_2$):
  AB2_hP6_194_c_ad-001 X5ZH
- Molybdenite (MoS_2, $C7$):
  AB2_hP6_194_c_f-001 A8HJ
- LiBC:
  ABC_hP6_194_c_d_a-001 F0CN
- Hypothetical Tetrahedrally Bonded Carbon with3-Member Rings:
  A_hP6_194_h-001 1BYJ
- ReB_2:
  A2B_hP6_194_f_c-003 TH7D
- Hexagonal High-Temperature NbS_2:
  AB2_hP6_194_b_f-002 Z5TL
- Ni_3Sn ($D0_{19}$):
  A3B_hP8_194_h_c-001 LJF8
- Na_3As ($D0_{18}$):
  AB3_hP8_194_c_bf-001 5M89
- $AlCCr_2$:
  ABC2_hP8_194_c_a_f-007 NEW2
- AsTi (B_i):
  AB_hP8_194_ac_f-004 E9RV
- ReB_3:
  A3B_hP8_194_af_c-001 72PY
- Hexagonal Delafossite ($CuFeO_2$):
  ABC2_hP8_194_a_c_f-005 Y6AL
- $SnTaS_2$:
  A2BC_hP8_194_e_a_c-001 DG69
- $NiMoP_2$:
  ABC2_hP8_194_b_a_f-001 D1PM
- LiO:
  AB_hP8_194_ac_f-003 JV7G
- β-GaSe:
  AB_hP8_194_f_f-003 BDG1
- Pt_2Sn_3 ($D5_b$):
  A2B3_hP10_194_f_bf-001 Y79W
- $Na_{0.74}CoO_2$:
  AB2C2_hP10_194_a_bc_f-001 6X9E

- $EuIn_2P_2$:
  AB2C2_hP10_194_a_f_f-001 PL9Q
- β-Be_3N_2:
  A3B2_hP10_194_bf_ac-001 CJUB
- $BaNiO_3$:
  ABC3_hP10_194_c_a_h-001 UTCF
- High temperature $GdBO_3$:
  ABC3_hP10_194_c_a_h-002 R6VB
- β-Tridymite (SiO_2, $C10$):
  A2B_hP12_194_cg_f-001 3KTM
- $MgZn_2$ Hexagonal Laves ($C14$):
  AB2_hP12_194_f_ah-001 LL0C
- CMo:
  AB_hP12_194_af_bf-001 Q5G8
- Covellite (CuS, $B18$):
  AB_hP12_194_cf_de-001 QP0Q
- Fe_3GeTe_2:
  A3BC2_hP12_194_ce_d_f-001 ANDB
- W_2B_5 ($D8_h$):
  A5B2_hP14_194_abcf_f-001 S78A
- AlN_3Ti_4:
  AB3C4_hP16_194_c_af_ef-001 53FU
- Ni_3Ti ($D0_{24}$):
  A3B_hP16_194_gh_ac-001 7D2A
- OP4-$LiNaCo_2O_4$:
  A2BC2D4_hP18_194_f_a_cd_ef-001 C4AH
- Disordered YBO_3:
  A3B5C_hP18_194_h_fh_a-001 3718
- CeH_9:
  AB9_hP20_194_c_bfk-001 B62K
- Proposed 300 GPa HfH_{10}:
  A10B_hP22_194_bhj_c-001 MK58
- Hexagonal Ti_6Sn_5:
  A5B6_hP22_194_ach_gh-001 09JW
- $MgNi_2$ Hexagonal Laves ($C36$):
  AB2_hP24_194_ef_fgh-001 HV5V
- Lu_2CoGa_3:
  AB3C2_hP24_194_f_k_bh-001 0GA4
- VCo_3:
  A3B_hP24_194_hk_bf-001 XEL5
- Hexagonal $PuAl_3$:
  A3B_hP24_194_hk_bf-002 E109
- Low temperature $NbSe_2$:
  AB2_hP24_194_bh_fk-001 YM9E
- $CeNi_3$:
  AB3_hP24_194_cf_abdk-001 1SSV
- Al_9Mn_3Si ($E9_c$):
  A9B3C_hP26_194_hk_h_a-001 KM59
- Hexagonal Vaterite ($CaCO_3$):
  A3BC9_hP26_194_h_a_hk-001 LCWU
- Na_9Pb_4 (δ'-NaPb):
  A9B4_hP26_194_ce3f_ef-001 J5ST
- Co_2Al_5 ($D8_{11}$):
  A5B2_hP28_194_ahk_ch-001 VX03
- $Cs_3Cr_2Cl_9$:
  A9B2C3_hP28_194_hk_f_bf-001 77Z6
- Hexagonal $Ba_3CoIr_2O_9$:
  A3BC2D9_hP30_194_bf_a_f_hk-001 BHER
- Hexagonal $BaTiO_3$:
  AB3C_hP30_194_bf_hk_af-001 VHHA
- $BaLi_4$:
  AB4_hP30_194_h_afhk-001 JAJR
- $Co_3W_9C_4$:
  A2B3C3_hP32_194_cg_2h_k-001 JSHF
- Hexagonal α-Ca_2SiO_4:
  A3B12C_hP32_194_af_2k_c-001 CEQR
- $S3_4$(II) (Catapleiite, $Na_2Zr(SiO_3)_3{\cdot}H_2O$)(*Obsolete*):
  A3B2C9D3E_hP36_194_g_f_hk_h_a-001 6TN8
- Ce_2Ni_7:
  A2B7_hP36_194_2f_aefhk-001 A0TL
- $Na_{13}Pb_5$ (γ-NaPb):
  A13B5_hP36_194_a2e4f_b2f-001 G1KV
- Th_2Ni_{17}:
  A17B2_hP38_194_fgjk_bc-001 DQFR
- Barlowite [$Cu_4FBr(OH)_6$]:
  AB6CD6E6_hP40_194_c_gh_b_k_k-001 GN34
- $Al_{23}V_4$:
  A23B4_hP54_194_fh3k_ah-001 W4P8
- $Ba_6Nd_2Ti_4O_{17}$:
  A6B2C17D4_hP58_194_ab2f_e_fh2k_2f-001 X8HZ
- β-Alumina ($D5_6$, Al_2O_3):
  A2B3_hP60_194_3fk_cdef2k-001 T15Z
- Magnetoplumbite ($PbFe_{12}O_{19}$):
  A12B19C_hP64_194_ab2fk_efh2k_c-001 5L5V
- $SrMg_4$:
  A4B_hP90_194_e2fgh4k_hk-001 DU5B

