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Volume 43

# Crystal Structures of Inorganic Compounds

Subvolume A

Structure Types

Part 1

Space groups (230) *Ia*-3*d* – (219) *F*-43*c*

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**Dedicated to Prof. E. Parthé, Geneva/Vienna, on the occasion of his 75th birthday.**

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# Preface

In the 1970s Landolt-Börnstein published a series of volumes containing crystallographic data for organic (III/5 Structure Data of Organic Crystals), intermetallic (III/6 Structure Data of Elements and Intermetallic phases) and inorganic compounds (III/7 Crystal Structure Data of Inorganic Compounds). During the 30 years that have passed, the experimental methods leading to a complete structure determination have considerably improved and the large number of crystal structures known today justifies the publication of a new compilation.

The present volume will cover both intermetallic and classical inorganic compounds, a clear limit having been drawn by excluding compounds that contain C-H bonds. Whereas the earlier edition listed space group/crystal system and cell parameters for different classes of compounds, we have here chosen a different approach by grouping known crystal structures into structure types. The structure type concept is widely used among inorganic compounds, where the number of isotypic compounds can reach several hundreds. The first subvolumes will contain complete crystallographic data sets, including atom coordinates, that represent distinct structure types, whereas the last subvolumes will list cell parameters of isotypic compounds. The crystallographic data are accompanied by remarks and crystallographic features common to isotypic compounds, such as the atomic environments, a brief description of the main structural features, and drawings of selected structure types.

In the definition used here, structures belonging to the same structure type crystallize in the same space group, have similar cell parameters and similar representative atom coordinates. The latter criterion requires that they are isopointal, i.e. they have the same Wyckoff sequence (sequence of Wyckoff positions). Following this scheme, the structure types are ordered according to the space group number and the Wyckoff sequence. The present subvolume, the first of the series, contains data for some 1000 cubic (space groups # 230 to 219) structure types, reported up to the year 2002.

We would like to thank the coauthors for their contribution and all other collaborators on the databases TYPIX and Pauling File, who have, through the years, helped in compiling and analyzing the large number of structural data that constitute the basis of this work.

Switzerland, March 2004 The Editors

# Contents of Subvolume III/43 A 1

# Introduction

## 1 Subject matter

### 1.1 General remarks on the contents

Inorganic compounds are here defined as compounds containing no C-H bonds.
The first series of subvolumes will contain complete crystallographic data sets representative of structure types found among inorganic compounds. The second series of subvolumes will contain lists of compounds crystallizing with these types.
The compilations TYPIX [1] and Pearson's Handbook [2] constitute a valuable basis for this work, but all data have been reprocessed from the original publications. Our aim is to cover the literature published up to two years before the release of the subvolume.

### 1.2 Structure type concept

According to the definition used here, isotypic compounds crystallize in the same space group, have similar cell parameter ratios, and occupy the same Wyckoff positions in the standardized description with the same or similar values of the atom coordinates [3]. If all these criteria are fulfilled, the coordination polyhedra should be similar and the main structural features respected. It follows from the definition that isotypic structures are isopointal (same Wyckoff positions), however, two isopointal structures are not necessarily isotypic. The last step in distinguishing different structure types is subjective and we have sometimes been guided by what is usually considered in the literature.
No distinction is made between structures with fully and partly occupied atom sites. Except for binary compounds, protons are not taken into consideration, so that e.g. ammonium and alkaline metal compounds are considered to be isotypic. Disordered structures are included in the classification and different models for site splitting can sometimes subdivide a conventional structure type into several types. Ordering variants are distinguished, mixed occupations by two or several chemical elements being considered as the same dummy element, independently of the proportions.

### 1.3 Data selection and checking

Each structure type is represented by a, if available, recent refinement of the structure of the compound for which this particular atom arrangement was first reported. In those cases where two isotypic structures were reported the same year, the date of submission of the manuscript was taken as criterion. In exceptional cases, preference has been given to a structure with less vacancies, or a lower degree of disorder. Thesis works have not been considered, and conference abstracts only in a few cases.
No systematic effort has been made to select the most recent refinement, and a more accurate refinement has sometimes been preferred to a routine phase analysis, without any claim on having selected here the "best" refinement. Preference has been given to structure determinations corresponding to ambient conditions.
The data have been submitted to extensive computer-aided checking and, as far as possible, misprints in the crystallographic data have been corrected. When relevant, the data have been transformed to a space group taking into consideration all symmetry elements effectively present in the structure. A few obviously wrong structures have been excluded from the compilation. References are sometimes added to more recent literature where the correctness of the structure determination is questioned, but no exhaustive literature search has been carried out in this sense.

### 1.4 Standardization of crystallographic data

The crystallographic data have been standardized following a method proposed by Parthé and Gelato [4], using the program STRUCTURE TIDY [5]. The standardization procedure applies criteria to select the space group setting, the cell parameters, the origin of the coordinate system, the representative atom coordinates, and the order of the atom sites.
(1) The coordinate system must be right-handed and refer to a space group setting defined in the International Tables for Crystallography [6], with the following additional constraints

- triclinic space groups: Niggli-reduced cell
- monoclinic space groups: b-axis unique, "best" cell
- orthorhombic space groups: $a \le b \le c$, when not fixed by the space group setting
- trigonal space groups with *R*-lattice: triple hexagonal cell
- space groups with two origin choices: origin choice 2 (origin at inversion center)
- enantiomorphic space groups: smallest index of the relevant screw axis

(2) The representative triplet of each atom site must obey a series of eliminative conditions listed below.

- first triplet in International Tables for Crystallography [6]
- $0 \le x, y, z < 1$
- minimum value of $(x^2 + y^2 + z^2)$
- minimum value of $x$

- minimum value of $y$
- minimum value of $z$

(3) For the 148 non-polar space groups there are between 1 and 24 possibilities to rotate, invert or shift the coordinate system, respecting the conditions listed above. For polar space groups the standardization program will prepare data sets where one atom site after the other, belonging to the "lowest Wyckoff set" (set of Wyckoff sites containing the earliest letters in the alphabet), fixes the origin on the polar axis. In each case, the standardized data set is selected based on the following eliminative conditions:

- minimum value of $\Gamma = \Sigma\,(x_j^2 + y_j^2 + z_j^2)^{1/2}$ summing over all atom sites
- minimum value of $\Sigma\, x_j$ summing over all atom sites
- minimum value of $\Sigma\, y_j$ summing over all atom sites
- minimum value of $\Sigma\, z_j$ summing over all atom sites
- minimum value of $x_n^2 + y_n^2 + z_n^2$ for the $n^{\text{th}}$ atom site

(4) Finally, the atom sites are reordered according to the eliminative criteria:

- inverse alphabetic order of the Wyckoff letters
- increasing $x$
- increasing $y$
- increasing $z$

(5) On extending the standardization procedure, originally designed for intermetallic compounds, to other inorganic compounds, it appeared sensible to consider protons apart, since their positions are often not determined. For compounds with more than two elements, the proton positions, when determined, are consequently not taken into consideration for the selection of the standardized description, but are listed at the end of the table of atom coordinates, respecting the same criteria for their internal ordering and selection of representative triplets as indicated above. It follows that proton positions are not considered in the Wyckoff sequence, and also not in the sum of multiplicities included in the Pearson symbol.

### 1.5 Atomic environments

The definition of the atomic environments (AE) [7] is based on the method of Brunner and Schwarzenbach [8], where the interatomic distances between an atom site and its nearest neighbors are plotted in a histogram. In the general case, the Atomic Environment Type (AET) is the polyhedron formed by the atoms to the left of the maximum gap appearing in the histogram. In those cases where the maximum gap rule leads to AEs with some of the selected atoms inside the polyhedron formed by the others, or to AEs with atoms located in the faces of the polyhedron, the maximum-convex-volume rule is applied. This rule is defined as the maximum volume around only one central atom enclosed by convex faces, with all the atoms situated at the intersections of at least three faces. The same rule was also used in those cases where no clear maximum gap was present. Whenever two or more equal or similar gaps were observed, the number of different AETs in a structure type was kept as small as possible.

For fully ordered intermetallic structures, the AETs can be assimilated to the conventional coordination polyhedra. Differences occur based on the fact that the atomic environment is a purely geometric concept and differences in chemical bonding, oxidation state (cations and anions are not distinguished) or atomic radii are not taken into consideration. All atom sites are further treated as being fully occupied, so that, for instance, the atomic environment of the phosphorus atom in an orientationally disordered phosphate group may be a cube, whereas the conventional coordination polyhedron is a tetrahedron.

The AETs are here designated by the name of the coordination polyhedron (when simple) and its composition. Positions belonging to atom sites with mixed occupation are represented by the majority element, or by the first element in alphabetic order, if identical proportions are reported. Protons are only taken into consideration in exceptional cases.

## 2 Selection and arrangement of the data

### 2.1 Framed data

- Chemical formula. Selected chemical units are distinguished and a particular order is adopted for the elements, which constitutes a compromise for chemical compounds ranging from intermetallic to ionic, including some coordination and covalent compounds. The coefficients are defined so that the number of formula units in the unit cell is an integer which takes into consideration at least the factor corresponding to the Bravais lattice.
- Pearson symbol [9]. A lower-case letter defines the crystal system (*a* for anorthic = triclinic, *m* for monoclinic, *o* for orthorhombic, *t* for tetragonal, *h* for hexagonal or trigonal, and *c* for cubic) and an upper-case letter the Bravais lattice (*P* for primitive, *S* for side-face centered, *F* for all-face centered, *I* for body centered, and *R* for rhombohedrally centered). The integer number following these two characters corresponds to the sum of the site multiplicities of all partly or fully occupied Wyckoff positions. Note that following the

recommendations of a subcommission of the International Union of Crystallography [10], we use the letter *S*, which groups *A*, *B* and *C*-face centered lattices, and that the triple hexagonal cell is considered for *R*-type Bravais lattices.

- Space group and Wyckoff sequence. The number assigned to the space group in the International Tables for Crystallography [6], indicated within parentheses, is followed by the Hermann-Mauguin symbol corresponding to the standardized data. The Wyckoff sequence lists the Wyckoff letters of all, fully or partly occupied atom sites in the structure. The letters are written in inverse alphabetic order, a superscript number being added when a particular Wyckoff position is present more than once.

### 2.2 General information about the structure type

- Alternative type names. These include chemical formulas of isotypic compounds that are sometimes used in the literature to designate the structure type, but also mineral names, colloquial names used within particular structure families, and Strukturbericht notations [11]. The alternative type names are listed in alphabetic order in the subject index.
- References. Each chemical formula is followed by a reference to the first structure determination.
- Structural features. A short description of the structure type, referring to the type-defining compound, emphasizes particular structural features such as the arrangement of close-packed layers or coordination polyhedra. Close relationships to other structure types, such as ordered substitution or filling-up of interstices, are sometimes mentioned.

### 2.3 General information about the selected data set

- First author(s) of the reference from which the crystallographic data are taken.
- Refined composition. An alphabetically sorted chemical formula as computed from the crystallographic data set.
- Cell parameters $a$, $b$, $c$, $\alpha$, $\beta$, $\gamma$, computed cell volume $V$, interaxial ratio(s), and the number of formula units per unit cell $Z$. The latter applies to the refined composition and to the chemical formula given in the frame, but not necessarily to the alternative type names.

### 2.4 Table of atom coordinates

- Atom site. The sites are named after the chemical element they are occupied by, or *M* if occupied by a mixture of two or several elements. The numbering is continuous through the table, starting from 1, and independent of the site occupation.
- Site multiplicity and Wyckoff letter, according to the International Tables for Crystallography [6].
- Site symmetry. Point symmetry (symmetry implying no translational component, *m* for mirror plane, 2 for 2-fold axis, etc.).
- Fractional positional coordinates with respect to the three crystallographic axes: $x/a$, $y/b$, $z/c$.
- Site occupancy. Normalized to 1 (omitted) for a fully occupied site.
- Atomic environment type (AET) as defined under 1.5.

### 2.5 Footnote to the table of atom coordinates

- When relevant, occupation of mixed sites normalized to a total occupancy 1.
- When relevant, transformation from the published data applied by the standardization procedure.
- When specified in the original publication, condensed information about the experimental procedure: single crystal/powder/thin film, diffractometer/photographs, X-rays/neutrons/electrons, the lowest of the published conventional reliability factors for the structure refinement R/wR/$R_p$/w$R_p$/$R_B$, temperature T, pressure p.

### 2.6 Remarks

The remarks given here include information about the stability range of the type-defining compound, the origin of mineral specimens, particularities concerning the structure refinement, short interatomic distances, corrections applied to the published data, related literature, etc.

### 2.7 References

Literature references are given for all publications mentioned in the data set. The journal names are abbreviated following the recommendations of the Chemical Abstracts Service.

### 2.8 Figures

Figures emphasizing particular structural features are presented for commonly occurring structure types. Some less common structure types are also shown, in order to illustrate the great variety of inorganic structures.

### 2.9 Order of the structure types

The data sets representing the distinct structure types are arranged according to features characterizing the standardized crystallographic description:

- decreasing order of the number assigned to the space group in the International Tables for Crystallography [6]

- increasing sum of site multiplicities (included in the Pearson symbol)
- alphabetic order of the Wyckoff sequence
- increasing value of the interaxial ratio *c*/*a*

An extensive index listing various type names found in the literature will help the user to find a particular structure type.