P23 (195):

- Cd_8As_7Cl:
  A7B12C_cP20_195_ag_3e_b-001 J7FX
- $PrRu_4P_{12}$:
  A12BC4_cP34_195_2j_ab_2e-001 8SJC

F23 (196):

- $Cu_2Fe[CN]_6$:
  A12B2C_cF60_196_h_ac_b-001 DJ7F
- $Ca_{14}Zn_6Al_{10}O_{35}$:
  A12B14C35D4_cF260_196_abeg_2ef_cef2h_e-001 JELG
- $Li_{22}Si_5$:
  A22B5_cF432_196_abcd6efg4h_2efg-001 GA7M

I23 (197):

- Ga_4Ni:
  A4B_cI40_197_cde_c-001 PBV9
- $Hf_{10}Ta_3S_3$:
  A11B3C2_cI64_197_cdf_e_c-001 8883
- γ-Bi_2O_3:
  A13B20_cI66_197_af_2cf-001 8111

$P2_13$ (198):

- α-CO ($B21$):
  AB_cP8_198_a_a-001 LCVR
- FeSi ($B20$):
  AB_cP8_198_a_a-002 93P7
- α-N ($P2_13$):
  A_cP8_198_2a-001 VHKA
- Ullmanite (NiSSb, $F0_1$):
  ABC_cP12_198_a_a_a-001 VHP8
- Ammonia (NH_3, $D0_1$):
  A3B_cP16_198_b_a-001 QTNQ
- Sodium Chlorate ($NaClO_3$, $G0_3$):
  ABC3_cP20_198_a_a_b-001 QEXW
- α-Carnegieite ($NaAlSiO_4$, $S6_5$):
  ABC4D_cP28_198_a_a_ab_a-001 M6W2
- Na_2CaSiO_4 ($S6_6$):
  AB2C4D_cP32_198_a_2a_ab_a-001 MFVM
- Cubic Cu_2OSeO_3:
  A2B4C_cP56_198_ab_2a2b_2a-001 PZ2V
- Low temperature CsW_2O_6:
  AB6C2_cP72_198_2a_4b_ab-001 WBDQ
- Langbeinite [$K_2Mg_2(SO_4)_3$]:
  A2B2C12D3_cP76_198_2a_2a_4b_b-001 98LD

$I2_13$ (199):
- CoU (B_a):
  AB_cI16_199_a_a-001 TFMD
- Corderoite (α-$Hg_3S_2Cl_2$):
  A2B3C2_cI28_199_a_b_a-002 VYHG
- $C26_a$ (NO_2) (*Obsolete*):
  AB2_cI36_199_b_c-001 VGMG

$Pm\bar{3}$ (200):
- $CsHgN_3O_6$:
  ABC3D6_cP11_200_a_b_c_f-001 4JP4
- C-AlRuNi ($Al_{20}Ni_3Ru_5$):
  A23B2C6_cP31_200_cij_ab_f-001 L1EN
- Mg_2Zn_{11} ($D8_c$):
  A2B11_cP39_200_f_begik-001 8FHP

$Pn\bar{3}$ (201):
- $KSbO_3$ (High-Temperature):
  AB3C_cP60_201_be_fh_g-001 WX0M
- $Bi_3Ru_3O_{11}$:
  A3B11C3_cP68_201_be_efh_g-001 0WEU
- $CuMo_3Cl_7$:
  A7BC3_cP88_201_e2h_e_h-001 HF2G
- KW_3Br_7:
  A28B5C12_cP90_201_e2h_bd_h-001 RMGB
- Ce_6Cd_{37}:
  A41B6_cP188_201_b2efg5h_h-001 D917

$Fm\bar{3}$ (202):
- α-$CuZrF_6$:
  AB12C_cF56_202_a_h_b-001 G65V
- $K_3Co(NO_2)_6$ ($J2_4$):
  AB3C6D12_cF88_202_a_bc_e_h-001 G8R0
- KB_6H_6:
  A6B6C_cF104_202_h_h_c-001 PZB0
- FCC C_{60} Buckminsterfullerene:
  A_cF240_202_h2i-001 TV0E

$Fd\bar{3}$ (203):
- Rb_3AsSe_{16}:
  AB3C16_cF160_203_a_bc_eg-001 HAGZ
- Pyrochlore ($Na_3Co(CO_3)_2Cl$):
  A2BCD3E6_cF208_203_e_c_d_f_g-001 LH7J
- Tychite ($Na_6Mg_2SO_4(CO_3)_4$):
  A4B2C6D16E_cF232_203_e_c_f_eg_b-001 LJXD

$Im\bar{3}$ (204):
- $Al_{12}W$:
  A12B_cI26_204_g_a-001 JDL2
- Skutterudite ($CoAs_3$, $D0_2$):
  A3B_cI32_204_g_c-001 9U6F
- $LaFe_4P_{12}$:
  A4BC12_cI34_204_c_a_g-001 GXVQ
- Modern $C26$ (NO_2):
  AB2_cI36_204_d_g-001 XJC7
- $NaMn_7O_{12}$:
  A7BC12_cI40_204_bc_a_g-001 M5NA
- $CaCu_3Mn_4O_{12}$:
  AB3C4D12_cI40_204_a_b_c_g-001 RGPS
- Ru_3Be_{17}:
  A17B3_cI160_204_def2gh_g-001 92TS
- Bergman [Mg_{32}(Al,Zn)$_{49}$]:
  AB32C48_cI162_204_a_2efg_2gh-001 9AQF
- YCd_6:
  A20B3_cI184_204_def3gh_g-001 HYXN

$Pa\bar{3}$ (205):
- α-N ($Pa\bar{3}$):
  A_cP8_205_c-001 84Y3
- Pyrite (FeS_2, $C2$):
  AB2_cP12_205_a_c-001 M44S
- SC16 (CuCl):
  AB_cP16_205_c_c-001 F4G8
- $NaSbF_6$:
  A6BC_cP32_205_d_a_b-001 N7XD
- $Pb(NO_3)_2$ ($G2_1$):
  A2B6C_cP36_205_c_d_a-001 LPJD
- SnI_4 ($D1_1$):
  A4B_cP40_205_cd_c-001 MJPK
- ZrP_2O_7 ($K6_1$) High-Temperature:
  A7B2C_cP40_205_ad_c_b-001 NTUQ
- $Zn(BrO_3)_2 \cdot 6H_2O$ ($J1_{10}$):
  A2B6C6D_cP60_205_c_d_d_a-001 Q0QA
- $H6_4$ [$Ni(NO_3)_2(NH_3)_6$] (*Obsolete*):
  A2B6CD6_cP60_205_c_d_a_d-001 GED2
- CaB_2O_4 (IV):
  A2BC4_cP84_205_d_ac_2d-001 TZRB
- $NaCr(SO_4)_2 \cdot 12H_2O$ Alum:
  AB12CD8E2_cP96_205_a_2d_b_cd_c-001 AUGT
- γ-Alum [$AlNa(SO_4)_2 \cdot 12H_2O$, $H4_{15}$]:
  AB24CD20E2_cP192_205_a_4d_b_c3d_c-001 VBLW
- α-Alum [$KAl(SO_4)_2 \cdot 12H_2O$, $H4_{13}$]:
  AB24CD28E2_cP224_205_a_4d_b_2c4d_c-001 MHB8
- Simple Cubic C_{60} Buckminsterfullerene:
  A_cP240_205_10d-001 3VYE
- β-Alum [$Al(NH_3CH_3)_2(SO_4)_2 \cdot 12H_2O$, $H4_{14}$]:
  AB2C36D2E20F2_cP252_205_a_c_6d_c_c3d_c-001 SFC7
- $Ca_3Al_2O_6$:
  A2B3C6_cP264_205_2d_ab2c2d_6d-001 Q2JD