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# Contents of Subvolume III/43 A 1

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| structure type | Pearson symbol | space group number, Wyckoff sequence | page |
|---|---|---|---|
| $Al_2([OH]_{1-x}F_x)_6{\cdot}H_2O$ | *cF*72 | 227,fcb | 77 |
| $Al(PO_3)_3$ | *cI*208 | 220,$e^4$c | 480 |
| $Al_2S_3$ cubic | *cF*56 | 227,ecb | 71 |
| $Al_{12}Si_{164}O_{338}$ | *cF*640 | 227,ihg$^3$e$^2$ | 135 |
| $Al_{52}Si_{140}O_{358}$ | *cF*672 | 227,ihg$^3$e$^3$ | 141 |
| (AlV) α | *cF*184 | 227,gfdca | 111 |
| $As_2O_3$ cubic | *cF*80 | 227,fe | 79 |
| $AuSb_3$ | *cI*8 | 229,ba | 15 |
| $AuZn_3$ rt | *cP*32 | 223,kca | 325 |
| B1 | *cF*8 | 225,ba | 198 |
| B2 | *cP*2 | 221,ba | 343 |
| B23 | *cI*44 | 229,hdba | 28 |
| B32 | *cF*16 | 227,ba | 67 |
| $Ba_8Al_{16}Ge_{30}$ | *cP*54 | 223,kidca | 330 |
| $Ba_4Al_7O_{12}(OH)_5{\cdot}H_2O$ | *cP*66 | 221,jihg$^2$feba | 381 |
| $Ba_{15}Al_{30}Si_{66}O_{192}{\cdot}1.6Ba(OH)_2{\cdot}11.9BaBr_2{\cdot}30H_2O$ | *cI*364 | 229,lk$^2$jihfe$^2$d | 50 |
| $Ba_{15}Al_{30}Si_{66}O_{192}{\cdot}1.7Ba(OH)_2{\cdot}12.5BaCl_2{\cdot}35H_2O$ | *cI*400 | 229,lk$^2$jih$^2$fe$^3$d | 52 |
| $Ba_{0.6}Bi_{0.4}F_{2.4}$ | *cF*92 | 225,hfcb | 233 |
| $BaBiO_3$ ht2 | *cF*40 | 225,ecba | 207 |
| $BaBi_3O_{5.5}$ ht | *cI*8 | 229,ba | 16 |
| $Ba_{2.4}Bi_{1.6}O_6$ cubic | *cF*112 | 225,jcba | 241 |
| $Ba_3Bi(PO_4)_3$ | *cI*140 | 220,e$^2$c$^2$a | 475 |
| $Ba_3C_{60}$ | *cP*126 | 223,l$^2$kc | 338 |
| $Ba_2Ca_{0.2}Cu_{1.2}O_3(CO_3)_{0.6}$ | *cP*76 | 221,jih$^2$gfedcba | 382 |
| $BaCaDy_2F_{10}$ | *cP*16 | 221,gdcba | 359 |
| $Ba_2CaWO_6$ | *cF*40 | 225,ecba | 207 |
| $BaCd_2Cl_6{\cdot}5H_2O$ | *cF*112 | 227,fedc | 93 |
| $Ba_3CdSn_2S_8$ | *cI*116 | 220,edc$^2$a | 474 |
| $Ba_{0.5}Ce_{0.5}F_{2.5}$ | *cF*64 | 225,hcba | 222 |
| $Ba_{0.5}Ce_{0.5}F_{2.5}$ | *cF*96 | 225,hfcba | 234 |
| $Ba_6Co_{25}S_{27}$ | *cP*58 | 221,mhgfeba | 378 |
| $Ba_3[Cr(CN)_6]_2{\cdot}20H_2O$ | *cI*336 | 229,k$^2$j$^3$ife$^2$c | 49 |
| $Ba_{44}Cu_{48}(CO_3)_6O_{87.9}$ | *cI*580 | 229,k$^4$j$^4$i$^2$hgfe$^2$d | 59 |
| $BaCuO_2$ | *cI*402 | 229,k$^3$j$^2$ih$^2$fe$^3$da | 53 |
| $Ba_{0.92}Cu_{1.01}O_{1.93}$ | *cI*406 | 229,k$^3$j$^2$ih$^2$fe$^3$db | 55 |
| $Ba_{0.92}Cu_{1.01}O_{2.17}$ | *cI*456 | 229,k$^3$j$^2$i$^2$h$^2$fe$^3$dba | 57 |
| $Ba_{0.92}Cu_{1.06}O_{2.14}$ | *cI*424 | 229,k$^3$ji$^2$h$^2$gfe$^3$d | 55 |
| $Ba_{0.92}Cu_{1.06}O_{2.28}$ | *cI*636 | 229,k$^3$j$^5$i$^2$h$^2$gfe$^4$dba | 60 |
| $Ba_{44}Cu_{45}O_{90}$ | *cI*400 | 229,k$^3$j$^2$ih$^2$fe$^3$d | 51 |
| $Ba_{44}Cu_{44}O_{88.5}Br$ | *cI*402 | 229,k$^3$j$^2$ih$^2$fe$^3$da | 54 |
| $Ba_{0.9}CuO_2{\cdot}xCO_2$ | *cI*472 | 229,k$^3$j$^2$i$^2$h$^2$gfe$^3$d | 58 |
| $Ba_{41}Cu_{44}O_{84}Cl_2$ | *cI*402 | 229,k$^3$j$^2$ih$^2$fe$^3$da | 53 |
| $Ba_8Ga_{16}Si_{30}$ | *cP*54 | 223,kidca | 329 |
| $Ba_2Ge_4S_{10}$ | *cF*128 | 227,fe$^2$c | 100 |
| $BaHg_{11}$ | *cP*36 | 221,jigca | 368 |
| $Ba_3La(PO_4)_3$ | *cI*124 | 220,e$^2$ca | 474 |
| $Ba_8Ni_6Ge_{40}$ | *cP*54 | 223,kidca | 330 |
| $Ba_2Ni(NO_2)_6$ | *cF*84 | 225,heca | 229 |
| $(Ba,Pb)_6(Cu,Fe,Ni)_{25}S_{27}$ | *cP*82 | 221,m$^2$hgfeba | 385 |

| structure type | Pearson symbol | space group number, Wyckoff sequence | page |
|---|---|---|---|
| $BaPb_{0.65}Sb_{0.3}Bi_{0.05}O_3$ | *cP*40 | 221,hgfedcba | 371 |
| $Ba_{11}Pd_{11}O_{20}(CO_3)_2$ | *cI*556 | 229,$k^3j^4i^2h^2fe^4d$ | 59 |
| $Ba_{0.73}Pr_{0.27}F_{2.27}$ | *cF*60 | 225,ica | 218 |
| $Ba_8Pt_4Y_3O_{17.5}$ | *cP*33 | 221,hgedca | 365 |
| "$Ba_{21}Si_2O_5$" | *cF*224 | 227,gfedcba | 117 |
| $Ba_3Te_2O_6Cl_2$ | *cF*296 | 227,hgfeca | 122 |
| $BaTiO_3$ cubic | *cP*56 | 221,ljhg | 377 |
| $BiF_3$ | *cF*16 | 225,cba | 200 |
| $BiMn_6PO_{12}$ | *cF*96 | 225,$f^2$dba | 234 |
| $Bi_2O_3$ δ | *cF*36 | 225,fa | 205 |
| $Bi_2O_3$ δ | *cF*44 | 225,fca | 209 |
| $Bi_4(SiO_4)_3$ | *cI*76 | 220,eca | 471 |
| $Bi_2Sn_2O_7$ ht | *cF*240 | 227,$g^2$ec | 118 |
| $(Br_2)_6{\cdot}46H_2O$ | *cP*52 | 223,kidc | 328 |
| C1 | *cF*12 | 225,ca | 199 |
| C3 | *cP*6 | 224,ba | 311 |
| C9 | *cF*104 | 227,ha | 89 |
| C15 | *cF*24 | 227,cb | 69 |
| C diamond cubic | *cF*8 | 227,a | 67 |
| $C_8$ | *cI*16 | 229,f | 19 |
| $C_{60}$ rt | *cF*1924 | 225,$l^{10}$a | 309 |
| $C_2Cl_6$ form III | *cI*28 | 229,fe | 21 |
| $(CF_3Ge)_4S_6$ | *cF*208 | 227,gf$e^2$ | 116 |
| "$Ca_3Ag_8$" | *cI*44 | 229,hec | 29 |
| $CaAg_4Al_7$ | *cP*36 | 221,jigca | 368 |
| $Ca_6Ag_{16}N$ | *cI*46 | 229,heca | 30 |
| $Ca_{19}Ag_8N_7$ | *cF*136 | 225,hf$e^2$ba | 254 |
| $Ca_{12}Al_{14}O_{33}$ | *cI*140 | 220,ed$^2$c$^2$b | 476 |
| $Ca_{12}Al_{14}O_{32}F_2$ | *cI*152 | 220,ed$^2$c$^2$ba | 477 |
| $Ca_3Al_2(OH)_{12}$ | *cI*136 | 230,hca | 2 |
| $Ca_3Al_2Si_3O_{12}$ | *cI*160 | 230,hdca | 3 |
| $Ca_6Al_{12}Si_{12}O_{48}$ | *cP*108 | 221,mki$^2$h$g^3$ | 407 |
| $Ca_{40}Al_{80}Si_{112}O_{384}$ | *cF*656 | 227,ih$g^3$e$^2$c | 138 |
| $Ca_{48}Al_{96}Si_{96}O_{384}$ | *cF*896 | 226,j$^2$i$^4$g$^2$ | 187 |
| $Ca_{48}Al_{96}Si_{96}O_{384}$ | *cF*992 | 226,j$^3$i$^3$g$^2$ | 191 |
| $Ca_{48}Al_{96}Si_{96}O_{384}$ | *cF*1000 | 226,j$^3$i$^3$g$^2$b | 191 |
| $Ca_6Al_{12}Si_{12}O_{48}{\cdot}xBr_2$ | *cP*136 | 221,ml$^2$kih$g^2$ | 433 |
| $Ca_{12}Al_{10.6}Si_{3.4}O_{32}Cl_{5.4}$ | *cI*128 | 220,edc$^2$ba | 475 |
| $Ca_{28.5}Al_{57}Si_{135}O_{384}{\cdot}xH_2O$ | *cF*800 | 227,ih$g^4$e$^4$ | 160 |
| $Ca_{40}Al_{80}Si_{112}O_{384}{\cdot}xH_2O$ | *cF*768 | 227,ih$g^4$e$^3$ | 156 |
| $Ca_6Al_{12}Si_{12}O_{48}{\cdot}28H_2O$ | *cP*140 | 221,m$^2$kih$g^5$ca | 436 |
| $CaB_6$ | *cP*7 | 221,fa | 350 |
| $Ca_3(BN_2)_2$ α | *cI*28 | 229,ecba | 20 |
| $Ca_3Bi(PO_4)_3$ | *cI*124 | 220,e$^2$ca | 474 |
| $CaC_2$ form IV | *cF*36 | 225,fa | 205 |
| $Ca_{15}(CBN)_6(C_2)_2O$ | *cI*312 | 230,h$^2$geca | 10 |
| $(Ca,Ce,Na)(Na,Ce)_3(Ti,Nb)_2Ti_2O_{12}$ | *cP*40 | 224,kdcba | 314 |
| $CaCu_{6.5}Al_{6.5}$ | *cF*112 | 226,iba | 179 |
| $CaCu_3Ti_4O_{12}$ | *cI*40 | 229,hcba | 27 |

| structure type | Pearson symbol | space group number, Wyckoff sequence | page |
|---|---|---|---|
| $CaF_2$ | *cF*12 | 225,ca | 199 |
| $Ca_{11}Ga_7$ | *cF*144 | 225,hf$^2$eba | 258 |
| $Ca_7Ge$ | *cF*32 | 225,dba | 202 |
| $Ca_{33}Ge$ | *cF*48 | 227,ec | 71 |
| "$Ca_3Hg$" | *cP*4 | 221,ca | 344 |
| $Ca_4(K,Ca,Sr,Ba)_3Cu_3Al_{12}Si_{12}O_{48}(OH)_8{\cdot}14H_2O$ | *cF*2476 | 225,l$^6$k$^7$j$^4$hf$^6$ea | 310 |
| $Ca_{48}Mg_{16}[Al(SiO_4)_4]_3\{(BO_3)_{17}(CO_3)_3\}(CO_3)_{16}{\cdot}4H_2O$ | *cF*520 | 227,igfe$^5$da | 129 |
| $Ca_5Mg_3ZnV_6O_{24}$ | *cI*160 | 220,e$^2$dcba | 477 |
| $(Ca_{1.04}Mn_{0.07}Na_{0.01})Sb_{0.65}(Sb_{0.99}Ti_{0.76}Fe_{0.19}Al_{0.06})O_6(OH)_{0.91}$ | *cF*184 | 227,gfdca | 113 |
| $Ca_3Mn_{2.26}(SiO_4)_{2.42}O_{2.32}$ | *cI*208 | 230,hgdca | 7 |
| $Ca_2NH$ | *cF*64 | 227,edc | 73 |
| $Ca_2NH$ | *cF*160 | 227,gedc | 108 |
| $Ca{\cdot}6NH_3$ | *cI*14 | 229,ea | 18 |
| $Ca_2Nb_2O_7$ cubic | *cF*88 | 227,fdca | 81 |
| $Ca_{0.8}Nd_{0.2}F_{2.2}$ | *cF*116 | 225,hfecb | 247 |
| "$Ca_3Pb$" | *cP*4 | 221,ca | 344 |
| $Ca_3PbO$ | *cP*5 | 221,dba | 345 |
| $CaPdH_2$ | *cP*5 | 221,dba | 345 |
| $Ca_4Rh_3H_{12}$ | *cI*38 | 229,edcb | 24 |
| $CaSnF_6$ rt | *cF*104 | 225,jba | 237 |
| $Ca_{0.9}Th_{0.1}F_{2.2}$ | *cF*76 | 225,f$^2$ca | 226 |
| $Ca_3(Ti_{0.5}Fe_{0.5})_2(Si_{0.67}Fe_{0.33})_3O_{12}$ | *cI*256 | 230,h$^2$dca | 8 |
| $CaTiO_3$ cubic | *cP*5 | 221,dba | 345 |
| $CaUS_2$ | *cI*40 | 220,cba | 468 |
| $Ca_{0.68}Y_{0.32}F_{2.32}$ | *cF*92 | 225,hfcb | 233 |
| $Ca_{0.90}Y_{0.10}F_{2.10}$ | *cF*92 | 225,ifca | 234 |
| $Ca_{0.13}Zr_{0.87}O_{1.87}$ | *cF*60 | 225,gca | 217 |
| $Cd_{11}Al_{12}Si_{12}O_{48}$ | *cP*134 | 221,m$^2$kihg$^4$f | 431 |
| $Cd_6Al_{12}Si_{12}O_{48}$ | *cP*80 | 221,mkihg | 384 |
| $Cd_6Al_{12}Si_{12}O_{48}$ | *cP*88 | 221,mkihg$^2$ | 388 |
| $Cd_{9.5}Al_{12}Si_{12}O_{48}Cl_4(OH)_3$ | *cP*163 | 221,m$^3$lkihg$^2$c | 447 |
| $Cd_{9.5}Al_{12}Si_{12}O_{48}Cl_4(OH)_3{\cdot}xH_2O$ | *cP*225 | 221,nm$^3$ljhg$^6$ed | 461 |
| $Cd_6Al_{12}Si_{12}O_{48}{\cdot}xH_2O$ | *cP*112 | 221,m$^2$kihg$^2$ | 412 |
| $Cd_6Al_{12}Si_{12}O_{48}{\cdot}xH_2O$ | *cP*152 | 221,m$^2$ki$^3$hg$^4$ | 444 |
| $Cd_6Al_{12}Si_{12}O_{48}{\cdot}31H_2O$ | *cP*192 | 221,m$^2$l$^2$kihg$^6$ | 454 |
| $Cd_9Al_{12}Si_{12}O_{48}{\cdot}3H_2O$ | *cP*160 | 221,m$^3$kihg$^5$ | 445 |
| $Cd_3B_7O_{13-x}(S_2)_x$ | *cF*272 | 219,hfe$^2$dcba | 492 |
| $Cd_{0.5}Bi_{1.5}O_{2.75}$ ht | *cI*40 | 230,da | 1 |
| $Cd(CN)_2{\cdot}CCl_4$ | *cF*144 | 227,geba | 104 |
| $Cd_3[Co(CN)_6]_2$ | *cF*56 | 225,e$^2$ba | 213 |
| $Cd_3[Co(CN)_6]_2{\cdot}12H_2O$ | *cF*344 | 225,lke$^2$ba | 290 |
| $Cd_3[Fe(CN)_6]_2{\cdot}15H_2O$ | *cF*208 | 225,kfe$^3$ba | 276 |
| CdNi | *cF*96 | 227,fec | 85 |
| $Cd[Pd(CN)_6]$ | *cF*56 | 225,e$^2$ba | 213 |
| $CdTm_4Mo_3O_{16}$ | *cP*96 | 222,ifedc | 342 |
| $CdY_4Mo_3O_{16}$ | *cP*96 | 222,ifedc | 342 |
| $Cd_{1.5}Zn_{1.5}[Co(CN)_6]_2{\cdot}12H_2O$ | *cF*120 | 225,fe$^3$cba | 250 |
| $CeCd_{11}$ | *cP*36 | 221,jigca | 368 |
| $CeCr_2Al_{20}$ | *cF*184 | 227,gfdca | 112 |

| structure type | Pearson symbol | space group number, Wyckoff sequence | page |
|---|---|---|---|
| $Cs_{0.95}H_{9.35}Al_{10.3}Si_{37.7}O_{96}\cdot 30H_2O$ | *cI*282 | 229,lkjiheb | 44 |
| $CsHgCl_3$ | *cP*11 | 221,edba | 354 |
| $Cs_8In_8Ge_{38}$ | *cP*54 | 223,kidca | 330 |
| $Cs_7K_5Al_{12}Si_{12}O_{48}$ | *cP*115 | 221,mkihg$^5$c | 417 |
| $Cs_{9.8}K_{13}Al_{22.8}Si_{73.2}O_{192}$ | *cI*328 | 229,lk$^2$jifed | 48 |
| $Cs_{6.0}K_{2.7}H_{13.0}Al_{21.7}Si_{74.3}O_{192}$ | *cI*312 | 229,lk$^2$jied | 47 |
| $CsLi_2C_{60}$ | *cF*16 | 225,cba | 200 |
| $Cs_2Li[Co(CN)_6]$ | *cF*64 | 225,e$^2$cba | 219 |
| $Cs_2MoOBr_5$ | *cF*60 | 225,e$^2$ca | 215 |
| $CsN_3$ β | *cP*8 | 221,eba | 351 |
| $CsNO_2$ | *cP*31 | 221,keb | 365 |
| $Cs_{11}Na_3Al_{12}Si_{12}O_{48}$ | *cP*119 | 221,mkjihg$^4$c | 422 |
| $Cs_7Na_5Al_{12}Si_{12}O_{48}$ | *cP*99 | 221,mkihg$^3$c | 396 |
| $Cs_9Na_{3.5}Al_{12}Si_{12}O_{48}$ | *cP*123 | 221,m$^2$kihg$^3$c | 426 |
| $Cs_{0.2}Na_{1.2}Cd_{4.8}Al_{11}Si_{37}O_{96}$ ht | *cI*166 | 229,kjifb | 41 |
| $Cs_6Na_8Ga_{14}Si_{34}O_{96}$ | *cI*208 | 230,hgfb | 8 |
| $Cs_3Na_{8.5}H_{0.5}Al_{12}Si_{12}O_{48}$ | *cP*95 | 221,mkjihgc | 393 |
| $Cs_3Na_8HAl_{12}Si_{12}O_{48}\cdot 6Ar$ | *cP*115 | 221,mkji$^2$hg$^2$c | 417 |
| $Cs_3Na_8HAl_{12}Si_{12}O_{48}\cdot 22H_2O$ | *cP*147 | 221,m$^2$lkihg$^3$c | 439 |
| $Cs_3Na_8HAl_{12}Si_{12}O_{48}\cdot 5Kr$ | *cP*111 | 221,mkjihg$^3$c | 411 |
| $Cs_3Na_8HAl_{12}Si_{12}O_{48}\cdot 2.5Xe$ | *cP*104 | 221,mkjihg$^2$ca | 403 |
| $Cs_3Na_8HAl_{12}Si_{12}O_{48}\cdot 5.25Xe$ | *cP*120 | 221,mkjihg$^4$ca | 424 |
| $Cs_8Na_{16}Si_{136}$ | *cF*160 | 227,gecba | 107 |
| $CsNbN_2$ | *cF*32 | 227,cba | 70 |
| $CsNd(PO_3)_4$ β | *cI*220 | 220,e$^4$ca | 481 |
| $Cs_7(NpO_2)_3Cl_{12}$ | *cI*112 | 220,edcba | 473 |
| $Cs_3P_{11}$ ht | *cF*188 | 225,khfcb | 268 |
| $Cs_3P_{8.33}$ β | *cF*548 | 225,lk$^2$jfecb | 298 |
| $CsPF_6$ | *cF*152 | 225,khba | 261 |
| $Cs_3(P_7)_{0.67}(P_{11})_{0.33}$ | *cF*592 | 225,lk$^2$jf$^2$e$^2$ | 301 |
| $Cs_{46}Pb_{37}Al_{88}Si_{104}O_{384}(OH)_{32}\cdot xH_2O$ | *cF*1632 | 227,i$^5$hg$^4$e$^6$ | 175 |
| $CsPbCl_3$ ht | *cP*14 | 221,hba | 356 |
| $CsPbCl_3$ ht | *cP*19 | 221,jfa | 362 |
| $Cs_6[(ReI)_6S_8]I_2$ | *cF*112 | 225,fe$^2$dc | 238 |
| $Cs_8Sn_{44}$ | *cP*54 | 223,kidca | 329 |
| $Cs_8Sn_{44}$ | *cP*78 | 223,k$^2$idca | 336 |
| $CsTaN_2$ | *cF*112 | 227,hba | 93 |
| $CsTi_2As_3O_{12}$ | *cI*608 | 230,h$^5$g$^2$ba | 13 |
| $CsTiAsO_5$ ht | *cF*552 | 227,i$^2$hfcb | 130 |
| $CsTiPO_5$ | *cF*168 | 227,hfcb | 110 |
| $CsTiSi_2O_{6.5}$ | *cI*352 | 230,h$^3$gb | 12 |
| $Cs_9Tl_3Al_{12}Si_{12}O_{48}$ | *cP*129 | 221,mlkihg$^3$fc | 430 |
| $CsVTeO_6$ | *cF*552 | 227,i$^2$hfcb | 130 |
| $Cs_6Zn_5(MoO_4)_8$ | *cI*104 | 220,ec$^2$ba | 472 |
| Cu | *cF*4 | 225,a | 198 |
| $Cu_{28}Al_{56}Si_{136}O_{384}$ | *cF*976 | 227,i$^2$hg$^3$e$^6$c | 167 |
| $Cu_{28}Al_{56}Si_{136}O_{384}\cdot xH_2O$ | *cF*1256 | 227,i$^3$hg$^5$e$^3$a | 172 |
| $Cu_8Al_{12}Si_{12}O_{48}(OH)_{0.5}\cdot xH_2O$ | *cP*115 | 221,mkjihg$^3$ea | 418 |
| $Cu_8Al_{12}Si_{12}O_{48}(OH)_4\cdot xH_2O$ | *cP*112 | 221,mkji$^2$hg$^2$ | 414 |

| structure type | Pearson symbol | space group number, Wyckoff sequence | page |
|---|---|---|---|
| $Cu_8Al_{12}Si_{12}O_{48}(OH)\cdot xH_2O$ | *cP*124 | 221,mkjihg$^5$ | 427 |
| $Cu_3As$ α | *cI*64 | 220,ec | 470 |
| $Cu_3Au$ | *cP*4 | 221,ca | 344 |
| $CuBiI_4$ | *cF*112 | 227,fecba | 89 |
| $Cu_9BiS_6$ | *cF*72 | 225,f$^2$ba | 225 |
| $Cu_2Cr_2Se_4$ | *cF*200 | 227,hfecb | 115 |
| $Cu_{1.5}Cr_2Se_3Br$ | *cF*152 | 227,hecb | 106 |
| $Cu_{1.1}Cr_{1.3}Sn_{0.7}S_{3.9}$ | *cF*72 | 227,edca | 76 |
| $Cu_2Cr_2Te_4$ | *cF*104 | 227,fecb | 88 |
| $Cu_2Fe(CN)_6\cdot xH_2O$ | *cF*64 | 225,e$^2$cba | 218 |
| $Cu_8[Fe(NH_3)_6]Sb_3S_{13}$ | *cF*248 | 219,hfe$^2$cba | 491 |
| $Cu_5FeS_4$ ht2 | *cF*196 | 225,la | 271 |
| CuI α | *cF*44 | 225,fca | 209 |
| $Cu_6InO_8Cl$ | *cF*64 | 225,fdba | 221 |
| $CuIn_2Se_3I$ hp2 | *cF*112 | 227,fecba | 89 |
| $Cu_2MnCl_4$ | *cF*40 | 225,fba | 208 |
| $Cu_2MnCl_4$ | *cF*48 | 225,fcba | 211 |
| $Cu_3N$ | *cP*4 | 221,da | 344 |
| $Cu_{24}Na_5H_{17}Cl_{15}Si_{137}Al_{55}O_{384}$ | *cF*720 | 227,ihg$^4$ec | 152 |
| $Cu_2O$ | *cP*6 | 224,ba | 311 |
| $Cu_{7.6}O_8(NO_3)$ | *cF*204 | 225,jfe$^2$da | 274 |
| $Cu_6PbO_8$ | *cF*60 | 225,edca | 216 |
| $Cu_6PbO_{8-x}(Cl,Br)_{2x}$ | *cF*64 | 225,fdba | 221 |
| $CuPt_7$ | *cF*32 | 225,dba | 202 |
| $Cu_9S_2$ ht | *cF*36 | 225,eca | 203 |
| $Cu_9S_5$ ht | *cF*44 | 225,fca | 209 |
| $Cu_3SbS_4$ form II | *cF*64 | 225,fdc | 221 |
| $Cu_2Se$ α | *cF*44 | 225,fca | 209 |
| $Cu_2Se$ α | *cF*48 | 225,fcba | 210 |
| $Cu_2Se$ α | *cF*68 | 225,f$^2$b | 222 |
| $Cu_{15}Si_4$ | *cI*76 | 220,eca | 470 |
| $Cu_{9.1}TeSb_3$ | *cP*32 | 223,kca | 325 |
| $Cu_2Th_4(MoO_4)_9$ | *cI*244 | 220,e$^4$dca | 482 |
| $Cu_6YO_8Cl$ | *cF*84 | 225,feda | 228 |
| $D0_3$ | *cF*16 | 225,cba | 200 |
| $D0_9$ | *cP*4 | 221,da | 344 |
| $D2_1$ | *cP*7 | 221,fa | 350 |
| $D2_3$ | *cF*112 | 226,iba | 179 |
| $D2_e$ | *cP*36 | 221,jigca | 368 |
| $D2_f$ | *cF*52 | 225,ia | 212 |
| $D5_4$ | *cF*80 | 227,fe | 79 |
| $D5_5$ | *cP*10 | 224,db | 311 |
| $D5_c$ | *cI*40 | 220,dc | 468 |
| $D7_2$ | *cF*56 | 227,ecb | 71 |
| $D7_3$ | *cI*28 | 220,ca | 467 |
| $D8_4$ | *cF*116 | 225,hfeca | 245 |
| $D8_6$ | *cI*76 | 220,eca | 470 |
| $D8_9$ | *cF*68 | 225,feca | 223 |
| $D8_a$ | *cF*116 | 225,f$^2$eda | 243 |