$Ia\bar{3}$ (206):
- BC8 (Si):
  A_cI16_206_c-001 83MZ
- Bixbyite (Mn_2O_3, $D5_3$):
  AB3C6_cI80_206_a_d_e-001 G3EF
- $AlLi_3N_2$ ($E9_d$):
  AB3C2_cI96_206_c_e_ad-001 WEUP
- $ZrTe_3O_8$:
  A8B3C_cI96_206_ce_d_a-001 3HHF

P432 (207):
- Palladseite ($Pd_{17}Se_{15}$):
  A17B15_cP64_207_acfk_eij-001 8LH0

$P4_232$ (208):
- H_3P:
  A3B_cP16_208_i_c-001 CCPW
- $Cs_2ZnFe[CN]_6$:
  A6B2CD6E_cP64_208_m_ad_b_m_c-001 0HGH
- $Na_{11}U_5O_{16}$:
  A11B16C5_cP64_208_bfh_adm_ce-001 NFNJ

F432 (209):
- KPF_6:
  A24BC_cF104_209_j_a_b-001 XBGM
- PCN-20 [$C_{14}CuO(H_2O)_4$]:
  A14BC8D5_cF1344_209_7j_g_4j_g2j-001 5WNB

$F4_132$ (210):
- $MgB_{12}H_{12}[H_2O]_{12}$:
  A12B36CD12_cF488_210_h_3h_a_fg-001 X29X
- $Te[OH]_6$:
  A12B6C_cF608_210_4h_2h_e-001 7K4Q

I432 (211):
- Hypothetical Cubic SiO_2:
  A2B_cI72_211_hi_i-001 NT1Y

$P4_332$ (212):
- $SrSi_2$:
  A2B_cP12_212_c_a-001 XX75
- Li_2Pd_3B:
  AB2C3_cP24_212_a_c_d-001 K791
- γ-Fe_2O_3 ($D5_7$):
  A2B3_cP60_212_acd_bce-001 J7V3

$P4_132$ (213):
- β-Mn ($A13$):
  A_cP20_213_cd-001 4VEQ
- Mg_3Ru_2:
  A3B2_cP20_213_d_c-001 6QE7
- $Co_8Zn_9Mn_3$:
  A2B3_cP20_213_c_d-001 KXT1
- Al_2Mo_3C:
  A2BC3_cP24_213_c_a_d-001 SRH0
- $SrCuTe_2O_6$:
  AB6CD2_cP120_213_d_3e_ac_e-001 1AJT

$I4_132$ (214):
- Petzite (Ag_3AuTe_2):
  A3BC2_cI48_214_f_a_e-001 3JDV
- Ca_3PI_3:
  A3B3C_cI56_214_g_h_a-001 4XVN
- $La_3Rh_4Sn_{13}$:
  A3B4C13_cI320_214_gh_abgh_e4i-001 1DPD

$P\bar{4}3m$ (215):
- Fe_4C:
  AB4_cP5_215_a_e-001 WNQX
- Sulvanite (Cu_3S_4V, $H2_4$):
  A3B4C_cP8_215_c_e_b-001 WCVT
- Cubic Lazarevićite ($AsCu_3S_4$):
  AB3C4_cP8_215_a_c_e-001 31D9
- Intermediate temperature $TmNi_2$:
  A2B_cP24_215_ei_ace-001 X751
- γ-brass (Cu_9Al_4, $D8_3$):
  A4B9_cP52_215_ei_3efgi-001 TRNX
- Palladseite ($Pd_{17}Se_{15}$):
  A17B15_cP64_215_acg2i_f2i-001 55EV