| structure type | Pearson symbol | space group number, Wyckoff sequence | page |
|---|---|---|---|
| $H4_{16}$ | *cP*116 | 224,k$^4$edba | 319 |
| $H4_{21}$ | *cF*656 | 227,g$^5$f$^2$e$^2$ba | 137 |
| $H5_8$ | *cF*72 | 225,fecba | 226 |
| $H6_4$ | *cF*132 | 225,keca | 253 |
| $H_{26}Ag_{70}Al_{96}Si_{96}O_{384}$ | *cF*856 | 226,ji$^5$g$^2$eb | 185 |
| $H_{2.2}Ag_{9.8}Al_{12}Si_{12}O_{48}\cdot 6Br_2$ | *cP*196 | 221,m$^2$lk$^3$j$^2$hg$^2$ | 455 |
| $H_{2.25}Ag_{12}Al_{12}Si_{12}O_{48}Cl_{2.25}\cdot 6Cl_2$ | *cP*180 | 221,mlk$^3$jihg$^3$ | 451 |
| $H_{22}Ag_{20}(ClO_4)_4O_{33}$ | *cF*1224 | 227,i$^2$hg$^6$fe$^3$cb | 171 |
| $H_{22}Ag_{18}Hg_2(ClO_4)_4O_{33}$ | *cF*840 | 227,i$^2$hg$^2$fe$^3$cb | 162 |
| $H_{105}Al_9Si_{151}O_{368}$ | *cF*608 | 227,ihg$^3$e | 132 |
| $H_{12}Al_{12}Si_{36}O_{96}$ ht | *cI*144 | 229,kji | 38 |
| HCl form I | *cF*52 | 225,ha | 212 |
| $H_{9.3}La_{15.9}Al_{57}Si_{135}O_{384}\cdot 1.4H_2O$ | *cF*704 | 227,ihg$^3$e$^4$ | 149 |
| $H_{92}La_{38}Al_{92}Si_{100}O_{384}O_{48}(OH)_{18}\cdot xH_2O$ | *cF*768 | 227,ihg$^4$e$^2$dc | 155 |
| $H_{60}Na_4Cu_{12}Al_{88}Si_{104}O_{384}\cdot 48NH_3\cdot 40H_2O$ | *cF*784 | 227,ihg$^4$fe$^2$ | 158 |
| $H_2Na_3Ni_{3.5}Al_{12}Si_{12}O_{48}\cdot 40H_2O$ | *cP*269 | 221,nm$^4$lkj$^2$i$^2$hg$^2$b | 462 |
| $H_{10}Ni_{24}Al_{58}Si_{134}O_{384}\cdot xH_2O$ | *cF*752 | 227,ihg$^3$e$^5$c | 154 |
| $H_2O$ form I cubic | *cF*40 | 227,ea | 70 |
| $H_2O$ form VII | *cP*10 | 224,ea | 312 |
| $H_2O$ form VII | *cP*20 | 224,ge | 313 |
| $(H_3O)_{28}La_{38}Al_{92}Si_{100}O_{384}(OH)_{50}\cdot 64H_2O$ | *cF*1176 | 227,i$^2$hg$^5$e$^6$cb | 169 |
| $(H_3O)_3[PW_{12}O_{40}]$ | *cP*112 | 224,k$^4$eda | 318 |
| $(H_3O)YbF_{10}\cdot H_2O$ | *cF*272 | 227,hf$^2$e$^2$c | 121 |
| $(H_3O)_5[(Zr_6BCl_{12})Cl_6]\cdot 19H_2O$ | *cI*98 | 229,khe$^2$a | 34 |
| $HPF_6\cdot 6H_2O$ | *cI*110 | 229,lda | 36 |
| $HPF_6\cdot 7.67H_2O$ | *cP*112 | 223,lkigdc | 337 |
| $HPF_6\cdot 5H_2O\cdot HF$ | *cI*62 | 229,kda | 33 |
| $H_3[PMo_{12}O_{40}]\cdot 30H_2O$ | *cF*472 | 227,g$^4$fea | 128 |
| $H_3[PW_{12}O_{40}]\cdot 29H_2O$ | *cF*656 | 227,g$^5$f$^2$e$^2$ba | 137 |
| $H_3[PW_{12}O_{40}]\cdot 30H_2O$ | *cF*472 | 227,g$^4$fea | 128 |
| $H_3[PW_{12}O_{40}]\cdot 5H_2O$ | *cP*116 | 224,k$^4$edba | 319 |
| $H_3[PW_{12}O_{40}]\cdot 6H_2O$ rt | *cP*130 | 224,k$^4$hea | 319 |
| $HSbO_3\cdot 0.5H_2O$ | *cF*128 | 227,fe$^2$d | 101 |
| $H_2[Ta_6Cl_{18}]\cdot 6H_2O$ | *cF*192 | 227,gf$^2$ | 114 |
| $HTaWO_6$ | *cF*64 | 227,fc | 74 |
| $HTaWO_6\cdot H_2O$ | *cF*96 | 227,fec | 86 |
| $HTl_2Ag_{10}Al_{12}Si_{12}O_{48}$ | *cP*122 | 221,m$^2$ki$^2$hge | 424 |
| $HTl_3Ag_9Al_{12}Si_{12}O_{48}$ | *cP*106 | 221,mki$^2$hg$^2$e | 404 |
| $HTl_5Ag_7Al_{12}Si_{12}O_{48}$ | *cP*126 | 221,mk$^2$ihg$^3$e | 427 |
| $HTl_{5.5}Ag_{6.5}Al_{12}Si_{12}O_{48}$ | *cP*138 | 221,mlki$^2$hg$^3$e | 434 |
| Heusler phase | *cF*16 | 225,cba | 200 |
| $Hf_2FeH_3$ | *cF*224 | 227,gfe$^2$c | 117 |
| $Hf_2FeH_5$ | *cF*512 | 227,ig$^2$fe$^2$c | 128 |
| $Hf_6Ni_7Al_{16}$ | *cF*116 | 225,f$^2$eda | 244 |
| $HfV_2H_4$ ht | *cF*152 | 227,gecb | 105 |
| $Hg_6O(OH)Cl_3$ | *cI*176 | 230,hge | 6 |
| $Hg_3S_2Cl_2$ β | *cP*224 | 223,lk$^4$jifedcba | 341 |
| $Hg_3TeO_6$ | *cI*160 | 230,hga | 5 |
| $Ho_6Fe_{23}H_{1.5}$ | *cF*152 | 225,f$^3$edba | 260 |

| structure type | Pearson symbol | space group number, Wyckoff sequence | page |
|---|---|---|---|
| $Ho_6Fe_{23}H_{15.7}$ | *cF*436 | 225,kj$^2$f$^3$eda | 293 |
| $Ho_6Fe_{23}H_{8.2}$ | *cF*244 | 225,kf$^3$eda | 279 |
| $In_{87}Al_{92}Si_{100}O_{384}$ | *cF*1256 | 227,i$^4$hg$^3$e$^3$a | 173 |
| $In_8Al_{12}Si_{12}O_{48}{\cdot}In_{0.75}(S_2)$ | *cP*225 | 221,n$^2$m$^2$kihg$^4$a | 460 |
| $In_3P_2O_8$ | *cI*104 | 220,edc$^2$ | 473 |
| $Ir_3Ge_7$ | *cI*40 | 229,fed | 26 |
| $Ir_3Sn_7$ | *cI*40 | 229,fed | 26 |
| $J1_1$ | *cF*36 | 225,eca | 204 |
| $J2_1$ | *cF*40 | 225,ecba | 206 |
| $J2_3$ | *cI*136 | 230,hca | 2 |
| J phase | *cP*58 | 221,mhgfeba | 378 |
| $K7_4$ | *cI*140 | 220,ed$^2$c$^2$b | 476 |
| $K_{1.3}Ag_{10.7}Al_{12}Si_{12}O_{48}$ | *cP*110 | 221,mki$^3$hge | 410 |
| $K_{2.7}Ag_{9.3}Al_{12}Si_{12}O_{48}$ | *cP*98 | 221,mki$^2$hge | 395 |
| $K_9Ag_3Al_{12}Si_{12}O_{48}{\cdot}xH_2O$ | *cP*134 | 221,mkji$^2$hg$^4$e | 432 |
| $KAg_3S_2$ | *cF*96 | 227,fec | 86 |
| $KAlSi_2O_6$ ht | *cI*160 | 230,hgb | 5 |
| $K_{11.5}Al_{11.5}Si_{12.5}O_{48}$ | *cP*118 | 221,mkji$^2$hg$^2$e | 420 |
| $K_{12}Al_{12}Si_{12}O_{48}$ | *cP*116 | 221,mki$^2$hg$^4$ | 419 |
| $K_{12.5}Al_{12}Si_{12}O_{48}$ | *cP*112 | 221,mkji$^2$hg$^2$ | 414 |
| $K_{13}Al_{12}Si_{12}O_{48}$ | *cP*103 | 221,mkjihg$^2$c | 398 |
| $K_{13}Al_{12}Si_{12}O_{48}$ | *cP*118 | 221,mkji$^2$hg$^2$e | 420 |
| $K_{22.4}Al_{22.4}Si_{73.6}O_{192}$ | *cI*336 | 229,lk$^2$jifedc | 49 |
| $K_{23}Al_{23}Si_{25}O_{96}$ | *cF*944 | 226,ji$^5$hg$^2$e | 189 |
| $K_{92}Al_{92}Si_{100}O_{384}$ | *cF*1056 | 227,ihg$^6$fe$^4$c | 168 |
| $K_{120}Al_{96}Si_{96}O_{384}$ | *cF*776 | 225,lk$^3$jhf$^4$e | 304 |
| $K_{136}Al_{96}Si_{96}O_{384}$ | *cF*784 | 225,lk$^4$jhf$^2$ | 305 |
| $K_{12}Al_{12}Si_{12}O_{48}{\cdot}20H_2O$ | *cP*148 | 221,m$^3$ljihg$^2$ | 441 |
| $K_2B_6H_6$ | *cF*56 | 225,e$^2$c | 214 |
| $KBSi_2O_6$ | *cI*160 | 220,e$^3$c | 478 |
| $K_6Ba_2CaU_6O_{24}$ | *cI*40 | 229,edcba | 25 |
| $K_2BaNi(NO_2)_6$ | *cF*136 | 225,jecba | 256 |
| $(K,Bi)_{1.5}Bi_2O_4{\cdot}H_2O$ | *cF*120 | 227,fedca | 97 |
| $(K,Bi)_{1.5}Bi_2(O,OH)_6(OH)_{0.8}$ | *cF*112 | 227,fedc | 92 |
| $KBi_6O_9I$ | *cI*272 | 230,hg$^2$fba | 9 |
| $K_9BiU_6O_{24}$ | *cP*40 | 221,hgfedcba | 370 |
| $K_3C_{60}$ | *cF*492 | 225,l$^2$jca | 296 |
| KCN form III | *cP*9 | 221,ga | 352 |
| KCN rt | *cF*28 | 225,ea | 201 |
| $K_2Cd(CN)_4$ | *cF*88 | 227,e$^2$cb | 80 |
| $KCo[Co(CN)_6]{\cdot}10H_2O$ | *cF*120 | 225,fe$^3$cba | 251 |
| $K_{7.77}[CoW_{12}O_{40}]{\cdot}9.7H_2O$ | *cP*127 | 221,m$^4$jgfdba | 428 |
| $KCu[Co(CN)_6]{\cdot}9H_2O$ | *cF*120 | 225,fe$^3$cba | 251 |
| $K_2Cu[Fe(CN)_6]$ | *cF*64 | 225,e$^2$cba | 219 |
| $K_2Cu[Fe(CN)_6]$ | *cF*112 | 225,jcba | 242 |
| $K_6Cu_{12}U_2S_{15}$ | *cI*280 | 230,h$^2$gca | 9 |
| $K_2Fe_8Al(SO_4)_{12}{\cdot}18H_2O$ | *cF*1712 | 228,h$^8$gcba | 66 |
| $K_3FeF_6$ | *cF*208 | 225,lcba | 276 |
| $K_8Ge_{46}$ | *cP*54 | 223,kidca | 329 |

| structure type | Pearson symbol | space group number, Wyckoff sequence | page |
|---|---|---|---|
| $K_3[H_{12}(AsO)_2AsV_{12}O_{40}]\cdot 12H_2O$ | *cP*84 | 221,mji$^2$gfeda | 386 |
| $K_5H(CN_2)_3$ | *cI*28 | 229,ecba | 20 |
| $K_6H[In(NO_3)_4(H_2O)_2]_3(NO_3)_4$ | *cI*316 | 220,e$^5$d$^2$ca | 483 |
| $K_8H_4Nb_4W_8O_{36}(O_2)_4\cdot 18H_2O$ | *cP*65 | 221,mi$^2$gfd | 381 |
| $K_2(H_3O)[PMo_{12}O_{40}]$ | *cP*112 | 224,k$^4$eda | 318 |
| $K_6H_3[ZnW_{11}AlO_{40}]\cdot 9.5H_2O$ | *cF*644 | 225,lk$^3$hfe$^2$dca | 303 |
| $K_2Hg(CN)_4$ | *cF*88 | 227,e$^2$cb | 80 |
| $K_{17}In_{41}$ | *cF*464 | 227,g$^4$e$^2$ba | 125 |
| $K_8In_6Ge_{40}$ | *cP*54 | 223,kidca | 330 |
| $KInI_4$ | *cF*160 | 219,heda | 489 |
| $K_6LiFe_{23}S_{26}Cl$ | *cP*58 | 221,mhgfeba | 378 |
| $KMnF_3$ | *cP*14 | 221,hba | 356 |
| $K_7[Mo_6Se_8(CN)_6]\cdot 8H_2O$ | *cF*196 | 225,hf$^2$e$^3$ca | 269 |
| $K_3NO_3$ | *cP*58 | 221,necb | 379 |
| $KNO_2$ form I | *cF*104 | 225,kba | 237 |
| $KNO_2$ form I | *cF*132 | 225,kfb | 254 |
| $K_2NaAlF_6$ | *cF*40 | 225,ecba | 207 |
| $K_{60}Na_{36}Al_{95}Si_{97}O_{384}$ | *cF*896 | 226,ji$^5$hg$^2$ | 187 |
| $K_{36.5}Na_{19.5}Al_{56}Si_{136}O_{384}\cdot 15H_2O$ | *cF*880 | 227,ihg$^5$e$^3$c | 166 |
| $K_2NaC_{60}\cdot NH_3$ | *cF*552 | 225,l$^2$jf$^2$c | 299 |
| $K_{68}Na_{12}Ca_{36}Al_{152}Si_{520}O_{1344}\cdot 705H_2O$ | *cI*2556 | 229,l$^{14}$k$^{12}$j$^8$i$^2$h$^2$gf$^3$e$^3$ | 61 |
| $K_2NaCrF_6$ | *cF*40 | 225,ecba | 207 |
| $K_{29}NaHg_{48}$ | *cP*156 | 223,lk$^3$idcba | 340 |
| $K_3Na_{26}In_{48}$ | *cP*154 | 223,lk$^3$idcb | 340 |
| $K_{5.5}Na_{1.5}[PW_{10}Cu_2(H_2O)_2O_{38}]\cdot 13H_2O$ | *cF*620 | 225,k$^4$ihfe$^3$dca | 302 |
| $K_3NbOF_6$ | *cF*512 | 225,l$^2$f$^4$ | 297 |
| $KNbWO_6\cdot xH_2O$ | *cF*128 | 227,fe$^2$d | 100 |
| $KNi[Fe(CN)_6]$ | *cF*64 | 225,e$^2$cba | 219 |
| $KPF_6$ | *cF*104 | 225,kba | 238 |
| $K_6[PMo_3W_9O_{40}]\cdot 13H_2O$ | *cF*544 | 225,k$^4$hfe$^2$dc | 298 |
| $K_{0.33}Pb_{0.67}F_{1.67}$ | *cI*20 | 229,dba | 19 |
| $K_{19}Pb_8O_4(OH)_3$ | *cF*136 | 225,hfe$^2$ba | 254 |
| $K_2PtCl_6$ | *cF*36 | 225,eca | 204 |
| $K_2PtH_6$ | *cF*36 | 225,eca | 204 |
| $K_3Rh(NO_2)_6$ | *cF*88 | 225,hecba | 232 |
| $K_3(SO_4)F$ α | *cP*13 | 221,gcba | 355 |
| $K_{0.51}Sb_{2.67}O_{6.26}$ | *cF*296 | 227,g$^2$feda | 121 |
| $K_8Si_{46}$ | *cP*54 | 223,kidca | 329 |
| $K_8[SiNb_4W_8O_{40}]\cdot 12H_2O$ | *cP*78 | 221,mji$^2$gfda | 383 |
| $(K,Sr,Na,Ca,H_2O)_{2-x}(Nb,Ti)_2(O,OH)_6$ | *cF*320 | 227,igdc | 123 |
| $KTaO_3$ | *cP*15 | 221,geb | 357 |
| $KTaO_3$:Li | *cP*11 | 221,ecba | 354 |
| $KTaO_3$:Li | *cP*18 | 221,geca | 361 |
| $KTaWO_6\cdot H_2O$ | *cF*80 | 227,fdc | 79 |
| $K_2TeBr_6$ α | *cF*36 | 225,eca | 204 |
| $K_3Ti(O_2)F_5$ | *cF*348 | 225,kj$^2$fea | 291 |
| $KTlBr_4\cdot 2H_2O$ | *cF*256 | 219,h$^2$eda | 492 |
| $KTlBr_4\cdot 2H_2O$ | *cF*560 | 226,j$^2$ifcb | 180 |
| $K_3UF_7$ cubic | *cF*520 | 225,l$^2$jecba | 297 |

| structure type | Pearson symbol | space group number, Wyckoff sequence | page |
|---|---|---|---|
| $Li_6NBr_3$ form I | *cF*112 | 225,jcba | 242 |
| $Li_6NBr_3$ form I | *cF*592 | 225,$l^3$cba | 300 |
| $Li_5NCl_2$ form I | *cF*116 | 225,g$f^2$a | 244 |
| $Li{\cdot}4NH_3$ | *cI*80 | 220,e$c^2$ | 471 |
| $Li_7N_2I$ | *cF*80 | 227,fcba | 78 |
| $Li_3Ni_{20}B_6$ | *cF*116 | 225,hfeca | 246 |
| $Li_2O$ | *cF*12 | 225,ca | 199 |
| $Li_{10}P_4N_{10}$ | *cF*216 | 227,$f^2e^3$da | 116 |
| $Li_3Pb$ | *cF*16 | 225,cba | 200 |
| $LiPt_7$ | *cF*32 | 225,dba | 202 |
| $LiRhO_2$ β | *cF*64 | 227,edc | 73 |
| $LiRuGa_2$ | *cF*16 | 225,cba | 200 |
| $LiTiO_2$ | *cF*64 | 227,edc | 73 |
| $Li_2Zr_6MnCl_{15}$ | *cI*56 | 229,hedba | 32 |
| $Mg_{28}Al_{45}$ | *cF*1832 | 227,ihg$^{14}$f$e^4$da | 176 |
| $MgAl_2O_4$ | *cF*56 | 227,ecb | 72 |
| $Mg_3B_7O_{13}Cl$ cubic | *cF*192 | 219,hedcba | 489 |
| $Mg_3Cr_2Al_{18}$ | *cF*184 | 227,gfdca | 113 |
| $MgCu_2$ | *cF*24 | 227,cb | 69 |
| $Mg_6Cu_{16}Si_7$ | *cF*116 | 225,$f^2$eda | 244 |
| $MgFe_2O_4$ | *cF*56 | 227,ecb | 72 |
| $Mg_{0.04}Fe_{2.96}O_4$ | *cF*200 | 227,hfecb | 115 |
| $Mg(H_2PO_2)_2{\cdot}6H_2O$ | *cF*132 | 225,keca | 253 |
| $Mg_3Mn_2Al_{18}$ | *cF*184 | 227,gfdca | 113 |
| $Mg_6MnO_8$ | *cF*60 | 225,edca | 216 |
| $Mg_3NF_3$ | *cP*7 | 221,dca | 348 |
| $Mg_3Ni_{20}B_6$ | *cF*116 | 225,hfeca | 246 |
| $Mg_2NiH_4$ ht | *cF*84 | 225,heca | 229 |
| $Mg_3Ni_{20}P_6$ | *cF*116 | 225,hfeca | 246 |
| "$Mg_3P_2$" | *cP*10 | 224,db | 311 |
| $Mg_3Pt_2Al$ | *cF*96 | 227,fec | 85 |
| $Mg_2RhH_{1.1}$ | *cF*152 | 227,fe$^2$dca | 105 |
| $Mg_2Si$ | *cF*12 | 225,ca | 199 |
| $Mg_xTiS_2$ | *cF*64 | 227,edc | 73 |
| $Mg_{0.125}Zr_{0.875}O_{1.825}$ | *cF*52 | 225,ga | 211 |
| $Mn_3AlC$ | *cP*5 | 221,dba | 345 |
| $Mn_3[Co(CN)_6]_2{\cdot}xH_2O$ | *cF*440 | 225,$l^2e^2$ba | 294 |
| $Mn_3[Co(CN)_6]_2{\cdot}12H_2O$ | *cF*120 | 225,fe$^3$cba | 250 |
| MnCoSb | *cF*120 | 227,fedca | 96 |
| $MnCu_2Al$ | *cF*16 | 225,cba | 200 |
| $Mn_3Cu_4Bi_4$ | *cF*88 | 225,fedc | 231 |
| $(Mn,Mg,Cu)_9MnAs_6O_{18}(OH,Cl)$ | *cI*696 | 230,$h^5g^4$d | 14 |
| $Mn_3[Mn(CN)_6]_2{\cdot}15H_2O$ | *cF*208 | 225,kfe$^3$ba | 275 |
| $Mn_3Ni_2Si$ | *cF*96 | 227,fec | 85 |
| $Mn_8O_{10}Cl_3$ ht | *cF*168 | 225,hgfecba | 265 |
| $MoBe_{22}$ | *cF*184 | 227,hfdca | 114 |
| $Mo_3N_2$ | *cP*8 | 221,dcba | 350 |
| $Mo_6Ni_6C$ | *cF*104 | 227,fecb | 87 |
| $Mo_7Zn_{40}Sn_{12}$ | *cF*944 | 226,$j^2i^3$hgfeba | 188 |