$F\bar{4}3m$ (216):
- Zincblende (ZnAs, $B3$):
  AB_cF8_216_a_c-001 TL8Z
- Half–Heusler (AgAsMg, $C1_b$):
  ABC_cF12_216_a_c_b-001 3BJR
- Quaternary Heusler (LiMgAuSn):
  ABCD_cF16_216_a_b_c_d-001 4CEX
- Hg_2TiCu Inverse Heusler:
  AB2C_cF16_216_a_bc_d-001 4M8A
- $AuBe_5$ ($C15_b$):
  AB5_cF24_216_a_ce-001 3454
- High-Temperature Cubic $KClO_4$ ($H0_5$):
  ABC4_cF24_216_a_b_e-001 Q1UZ
- Theoretical cF40 AlN:
  AB_cF40_216_ae_be-001 3QP3
- Room temperature $GaMo_4S_8$:
  AB4C8_cF52_216_a_e_2e-001 BEEG
- $LiGaCr_4O_8$:
  A4BCD8_cF56_216_e_a_c_2e-001 1XJV
- $Al_{13}Cr_4Si_4$:
  A13B4C4_cF84_216_afg_e_e-001 5ADG
- Cubic Cr_4PtGa_{17}:
  A4B17C_cF88_216_e_aefg_c-001 9Q9K
- Gd_4RhIn:
  A4BC_cF96_216_efg_e_e-001 39CF
- $Ba_3In_2Zn_5O_{11}$:
  A3B2C11D5_cF168_216_f_e_ab2eh_eg-001 Z69R
- Low temperature $TmNi_2$:
  A2B_cF192_216_2e2h_ab2eg-001 5WAR
- Zunyite [$Al_{13}(OH,F)_{18}Si_5O_{20}Cl$ ($S0_8$)]:
  A13BC18D20E5_cF228_216_ah_c_gh_2eh_be-001 R5TJ
- Murataite [$(Y,Na)_6(Zn,Fe)_5Ti_{12}O_{29}(O,F)_{10}F_4$]:
  A16B40C12D6E5_cF316_216_eh_e2g2h_h_f_ae-001 ZX49
- Pt_3Zn_{10}:
  A2B5_cF392_216_4efg_4ef4h-001 V17U
- δ-$Cu_{41}Sn_{11}$:
  A41B11_cF416_216_7e2fg3h_egh-001 1MZW
- $Li_{17}Pb_4$:
  A17B4_cF420_216_a6efg4h_2efg-001 4E2L
- $Sm_{11}Cd_{45}$:
  A45B11_cF448_216_ac4efg5h_bd2eh-001 LZ4J

$I\bar{4}3m$ (217):
- SiF_4 ($D1_2$):
  A4B_cI10_217_c_a-001 WBME
- Theoretical cI16 AlN:
  AB_cI16_217_c_c-001 6RJH
- Tl_3VS_4:
  A4B3C_cI16_217_c_b_a-001 YOMN
- γ-Brass (Cu_5Zn_8, $D8_2$):
  A5B8_cI52_217_ce_cg-001 AYKC
- α-$Ba_8Ga_{16}Sn_{30}$ Clathrate:
  A4B4C6D13_cI54_217_c_c_d_ag-001 YXNP
- α-Mn ($A12$):
  A_cI58_217_ac2g-001 SV19
- $Mg_{17}Al_{12}$:
  A12B17_cI58_217_g_acg-001 56N2
- Tennantite ($Cu_{12}As_4S_{13}$):
  A4B24C13_cI82_217_c_deg_ag-001 5PAV

$P\bar{4}3n$ (218):
- $Ag_3(PO_4)$ ($H2_1$):
  A3B4C_cP16_218_c_e_a-001 X143
- Sodalite [$Na_4(AlSiO_4)_3Cl$, $S6_2$]:
  A3BC4D12E3_cP46_218_c_a_e_i_d-001 NYVB
- KGe:
  AB_cP64_218_ei_ei-001 RUTB
- Hauyne[$(Na_{0.5}Ca_{0.3}K_{0.2})_8(Al_6Si_6O_{24})(SO_4)_{1.5}$, $S6_9$]:
  A3B4C4D4E16F4G3_cP76_218_c_e_e_e_ei_e_d-001 BCKL
- Li_7MnN_4:
  A7BC4_cP96_218_bcefi_ad_ei-001 HJWV
- γ-HBO_2 (cubic):
  ABC2_cP96_218_i_i_2i-001 W9M1

$F\bar{4}3c$ (219):
- Si_3Cl_8:
  A8B3_cF176_219_eh_abe-001 ZRK3
- Boracite ($Mg_3B_7ClO_{13}$):
  A7BC3D13_cF192_219_ce_a_d_bh-001 0WNV
- $Sn[Co(CO)_4]_4$:
  A16B4C16D_cF296_219_eh_e_eh_a-001 6J8K