| structure type | Pearson symbol | space group number, Wyckoff sequence | page |
|---|---|---|---|
| $Na_{93}Al_{93}Si_{99}O_{384}$ ht | *cF*832 | 226,ji$^5$hg | 183 |
| $Na_{30}Al_{30}Si_{66}O_{192}\cdot 1.7BaCl_2\cdot 72H_2O$ | *cI*446 | 229,lk$^2$j$^3$if$^2$edb | 57 |
| $Na_{12}Al_{12}Si_{12}O_{24}\cdot 6Br_2$ | *cP*128 | 221,nmkihg | 429 |
| $NaAlSi_2O_6\cdot H_2O$ | *cI*184 | 230,hgcb | 6 |
| $Na_{12}Al_{12}Si_{12}O_{48}\cdot 27H_2O$ | *cF*1864 | 226,j$^7$i$^4$g$^2$a | 194 |
| $Na_{12}Al_{12}Si_{12}O_{48}\cdot 27H_2O$ | *cP*92 | 221,mki$^2$hg | 392 |
| $Na_{15}Al_{15}Si_{33}O_{96}\cdot 98H_2O$ | *cI*304 | 229,lk$^2$jif | 46 |
| $Na_{30}Al_{30}Si_{66}O_{192}\cdot xH_2O$ | *cI*288 | 229,lk$^2$ji | 45 |
| $Na_{51}Al_{51}Si_{141}O_{384}\cdot xH_2O$ | *cF*800 | 227,ihg$^4$e$^4$ | 159 |
| $Na_{56}Al_{56}Si_{136}O_{384}\cdot 19H_2O$ | *cF*880 | 227,ihg$^5$e$^3$c | 165 |
| $Na_{76}Al_{76}Si_{116}O_{384}\cdot xH_2O$ | *cF*624 | 227,ihg$^3$ec | 134 |
| $Na_{81}Al_{81}Si_{111}O_{384}\cdot 240H_2O$ | *cF*1856 | 227,i$^4$hg$^8$fe$^5$c | 177 |
| $Na_{81}Al_{81}Si_{111}O_{384}\cdot 240H_2O$ | *cF*1872 | 227,i$^4$hg$^9$e$^4$c | 178 |
| $Na_{12}Al_{12}Si_{12}O_{48}\cdot 12H_2S$ | *cP*160 | 221,m$^2$lkj$^2$ihg$^2$ | 445 |
| $Na_{11}Al_{11}Si_{13}O_{48}\cdot 32NH_3$ | *cP*150 | 221,m$^2$lkihg$^3$e | 443 |
| $Na_{12}Al_{12}Si_{12}O_{48}\cdot 8NH_3$ | *cP*116 | 221,m$^2$kjihg | 418 |
| $Na_{12}Al_{12}Si_{12}O_{48}\cdot NaAlO_2\cdot 29H_2O$ | *cP*72 | 221,mkih | 382 |
| $Na_{12}Al_{12}Si_{12}O_{48}\cdot 10NaNO_3\cdot 6.6H_2O$ | *cP*278 | 221,m$^4$lk$^2$jihg$^6$f$^2$e$^2$ba | 463 |
| $Na_{12}Al_{12}Si_{12}O_{48}\cdot 9.3NaNO_3\cdot 6.7H_2O$ | *cP*187 | 221,m$^3$lj$^2$i$^2$hg$^3$ea | 453 |
| $Na_5Al_{15}Si_{177}O_{363}(OH)_{32}$ | *cF*656 | 227,ihg$^3$e$^2$d | 140 |
| $Na_{11}Al_{11}Si_{13}O_{48}\cdot 2S_8$ | *cP*140 | 221,m$^2$lkj$^2$hg | 436 |
| $Na_{12}Al_{12}Si_{12}O_{48}\cdot 7Xe$ | *cP*201 | 221,nm$^3$kji$^2$hga | 457 |
| $Na_7As_2O_8F\cdot 19H_2O$ | *cF*1312 | 228,h$^6$edca | 65 |
| $Na_{6.6}Ba_{1.2}Ag_3Al_{12}Si_{12}O_{48}\cdot xH_2O$ | *cP*108 | 221,mki$^2$hg$^3$ | 408 |
| $Na_2Ba_{41}Al_{84}Si_{108}O_{384}\cdot 51.3H_2O$ | *cF*816 | 227,ihg$^4$e$^4$c | 161 |
| $NaBa_2(CN_2)(CN)_3$ lt | *cF*248 | 227,gfe$^2$dcb | 120 |
| $NaBa_2(CN_2)(CN)_3$ rt | *cF*240 | 227,gfe$^2$dc | 119 |
| $Na_{14}Ba_{14}CaN_6$ | *cF*140 | 225,f$^2$e$^2$da | 257 |
| $NaBaLiNiF_6$ | *cF*40 | 225,dcba | 206 |
| $Na_{16}Ba_6N$ | *cI*46 | 229,heca | 30 |
| $Na_3Bi_5(PO_4)_6$ | *cI*92 | 220,ec$^2$a | 472 |
| $NaBiS_2$ | *cF*8 | 225,ba | 198 |
| $Na_2C_{60}$ | *cF*12 | 225,ca | 199 |
| $Na_3C_{60}$ | *cF*16 | 225,cba | 200 |
| $Na_6C_{60}$ | *cF*44 | 225,fca | 209 |
| $Na_4Ca_4Al_7F_{33}$ | *cI*136 | 229,k$^2$edcba | 37 |
| $Na_{16}Ca_{40}Al_{96}Si_{96}O_{384}$ | *cF*704 | 226,ji$^4$g$^2$ | 181 |
| $Na_4Ca_4Al_{12}Si_{12}O_{48}$ | *cP*88 | 221,mkihg$^2$ | 388 |
| $Na_4Ca_4Al_{12}Si_{12}O_{48}$ | *cP*89 | 221,mkihg$^2$a | 389 |
| $Na_4Ca_4Al_{12}Si_{12}O_{48}$ | *cP*103 | 221,mki$^2$hg$^2$c | 398 |
| $Na_4Ca_4Al_{12}Si_{12}O_{48}$ | *cP*104 | 221,mkihg$^4$ | 401 |
| $Na_{0.4}Ca_{5.3}Al_{11}Si_{13}O_{48}\cdot(Al_{0.3}O_{0.6}H_{0.3})$ | *cP*97 | 221,mkihg$^3$a | 394 |
| $Na_4Ca_4Al_{12}Si_{12}O_{48}\cdot 6Br_2$ | *cP*136 | 221,ml$^2$kihg$^2$ | 433 |
| $Na_{16}Ca_{40}Al_{48}Si_{96}O_{384}\cdot 40CO\cdot 6.2[AlO(OH)_3]$ | *cF*1032 | 226,j$^2$i$^4$g$^4$b | 192 |
| $Na_4Ca_4Al_{12}Si_{12}O_{48}\cdot xH_2O$ | *cP*80 | 221,mkihg | 384 |
| $Na_4Ca_4Al_{12}Si_{12}O_{48}\cdot xH_2O$ | *cP*97 | 221,mkihg$^3$a | 394 |
| $Na_4Ca_4Al_{12}Si_{12}O_{48}\cdot xH_2O$ | *cP*106 | 221,mkihg$^4$ba | 406 |
| $Na_4Ca_4Al_{12}Si_{12}O_{48}\cdot xH_2O$ | *cP*119 | 221,mkihg$^5$ea | 421 |

| structure type | Pearson symbol | space group number, Wyckoff sequence | page |
|---|---|---|---|
| $Na_{28.8}Ca_{14.4}Al_{57.6}Si_{134.4}O_{384}{\cdot}263H_2O$ | *cF*672 | 227,ihg$^3$e$^3$ | 142 |
| $Na_{29}Ca_{14.5}Al_{58}Si_{134}O_{384}{\cdot}267H_2O$ | *cF*640 | 227,ihg$^3$e$^2$ | 134 |
| $Na_4Ca_4Al_{12}Si_{12}O_{48}{\cdot}5.65I_2$ | *cP*128 | 221,ml$^2$kihg | 429 |
| $NaCaNb_2O_6F$ | *cF*88 | 227,fdca | 82 |
| $NaCd_2$ | *cF*1192 | 227,ihg$^7$fe$^5$cb | 170 |
| $Na_{35}Cd_{24}Ga_{56}$ | *cF*464 | 227,g$^4$e$^2$ba | 126 |
| $Na_{22}Ce_{12}Al_{58}Si_{134}O_{384}{\cdot}270H_2O$ | *cF*704 | 227,ihg$^3$e$^4$ | 148 |
| $Na_{23}Ce_{12}Al_{59}Si_{133}O_{384}{\cdot}xH_2O$ | *cF*688 | 227,ihg$^3$e$^3$c | 147 |
| NaCl | *cF*8 | 225,ba | 198 |
| $NaClO_4$ ht | *cF*104 | 225,jba | 236 |
| $NaClO_4$ ht | *cF*264 | 225,kjf$^2$ba | 281 |
| $Na_4Co_4Al_{12}Si_{12}O_{48}{\cdot}4CO$ | *cP*104 | 221,mkihg$^4$ | 400 |
| $Na_{12}Co_{42}Al_{96}Si_{96}O_{384}{\cdot}12CO{\cdot}6Al(OH)_3$ | *cF*968 | 226,ji$^4$g$^6$b | 189 |
| $Na_4Co_4Al_{12}Si_{12}O_{48}{\cdot}4CS_2$ | *cP*196 | 221,nm$^2$lkj$^2$hg$^2$ | 455 |
| $Na_4Co_4Al_{12}Si_{12}O_{48}{\cdot}4Cl_2$ | *cP*148 | 221,mlk$^2$jh$^2$g$^2$ | 442 |
| $Na_4Co_4Al_{12}Si_{12}O_{48}{\cdot}35H_2O$ | *cP*391 | 221,n$^5$m$^3$kihg$^3$fa | 465 |
| $Na_4Co_4Al_{12}Si_{12}O_{48}{\cdot}11H_2S$ | *cP*134 | 221,m$^2$lkjhge | 431 |
| $Na_5Co_{3.5}Al_{12}Si_{12}O_{48}{\cdot}2.5I_2$ | *cP*148 | 221,ml$^2$ki$^2$hg$^2$ | 441 |
| $Na_4Co_4Al_{12}Si_{12}O_{48}{\cdot}2NO_2$ | *cP*144 | 221,m$^3$kihg$^3$ | 438 |
| $Na_4Co_4Al_{12}Si_{12}O_{48}{\cdot}3NO$ | *cP*140 | 221,m$^2$ki$^2$hg$^4$ | 435 |
| $Na_4Co_4Al_{12}Si_{12}O_{48}{\cdot}2S_8$ | *cP*144 | 221,m$^2$lkihg$^3$ | 438 |
| $Na_4[CoBr_3]_4Al_{12}Si_{12}O_{48}{\cdot}2Br_2$ | *cP*144 | 221,ml$^2$kihg$^3$ | 439 |
| $Na_{0.5}Eu_{5.75}Al_{12}Si_{12}O_{48}$ | *cP*103 | 221,mkjihg$^2$c | 399 |
| $Na_3Eu_{4.5}Al_{12}Si_{12}O_{50.75}$ | *cP*120 | 221,mkji$^2$hg$^3$ | 423 |
| $Na_2Eu_{5.5}Al_{12}Si_{12}O_{48}Cl_8$ | *cP*102 | 221,mkihg$^3$f | 397 |
| $Na_2Eu_5Al_{12}Si_{12}O_{48}{\cdot}21H_2O$ | *cP*208 | 221,nm$^4$kihg$^2$ | 457 |
| $Na_{6.6}Fe_{2.7}Al_{12}Si_{12}O_{48}{\cdot}xH_2O$ | *cP*161 | 221,m$^3$lkihg$^2$a | 446 |
| $Na_{17}Fe_{13}Al_{56}Si_{136}O_{384}{\cdot}41H_2O$ | *cF*688 | 227,ihg$^3$e$^3$c | 145 |
| $Na_{17}Ga_{29}In_{12}$ | *cF*464 | 227,g$^4$e$^2$ba | 127 |
| $Na_{57}Ga_{57}Si_{135}O_{384}$ | *cF*752 | 227,ihg$^4$e$^2$c | 154 |
| $Na_{72}Ga_{72}Si_{120}O_{384}$ | *cF*848 | 227,i$^2$hg$^3$e$^2$c | 163 |
| $Na_{85}Ga_{85}Si_{107}O_{384}$ | *cF*736 | 227,ihg$^4$e$^2$ | 153 |
| $Na_7Gd_{27}Al_{88}Si_{104}O_{384}{\cdot}xH_2O$ | *cF*960 | 227,i$^2$hg$^4$e$^3$ | 167 |
| $Na_6H_{3.33}Ag_{5.91}Al_{12}Si_{12}O_{48}$ | *cP*132 | 221,mlkjihg$^3$ | 430 |
| $Na_{7.4}H_{2.8}Ag_{3.6}Al_{12}Si_{12}O_{48}$ | *cP*172 | 221,m$^4$ljihg$^2$ | 449 |
| $Na_{21}H_{1.4}Al_{22.4}Si_{73.6}O_{192}$ | *cI*324 | 229,lk$^2$jifdc | 47 |
| $Na_3H_{53}Al_{56}Si_{136}O_{384}$ | *cF*592 | 227,ihg$^3$c | 131 |
| $Na_{85}H_{17}Al_{92}Si_{100}Te_5O_{384}$ | *cF*776 | 227,ihg$^4$e$^3$a | 157 |
| $NaH_{52}CaAl_{55}Si_{137}O_{384}$ | *cF*608 | 227,ihg$^3$e | 132 |
| $Na_{13}H_{40}CaAl_{55}Si_{137}O_{384}$ | *cF*624 | 227,ihg$^3$ec | 134 |
| $Na_{8.1}H_{23}Ce_{8.3}Al_{56}Si_{136}O_{384}$ | *cF*656 | 227,ihg$^3$e$^2$c | 139 |
| $Na_{8.1}H_{20.8}Ce_{8.3}Al_{56}Si_{136}O_{384}{\cdot}xH_2O$ | *cF*688 | 227,ihg$^3$e$^3$c | 146 |
| $Na_5H_{17}Cu_{24}Al_{55}Si_{137}O_{384}Cl_{15}{\cdot}xH_2O$ | *cF*832 | 227,ihg$^5$edc | 162 |
| $Na_{1.8}H_{45.5}La_{4.9}Al_{62}Si_{130}O_{384}{\cdot}xH_2O$ | *cF*648 | 227,ihg$^3$e$^2$a | 137 |
| $Na_{92.7}(H_3O)_{2.3}Al_{95}Si_{97}O_{384}{\cdot}250H_2O$ | *cF*2120 | 226,j$^7$i$^5$hg$^3$a | 197 |
| $Na_{92.7}(H_3O)_{2.3}Al_{95}Si_{97}O_{384}{\cdot}4.6H_2O$ | *cF*1600 | 226,j$^5$i$^5$hg | 193 |
| $Na_{11}H_{39}Pb_{26}Al_{55}Si_{137}S_{23.5}O_{384}$ | *cF*688 | 227,ihg$^3$e$^3$c | 145 |
| $Na_{9.3}H_{46.6}Pd_{13.7}Al_{55.9}Si_{136.1}O_{384}$ | *cF*688 | 227,ihg$^3$e$^3$c | 144 |
| $Na_{17}H_{30}Zn_{19.5}Al_{54}Si_{138}O_{384}(OH)_{32}$ | *cF*768 | 227,ihg$^3$e$^6$ | 155 |