$I\bar{4}3d$ (220):
- High-pressure cI16 Li:
  A_cI16_220_c-001 BTF5
- Theoretical cI24 AlN:
  AB_cI24_220_a_b-001 MH9E
- Th_3P_4 ($D7_3$):
  A4B3_cI28_220_c_a-001 JM9C
- Pu_2C_3 ($D5_c$):
  A3B2_cI40_220_d_c-001 M1ZX
- $Y_3Au_3Sb_4$:
  A3B4C3_cI40_220_a_c_b-001 GET1

- $Cu_{15}Si_4$ ($D8_6$):
  A15B4_cI76_220_ae_c-001 MVX2
- Eulytine ($Bi_4(SiO_4)_3$, $S1_5$):
  A4B12C3_cI76_220_c_e_a-001 VQL6
- Mayenite (12 $CaO{\cdot}7Al_2O_3$, $K7_4$, C12A7):
  A7B12C19_cI152_220_ac_2d_bce-001 L8NP
- $Al(PO_3)_3$ ($G5_2$):
  AB9C3_cI208_220_c_3e_e-001 2BX1

$Pm\bar{3}m$ (221):

- α-Po (A_h, simple cubic):
  A_cP1_221_a-001 NG7Y
- CsCl ($B2$):
  AB_cP2_221_a_b-002 QM6B
- NH_4NO_3 I ($G0_8$):
  AB_cP2_221_a_b-001 5YKM
- α-ReO_3 ($D0_9$):
  A3B_cP4_221_c_b-001 3DRV
- Bogdanovite (Cu_3Au, $L1_2$):
  AB3_cP4_221_a_c-001 NK1T
- Cubic Perovskite ($CaTiO_3$, $E2_1$):
  AB3C_cP5_221_a_c_b-001 QUKL
- *Erroneous* $L'1_0$:
  A4B_cP5_221_bc_a-001 Q52R
- γ'-Fe_4N ($L'1_0$):
  A4B_cP5_221_ac_b-002 TEA9
- NbO:
  AB_cP6_221_c_d-001 H75X
- CaB_6 ($D2_1$):
  A6B_cP7_221_e_b-001 GKJM
- S_3U_4:
  A3B4_cP7_221_d_ac-001 62DR
- Predicted High-pressure $YCaH_{12}$:
  AB12C_cP14_221_a_h_b-001 SQ16
- Model of Ferrite (cP16):
  AB11CD3_cP16_221_a_dg_b_c-001 729N
- Model of Austenite (cP32):
  AB27CD3_cP32_221_a_dij_b_c-001 3F7M
- $Ca_3Al_2O_6$ ($E9_1$):
  A2B3C6_cP33_221_cd_ag_fh-001 TZEN
- $Ce_8Pd_{24}Sb$:
  A8B24C_cP33_221_g_efh_a-001 CLMU
- $BaHg_{11}$ ($D2_e$):
  AB11_cP36_221_c_agij-001 2EDD
- Palladseite ($Pd_{17}Se_{15}$):
  A17B15_cP64_221_acfm_eij-001 RWLL

$Pn\bar{3}n$ (222):

- $Ce_5Mo_3O_{16}$:
  A5B3C16_cP96_222_ce_d_fi-001 3NUA
- $Co(H_2O)_2(C_4O_4)$:
  A4BC4D6_cP360_222_2i_h_2i_3i-001 7XG8

$Pm\bar{3}n$ (223):

- Cr_3Si ($A15$):
  A3B_cP8_223_c_a-001 7MHE
- SrB_3C_3 Clathrate:
  A3B3C_cP14_223_c_d_a-001 FACW
- $NaPt_3O_4$:
  AB4C3_cP16_223_a_e_c-001 R1MG
- β-UH_3:
  A3B_cP32_223_k_ac-001 4UMV
- $Yb_3Rh_4Sn_{13}$:
  A4B13C3_cP40_223_e_ak_c-001 GYST
- Si_{46} Clathrate:
  A_cP46_223_cik-001 VFEB
- β-$Ba_8Ga_{16}Sn_{30}$ Clathrate:
  A13B3C8D12_cP72_223_ak_c_i_k-001 KF6U
- "A15" Fullerene (Ba_3C_{60}):
  AB20_cP126_223_c_k2l-001 HV0S
- β-$Hg_3S_2Cl_2$:
  A2B3C2_cP224_223_abcdefk_j3k_il-001 UWQ4

$Pn\bar{3}m$ (224):

- Cuprite (Cu_2O, $C3$):
  A2B_cP6_224_b_a-001 WUJH
- Mg_3P_2 ($D5_5$):
  A3B2_cP10_224_d_b-001 LQ7A
- $PW_{12}O_{40}{\cdot}3H_3O$:
  A3B40CD12_cP112_224_d_e3k_a_k-001 R1HF
- 12-phosphotungstic acid $[H_3PW_{12}O_{40}{\cdot}5H_2O](H4_{16})$:
  A5B40CD12_cP116_224_bd_e3k_a_k-001 E8XB
- Dodecatungstophosphoric Acid Hexahydrate($H_3PW_{12}O_{40}{\cdot}6H_2O$):
  A27B52CD12_cP184_224_dl_eh3k_a_k-001 XBJQ

$Fm\bar{3}m$ (225):

- Face-Centered Cubic (Cu, $A1$, fcc):
  A_cF4_225_a-001 6EYD
- Rock Salt/Halite (NaCl, $B1$):
  AB_cF8_225_a_b-001 Q53X
- Fluorite (CaF_2, $C1$):
  AB2_cF12_225_a_c-001 8VXQ
- Heusler (Cu_2AlMn, $L2_1$):
  AB2C_cF16_225_a_c_b-001 02WQ
- BiF_3 ($D0_3$):
  AB3_cF16_225_a_bc-001 KFY2
- Ca_7Ge:
  A7B_cF32_225_ad_b-001 CAN8
- $L1_a$ (disputed $CuPt_3$):
  AB7_cF32_225_a_bd-001 3APN
- α'-$CuZrF_6$:
  AB6C_cF32_225_a_e_b-001 2016
- K_2PtCl_6 ($J1_1$):
  A6B2C_cF36_225_e_c_a-001 L6LF
- δ-Bi_2O_3:
  AB8_cF36_225_a_f-001 X2Q7
- Double Perovskite (Ba_2MnWO_6):
  A2BC6D_cF40_225_c_a_e_b-001 83J5
- Room temperature KBD_4:
  AB8C_cF40_225_a_f_b-001 WSA1
- LaH_{10} High-T_c Superconductor:
  A10B_cF44_225_cf_a-001 8F2Q
- UB_{12} ($D2_f$):
  A12B_cF52_225_h_b-001 JTKK
- Mg_6MnO_8:
  A6BC8_cF60_225_d_a_ce-001 4YGB
- Co_9S_8 ($D8_9$):
  A9B8_cF68_225_af_ce-001 X1EM
- Sulphohalite $[Na_6ClF(SO_4)_2, H5_8]$:
  ABC6D8E2_cF72_225_a_b_e_f_c-001 8Y3K
- High temperature Cu_2Se:
  A18B_cF76_225_c2f_a-001 7K0D
- $Cu_3[Fe(CN)_6]_2 \cdot xH_2O$ ($J2_5$):
  A6B9CD2E6_cF96_225_e_af_b_c_e-001 N4GS
- Model of Austenite (cF108):
  AB18C8_cF108_225_a_eh_f-001 VR5Q
- $Cr_{23}C_6$ ($D8_4$):
  A6B23_cF116_225_e_acfh-001 EY4X
- Th_6Mn_{23} ($D8_a$):
  A23B6_cF116_225_ad2f_e-001 W8MF
- $Mg_6Si_7Cu_{16}$:
  A16B6C7_cF116_225_2f_e_ad-001 NHP2

- Model of Ferrite (cF128):
  A9B16C7_cF128_225_acd_2f_be-001 FENM
- $(NH_4)_3AlF_6$ ($J2_1$):
  AB30C16D3_cF200_225_a_ej_2f_bc-001 U8XN
- Intermediate temperature Bornite($Cu_{5/6}Fe_{1/6})_3S_2$:
  A7B_cF256_225_f2k_ce-001 EMLR
- fcc Fullerene (K_3C_{60}):
  A40B_cF492_225_j2l_ac-001 54ZJ

Fm$\bar{3}$c (**226**):

- $NaZn_{13}$ ($D2_3$):
  AB13_cF112_226_a_bi-001 DCLX

Fd$\bar{3}$m (**227**):