| structure type | Pearson symbol | space group number, Wyckoff sequence | page |
|---|---|---|---|
| $Na_{26}In_4O_{19}$ | *cI*200 | 220,$e^3c^2ba$ | 480 |
| $Na_{2.1}La_{20.1}Al_{62}Si_{130}O_{384}\cdot xH_2O$ | *cF*648 | 227,$ihg^3e^2a$ | 136 |
| $Na_{13.4}La_{16.3}Al_{55}Si_{137}O_{384}[OH]_{7.3}.xH_2O$ | *cF*664 | 227,$ihg^3e^2ca$ | 140 |
| $Na_{5.2}Li_{46.0}H_{5.8}Al_{57}Si_{135}O_{384}$ | *cF*640 | 227,$ihg^3e^2$ | 134 |
| $NaLi_2Sb$ | *cF*16 | 225,cba | 200 |
| $Na_{64}Mg_{16}Al_{96}Si_{96}O_{384}\cdot 6H_2O$ | *cF*864 | 226,$ji^5g^3$ | 186 |
| $Na_3Mn_{4.5}Al_{12}Si_{12}O_{48}\cdot xH_2O$ | *cP*151 | 221,$ml^2kihg^3fa$ | 444 |
| $Na_{17.4}Mn_{19.3}Al_{56}Si_{136}O_{384}\cdot 5.1H_2O$ | *cF*688 | 227,$ihg^3e^3c$ | 144 |
| $Na_{17.4}Mn_{19.3}Al_{56}Si_{136}O_{384}\cdot xH_2O$ irradiated | *cF*672 | 227,$ihg^3e^3$ | 142 |
| $Na_3NO_3$ | *cP*16 | 221,$e^2cb$ | 358 |
| $Na_3NO_3$ | *cP*34 | 221,kecb | 367 |
| $Na_2Nb_7Br_4F_{17}$ | *cP*52 | 221,$j^2hfeca$ | 376 |
| $NaNb_6Cl_{15}$ rt | *cI*384 | 230,$h^3gf$ | 12 |
| $Na_2Nb_7Cl_{18}F_{13}$ | *cP*40 | 221,jhfeca | 371 |
| $NaNb_{1.25}F_6$ | *cF*56 | 225,edba | 215 |
| $Na_{16.9}Nd_{11}Al_{50}Si_{142}O_{384}\cdot xH_2O$ | *cF*1248 | 227,$i^4hg^3e^3$ | 172 |
| $Na_{20}Nd_{20}Al_{80}Si_{112}O_{384}\cdot xH_2O$ | *cF*1160 | 227,$i^2hg^5fe^4da$ | 169 |
| $Na_{40}Nd_{13.3}Al_{80}Si_{112}O_{384}\cdot xH_2O$ | *cF*1360 | 227,$i^2hg^8e^3c$ | 174 |
| $Na_7Ni_{30}Al_{55}Si_{137}O_{384}Cl_{12}$ | *cF*784 | 227,$ihg^4e^3c$ | 158 |
| $Na_7Ni_{30}Al_{55}Si_{137}O_{384}Cl_{12}\cdot xH_2O$ | *cF*848 | 227,$ihg^5e^2c$ | 164 |
| $Na_6Ni_3Al_{12}Si_{12}O_{48}\cdot xH_2O$ | *cP*216 | 221,$nm^3lkihg^3$ | 459 |
| $Na_{84.8}Ni_4Al_{92.8}Si_{99.2}O_{384}\cdot 212H_2O$ | *cF*1312 | 226,$j^3i^5g^4$ | 192 |
| $Na_3O(CN)$ | *cP*16 | 221,$e^2cb$ | 358 |
| $NaPF_6$ | *cF*200 | 225,lba | 273 |
| $Na_{10}[P_4(NH)_6N_4](NH_2)_6(NH_3)_{0.5}$ | *cF*292 | 225,$jgf^3e^2a$ | 285 |
| $Na_3PO_4$ form II | *cF*396 | 225,$lj^2ca$ | 291 |
| $Na_3PO_4$ form II | *cF*440 | 225,$lj^2ic$ | 294 |
| $Na_3PO_4$ form II | *cF*988 | 225,$l^5ea$ | 306 |
| $Na_3PO_4$ form II | *cF*1156 | 225,$l^6a$ | 308 |
| $Na_7P_2O_8F\cdot 19H_2O$ | *cF*1312 | 228,$h^6edca$ | 65 |
| $Na_{11}Pb_{26}Al_{55}Si_{137}O_{384}S_4$ | *cF*656 | 227,$ihg^3e^2c$ | 139 |
| $Na_{1.5}Pb_{0.75}PSe_4$ | *cI*128 | 220,$ed^2c^2$ | 474 |
| $NaPt_3O_4$ | *cP*16 | 223,eca | 323 |
| $Na_6(SO_4)_2ClF$ | *cF*72 | 225,fecba | 226 |
| $Na_6(SO_4)_2O$ | *cF*68 | 225,feca | 224 |
| $NaSbF_6$ | *cF*32 | 225,eba | 203 |
| $NaSbO_3$ | *cF*80 | 227,fdc | 78 |
| $Na_8Si_{46}$ | *cP*54 | 223,kidca | 329 |
| $Na_xSi_{136}$ | *cF*144 | 227,geba | 104 |
| $Na_xSi_{136}$ | *cF*160 | 227,gecba | 106 |
| $Na_8SnSb_4$ | *cF*104 | 227,feca | 87 |
| $NaSr_4(BN_2)_3$ | *cI*28 | 229,ecba | 21 |
| $Na_xTh_6FeBr_{15}$ | *cI*56 | 229,hedba | 32 |
| NaTl | *cF*16 | 227,ba | 67 |
| $Na_{32}Tl_{60}Al_{92}Si_{100}O_{384}$ | *cF*864 | 226,$ji^5g^3$ | 185 |
| $Na_3[VMo_{12}O_{40}]\cdot 19H_2O$ | *cF*600 | 225,$k^4ihfe^2dcba$ | 301 |
| $Na_{3.2}(V_5O_9)(PO_4)_2(OH)_{0.1}\cdot 8H_2O$ | *cI*430 | 229,$k^4j^2h^2f^2e^3dcb$ | 56 |
| $Na_{1.08}V_{0.43}Sb_{2.14}O_{6.84}$ | *cF*304 | 227,$g^2fedc$ | 123 |
| $Na_{0.75}WO_3$ | *cI*110 | 229,$k^2cb$ | 35 |

| structure type | Pearson symbol | space group number, Wyckoff sequence | page |
|---|---|---|---|
| $NaY_3F_{10}$ | *cP*16 | 221,gdcba | 359 |
| $NaZn_{13}$ | *cF*112 | 226,iba | 179 |
| $Na_2Zn_5Al_{12}Si_{12}O_{48}{\cdot}xH_2O$ | *cP*199 | 221,$m^2lk^2j^2hg^3e^3b$ | 456 |
| $Na_4Zn_4(P_4O_{12})_3$ | *cI*224 | 220,$e^4c^2$ | 482 |
| $Na_{21}Zn(SO_4)_{10}Cl_3$ | *cI*300 | 220,$e^4d^2c^3a$ | 483 |
| $Na_{21}Zn(SO_4)_{10}Cl_3$ | *cI*324 | 220,$e^5dc^3a$ | 484 |
| $Na_{0.5}Zr_6Cl_{15}C$ | *cI*400 | 230,$h^3g^2a$ | 13 |
| $Nb_{3.16}Al_{0.84}H_{2.52}$ | *cP*54 | 223,kidca | 331 |
| $Nb_3AuH_x$ | *cP*30 | 223,idca | 324 |
| $NbBi_3O_7$ | *cF*52 | 225,ga | 211 |
| $[Nb_6Br_{12}(H_2O)_6]HgBr_4{\cdot}12H_2O$ | *cF*328 | 227,$g^2f^2eb$ | 124 |
| $Nb_4C_3$ cubic | *cP*7 | 221,dca | 347 |
| $[Nb_6Cl_{12}(H_2O)_6](OH)_2{\cdot}8H_2O$ | *cF*136 | 225,$hfe^2c$ | 255 |
| $Nb_6F_{15}$ | *cI*42 | 229,heb | 27 |
| $Nb_5Ni$ | *cF*96 | 227,fec | 85 |
| $Nb_2Ni_{21}B_6$ | *cF*116 | 225,hfeca | 246 |
| NbO | *cP*6 | 221,dc | 347 |
| $NbO_{1.66}$ | *cP*112 | 221,$l^2k^2gdcba$ | 412 |
| $Nb_2(O,OH)_6{\cdot}xH_2O$ | *cF*240 | 227,$gfe^2dc$ | 119 |
| $Nb_3Sb_2Te_5$ | *cI*40 | 229,fed | 27 |
| $Nb_3SnH$ | *cP*14 | 223,dca | 322 |
| $Nb_2ZnC_x$ | *cF*120 | 227,fedca | 94 |
| $Nd_2Fe_{23}B_3$ | *cI*224 | 220,$e^3d^2c^2$ | 481 |
| $Nd_5Mo_3O_{16}$ | *cP*96 | 222,ifedc | 342 |
| $Nd_2O_3$ form X | *cI*26 | 229,ga | 20 |
| $Ni_{20}AlB_{14}$ | *cF*140 | 225,$hf^2ea$ | 258 |
| $Ni_{20}Al_3B_{9.75}$ | *cF*164 | 225,$hfe^3ca$ | 263 |
| $Ni_3Ga_4$ | *cI*112 | 230,gfa | 1 |
| $NiHg_4$ | *cI*10 | 229,ca | 16 |
| $Ni_{21}In_2P_6$ | *cF*116 | 225,hfeca | 246 |
| $Ni(NCNH_2)_4Cl_2$ | *cI*114 | 229,$kh^2eb$ | 36 |
| $[Ni(NH_3)_6](NO_3)_2$ | *cF*132 | 225,keca | 253 |
| $Ni_3[Re_6Se_8(CN)_6]_2{\cdot}33H_2O$ | *cF*272 | 225,$jf^2e^4cba$ | 282 |
| $Ni_3ZnGa_3$ | *cI*112 | 230,gfa | 1 |
| $Ni_7Zn_6Ge_2$ | *cF*120 | 227,fedca | 97 |
| $O_2$ γ | *cP*64 | 223,li | 333 |
| $Pb_{26}Ag_9Cu_{24}(OH)_{48}Cl_{62}$ | *cP*169 | 221,$m^3kj^2hg^2fe^2d$ | 448 |
| $Pb_2Ag(OH)Cl_3F$ | *cF*128 | 227,$fe^2c$ | 99 |
| $Pb_6Al_{12}Si_{12}O_{48}$ | *cP*112 | 221,$mk^2ihg^2$ | 413 |
| $Pb_9Al_{12}Si_{12}O_{48}(OH)_8{\cdot}3H_2O$ | *cP*280 | 221,$n^2m^4kihg^5$ | 464 |
| $Pb_9Al_{12}Si_{12}O_{49}(OH)_4{\cdot}xH_2O$ | *cP*188 | 221,$m^4kjihg^4$ | 453 |
| $Pb_{0.4}Bi_{0.6}O_{0.6}F_{1.4}$ | *cF*116 | 225,ifeca | 247 |
| $Pb_{0.4}Bi_{0.6}O_{0.6}F_{1.4}$ | *cF*484 | 225,$l^2f^3b$ | 295 |
| $Pb_{0.95}Bi_{0.05}O_{0.05}F_{1.95}$ | *cF*84 | 225,ieca | 230 |
| $Pb_3[Co(NO_2)_6]_2{\cdot}xH_2O$ | *cP*82 | 224,lkdb | 317 |
| $Pb_2CoWO_6$ | *cF*200 | 225,kjba | 272 |
| $PbFe_{0.5}Nb_{0.5}O_3$ ht | *cP*10 | 221,fda | 353 |
| $PbFe_{0.5}Nb_{0.5}O_3$ ht | *cP*19 | 221,hfa | 361 |
| $Pb_{54}(H_3O)_{12}Al_{88}Si_{104}O_{384}(OH)_{32}{\cdot}xH_2O$ | *cF*1568 | 227,$i^3hg^8e^4$ | 174 |