- Diamond ($A4$):
  A_cF8_227_a-001 X5M8
- NaTl ($B32$):
  AB_cF16_227_a_b-001 CHL9
- Ideal β-Cristobalite (SiO_2, $C9$):
  A2B_cF24_227_c_a-001 QDSV
- Cu_2Mg Cubic Laves ($C15$):
  A2B_cF24_227_c_b-001 8YL7
- Cubic CuPt [$L1_3(I)$, $D4$]:
  AB_cF32_227_c_d-001 0HDN
- T-Carbon:
  A_cF32_227_e-001 WPN9
- Ti_2C:
  AB2_cF48_227_c_e-001 PR5K
- Spinel (Al_2MgO_4, $H1_1$):
  A2BC4_cF56_227_c_b_e-001 MZYE
- Spinel (Co_3O_4, $D7_2$):
  A3B4_cF56_227_ad_e-001 SV6X
- β-Alane (AlD_3):
  AB3_cF64_227_c_f-001 9LSQ
- Senarmontite ($D6_1$, Sb_2O_3):
  A3B2_cF80_227_f_e-002 UHQ6
- Pyrochlore Iridate ($Eu_2Ir_2O_7$, $E8_1$):
  A2B2C7_cF88_227_c_d_af-001 0R9R
- $NiTi_2$:
  AB2_cF96_227_e_cf-001 AVWT
- $D6_2$ (Sb_2O_4, *Obsolete*):
  A2B_cF96_227_abf_cd-001 UGWY
- η-carbide (Fe_3W_3C, $E9_3$):
  AB3C3_cF112_227_c_de_f-001 WVM5
- γ-Ga_2O_3:
  A11B4_cF120_227_acdf_e-001 VTDR
- Si_{34} Clathrate:
  A_cF136_227_aeg-001 U115
- Dy_5Pd_2:
  A7B2_cF144_227_2ef_e-001 WYVV
- Predicted Li_2MgH_{16} High-T_c Superconductor(250 GPa):
  A16B2C_cF152_227_eg_c_b-001 WZBC
- $Al_{10}V$:
  A10B_cF176_227_cfg_d-001 WWX6
- $Mg_3Cr_2Al_{18}$:
  A18B2C3_cF184_227_fg_d_ac-001 3DEV
- $Zn_{22}Zr$:
  A22B_cF184_227_cdfg_a-001 MX6R
- $G7_3$ [$Na_3MgCl(CO_3)_2$] (*Obsolete*):
  A2BCD3E6_cF208_227_e_c_d_f_g-001 8XP6
- $H5_6$ [Tychite, $Na_6Mg_2SO_4(CO_3)_4$)] (*Obsolete*):
  A4B2C6D16E_cF232_227_e_c_f_eg_b-001 Y05P
- $H_3PW_{12}O_{40}{\cdot}29H_2O$ ($H4_{21}$):
  A29B40CD12_cF656_227_ae2fg_e3g_b_g-001 3VYY

Fd$\bar{3}$c (**228**):

- $Te[OH]_6$ (*Obsolete*):
  A6B_cF224_228_h_c-001 MSL9
- $CuCrCl_5[NH_3]_6$:
  A5BCD6_cF416_228_eg_c_b_h-001 19XK
- Voltaite ($K_2Fe_8Al[SO_4]_{12}{\cdot}18H_2O$):
  AB8C24D2E84F12_cF2096_228_a_cg_2h_b_7h_h-001 E4V9

Im$\bar{3}$m (**229**):

- Body-centered cubic (W, $A2$, bcc):
  A_cI2_229_a-001 7W8F
- High-pressure (200 GPa) H_3S:
  A3B_cI8_229_b_a-001 VV0Z
- β-Hg_4Pt:
  A4B_cI10_229_c_a-001 78LF
- Pt_3O_4:
  A4B3_cI14_229_c_b-001 BYND
- High pressure cubic CaH_6:
  AB6_cI14_229_a_d-001 N2LT
- Model of Ferrite (cI16):
  AB4C3_cI16_229_a_c_b-001 YRPB
- Model of Austenite (cI32):
  AB12C3_cI32_229_a_h_b-001 L6PB
- Ir_3Ge_7 ($D8_f$):
  A7B3_cI40_229_df_e-001 9SK5
- α-AgI ($B23$):
  A21B_cI44_229_bdh_a-001 QV5K
- $Ce_3Ni_6Si_2$:
  A3B6C2_cI44_229_e_h_c-001 BC5E
- $Dy_6Fe_{16}O$:
  A6B16C_cI46_229_e_ch_a-001 Y3T5
- γ-brass (Fe_3Zn_{10}, $D8_1$):
  A3B10_cI52_229_e_fh-001 TJ2T
- Sb_2Tl_7 ($L2_2$):
  A2B7_cI54_229_e_afh-001 KM4R

Ia$\bar{3}$d (**230**):

- Ga_4Ni_3:
  A4B3_cI112_230_af_g-001 K0Z6
- $RhBi_4$:
  A4B_cI120_230_h_c-001 V61M
- Garnet [$S1_4$, $Co_3Al_2(SiO_4)_3$]:
  A2B3C12D3_cI160_230_a_c_h_d-001 YMRU
- $Ca_3Al_2(OH)_{12}$ ($J2_3$):
  A2B3C12D12_cI232_230_a_c_h_h-001 LL0W

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