| structure type | Pearson symbol | space group number, Wyckoff sequence | page |
|---|---|---|---|
| $PbHf_{0.4}Ti_{0.6}O_3$ ht | *cP*22 | 221,jeda | 362 |
| $Pb_2HoAl_3O_8$ | *cP*56 | 224,kfe$^2$b | 316 |
| $Pb_{0.985}La_{0.01}Mg_{0.33}Nb_{0.67}O_3$ | *cP*17 | 221,icba | 360 |
| $PbMg_{0.33}Nb_{0.67}O_3$ | *cP*16 | 221,jda | 360 |
| $PbMg_{0.33}Nb_{0.67}O_3$ rt | *cP*42 | 221,mhe | 372 |
| $PbMg_{0.33}Nb_{0.67}O_3$ rt | *cP*49 | 221,jig$^2$ed | 375 |
| $PbMg_{0.33}Nb_{0.67}O_3$ rt | *cP*142 | 221,nmkjig$^2$e | 437 |
| $Pb_2MgWO_6$ form I | *cF*296 | 225,lkba | 286 |
| PbS | *cF*8 | 225,ba | 198 |
| $Pb_{0.9}Th_{0.1}F_{2.2}$ | *cF*124 | 225,hf$^2$cb | 252 |
| $Pb_{0.95}Th_{0.05}F_{2.1}$ | *cF*76 | 225,f$^2$ca | 226 |
| $Pb_{0.975}Th_{0.025}F_{2.05}$ | *cF*60 | 225,ica | 218 |
| $Pb_{0.825}Zr_{0.175}F_{2.35}$ | *cF*116 | 225,ifeca | 247 |
| $Pb_{0.85}Zr_{0.15}F_{2.3}$ | *cF*204 | 225,k$^2$ca | 274 |
| $Pb_{0.875}Zr_{0.125}F_{2.25}$ | *cF*156 | 225,kica | 262 |
| $Pb_{0.95}Zr_{0.05}F_{2.1}$ | *cF*108 | 225,kca | 238 |
| $PbZr_3O_4F_6$ | *cF*112 | 225,ifec | 241 |
| $PdH_{1.33}$ ht | *cP*14 | 221,hba | 355 |
| $PdH_{0.65}$ lt | *cP*64 | 223,kfedcba | 333 |
| $Pd_{17}Se_{15}$ | *cP*64 | 221,mjifeca | 380 |
| $Pd_{3.5}Te$ | *cF*120 | 227,fedca | 96 |
| Po α | *cP*1 | 221,a | 343 |
| $Pr_3Rh_4Sn_{13}$ | *cP*40 | 223,keca | 326 |
| $Pr_{30}Ti_{24}Se_{58}O_{25}I_8$ | *cF*580 | 225,k$^2$jihf$^3$e$^3$da | 300 |
| Prussian blue | *cF*120 | 225,fe$^3$cba | 249 |
| Prussian blue | *cP*88 | 221,h$^3$gf$^3$e$^3$dcba | 387 |
| Prussian blue dehydrated | *cF*200 | 225,k$^2$ba | 272 |
| Prussian blue family | *cF*120 | 225,fe$^3$cba | 250 |
| Prussian blue family | *cF*120 | 225,fe$^3$cba | 251 |
| Prussian blue family | *cF*120 | 225,fe$^3$cba | 251 |
| Prussian blue family | *cF*152 | 225,f$^2$e$^3$cba | 259 |
| Prussian blue family | *cF*192 | 225,f$^2$e$^5$ba | 268 |
| Prussian blue family | *cF*208 | 225,kfe$^3$ba | 275 |
| Prussian blue family | *cF*208 | 225,kfe$^3$ba | 276 |
| Prussian blue family | *cF*276 | 225,j$^2$e$^2$dca | 283 |
| Prussian blue family | *cF*344 | 225,lke$^2$ba | 290 |
| Prussian blue family | *cF*344 | 225,lke$^2$ba | 290 |
| Prussian blue family | *cF*440 | 225,l$^2$e$^2$ba | 294 |
| $PtHg_4$ | *cI*10 | 229,ca | 16 |
| $PtIn_6(GaO_4)_2$ | *cF*68 | 225,feca | 225 |
| $Pt_3O_4$ | *cI*14 | 229,cb | 17 |
| $Pt_3O_4$ | *cP*14 | 223,ec | 323 |
| $Pt_{3.4}O_4$ | *cP*16 | 223,eca | 323 |
| $Pu_2C_3$ | *cI*40 | 220,dc | 468 |
| $Rb_{11}Ag_{3.4}Al_{12}Si_{12}O_{48}$ | *cP*109 | 221,mljihg$^2$ed | 409 |
| $Rb_2Cd_5Al_{12}Si_{12}O_{48}$ | *cP*91 | 221,mkihg$^2$c | 391 |
| $Rb_4Cd_4Al_{12}Si_{12}O_{48}$ | *cP*91 | 221,mkihg$^2$c | 391 |
| $RbCrNiF_6$ | *cF*72 | 227,fcb | 77 |
| $Rb_{18}Cu_{31}Cl_{49}$ | *cI*396 | 220,e$^6$d$^2$c$^3$a | 485 |

| structure type | Pearson symbol | space group number, Wyckoff sequence | page |
|---|---|---|---|
| $Rb_4H_8[H_2W_{12}O_{40}]\cdot 18H_2O$ | *cF*608 | 225,$k^5$hfed | 302 |
| $Rb_{4.4}[H_{0.6}V_{0.6}Mo_{12}0_{40}]\cdot 14H_2O$ | *cF*656 | 225,$k^4ih^2f^2e^2$cba | 304 |
| $Rb_3Hg_{20}$ | *cP*46 | 223,kedca | 327 |
| $Rb_2KScF_6$ rt | *cF*112 | 225,jcba | 241 |
| $RbNO_3$ form I | *cF*132 | 225,kfb | 254 |
| $RbNO_3$ form I | *cF*184 | 225,khfba | 267 |
| $RbNO_3$ form III | *cP*46 | 221,migba | 373 |
| $Rb_{11}NaAl_{12}Si_{12}O_{48}$ | *cP*115 | 221,mkihg$^5$c | 416 |
| $Rb_3Na_9Al_{12}Si_{12}O_{48}$ | *cP*104 | 221,mkji$^2$hg | 402 |
| $Rb_{30}Na_{22}Al_{52}Si_{140}O_{384}$ | *cF*720 | 227,ihg$^3$e$^4$c | 151 |
| $Rb_{11}NaAl_{12}Si_{12}O_{48}$:Ba | *cP*107 | 221,mkihg$^4$c | 407 |
| $Rb_{11}NaAl_{12}Si_{12}O_{48}\cdot xH_2O$ | *cP*163 | 221,m$^2$lkji$^2$hg$^2$c | 447 |
| $Rb_{27.5}Na_{27.5}Al_{55}Si_{137}O_{384}\cdot 4.5H_2O$ | *cF*720 | 227,ihg$^3$e$^4$c | 150 |
| $Rb_{79}Na_2Ba_5Al_{91}Si_{101}O_{384}$ | *cF*856 | 226,ji$^4$g$^4$d | 184 |
| $Rb_7Na_{16}Sb_7$ | *cF*164 | 225,if$^2$eda | 264 |
| $RbNb_2O_5F$ | *cF*128 | 227,fe$^2$c | 99 |
| $Rb_{19}O_3$ | *cF*176 | 226,ifdb | 180 |
| $Rb_2O_3$ | *cI*40 | 220,dc | 468 |
| $Rb_3P_7$ ht | *cF*284 | 225,kjfe$^2$ca | 284 |
| $Rb_3ReH_{10}$ rt | *cP*53 | 221,mkcba | 376 |
| $Rb_3Sb$ β | *cF*16 | 227,ba | 67 |
| $RbSeO_2F$ | *cP*8 | 221,eba | 351 |
| $Rb_{10}Tc_6S_{14}$ | *cF*172 | 225,hf$^2$e$^2$ca | 266 |
| $RbTlBr_4\cdot H_2O$ | *cF*416 | 219,h$^4$da | 494 |
| $Rb_{1.10}W_{1.66}O_{5.53}$ form III | *cF*168 | 227,gfcb | 109 |
| $ReO_3$ | *cP*4 | 221,da | 344 |
| Reinecke's salt | *cI*100 | 229,h$^3$ecba | 35 |
| $RhBi_4$ α | *cI*120 | 230,hc | 2 |
| $Rh_{17}S_{15}$ | *cP*64 | 221,mjifeca | 380 |
| $RuCo_8S_8$ | *cF*68 | 225,feca | 224 |
| $[Ru(NH_3)_6](BF_4)_3$ | *cF*152 | 225,gf$^2$ecba | 261 |
| $[Ru(NH_3)_6]Br(SO_4)$ | *cF*156 | 225,kfea | 262 |
| $[Ru(NH_3)_5N_2]Cl_2$ | *cF*60 | 225,e$^2$ca | 216 |
| $Ru_3Sn_7$ | *cI*40 | 229,fed | 26 |
| $RuSn_6(Al_{0.33}O_4)_2$ | *cF*100 | 225,f$^2$eca | 235 |
| $S1_4$ | *cI*160 | 230,hdca | 3 |
| $S1_5$ | *cI*76 | 220,eca | 471 |
| $S6_1$ | *cI*184 | 230,hgcb | 6 |
| $SF_4$ | *cF*100 | 225,ja | 235 |
| $SF_6$ rt | *cI*14 | 229,ea | 17 |
| "$SbO_2$" | *cF*96 | 227,fdcba | 83 |
| $Sb_2O_3$ cubic | *cF*80 | 227,fe | 79 |
| $Sb_6O_{13}$ | *cF*88 | 227,fdca | 82 |
| "$Sb_3O_6OH$" | *cF*88 | 227,fdca | 82 |
| $Sc_{11}Ir_4$ | *cF*120 | 225,f$^2$edba | 248 |
| $Sc_6Ni_7Al_{16}$ | *cF*116 | 225,f$^2$eda | 244 |
| $SiC_2N_4$ β | *cP*14 | 224,eba | 313 |
| $Si_3Cl_8$ | *cF*176 | 219,he$^2$ba | 489 |
| $SiO_2$ cristobalite β | *cF*24 | 227,ca | 68 |

| structure type | Pearson symbol | space group number, Wyckoff sequence | page |
|---|---|---|---|
| $Th_6Mn_{23}H_{30}$ | *cF*292 | 225,khf$^3$eda | 286 |
| $Th_3P_4$ | *cI*28 | 220,ca | 467 |
| $ThZr_2H_7$ | *cF*80 | 227,fcba | 78 |
| $TiC_2$ | *cP*7 | 221,fa | 349 |
| $Ti_2C$ | *cF*48 | 227,ec | 71 |
| $TiC_xN_yH_z$ | *cF*64 | 227,edc | 73 |
| $Ti_3IrH_{3.63}$ | *cP*38 | 223,kdca | 325 |
| $Ti_2Ni$ | *cF*96 | 227,fec | 84 |
| $Ti_3NiAl_2C$ | *cF*112 | 227,fedc | 91 |
| $Ti_2NiH$ | *cF*128 | 227,fedcba | 103 |
| $Ti_4Ni_2O$ | *cF*112 | 227,fedc | 90 |
| $TiS_2$ | *cF*48 | 227,ec | 71 |
| $Ti_{12}Sn_3O_{10}$ | *cF*248 | 225,jgf$^2$ecba | 280 |
| $Ti_{18}Zn_2S_{32}$ | *cF*72 | 227,edca | 75 |
| $Tl_4Ag_8Al_{12}Si_{12}O_{48}$ | *cP*114 | 221,mki$^2$hg$^3$e | 415 |
| $Tl_7Ag_{36}Te_{22}$ | *cF*260 | 225,kihfeca | 281 |
| $Tl_{11}Al_{11}Si_{13}O_{48}$ | *cP*100 | 221,mki$^2$hg$^2$ | 397 |
| $Tl_{12}Al_{12}Si_{12}O_{48}$ | *cP*124 | 221,m$^2$ki$^2$hg$^2$ | 426 |
| $Tl_{12}Al_{12}Si_{12}O_{48}\cdot 18H_2O$ | *cP*148 | 221,mlk$^2$i$^2$hg$^2$ | 442 |
| $Tl_{13}Al_{12}Si_{12}O_{48}(OH)\cdot 9H_2O$ | *cP*184 | 221,nmlkji$^2$hg$^2$ | 452 |
| $Tl_2Cd_5Fe_3Al(SO_4)_{12}\cdot 18H_2O$ | *cF*1424 | 228,h$^6$gfcba | 65 |
| $TlNO_3$ form I | *cP*37 | 221,ke$^2$b | 369 |
| $Tl_2Nb_2O_{6.07}$ | *cF*104 | 227,feda | 88 |
| $TlNb_2O_5F$ | *cF*96 | 227,fec | 86 |
| $TlPd_3O_4$ | *cF*64 | 225,fdba | 220 |
| $Tl_7Sb_2$ | *cI*54 | 229,hfea | 31 |
| $Tl_{0.51}Sb_{2.71}O_{6.32}$ | *cF*232 | 227,gfe$^2$da | 118 |
| $Tl_2Ta_2O_6$ | *cF*96 | 227,fec | 86 |
| $Tl_{1.5}Ta_{1.5}W_{0.5}O_6$ | *cF*112 | 227,fedc | 91 |
| $Tl_{1.5}Ta_{1.5}W_{0.5}O_6$ | *cF*128 | 227,fe$^2$d | 101 |
| $Tl_2Zn(CN)_4$ | *cF*704 | 219,h$^5$e$^6$ca | 494 |
| $Tm_{11}Ni_{60}C_6$ | *cI*154 | 229,kjfe$^2$db | 39 |
| $TmRuGa_3$ | *cP*15 | 221,gdca | 356 |
| $UAl_3$ | *cP*4 | 221,ca | 344 |
| $UB_{12}$ | *cF*52 | 225,ia | 212 |
| $UH_3$ α | *cP*8 | 223,ca | 322 |
| $UH_3$ β | *cP*32 | 223,kca | 325 |
| $UO_2$ | *cF*36 | 225,fa | 205 |
| $UO_{2.12}$ | *cF*92 | 225,ifca | 234 |
| $UO_{2.12}$ | *cF*116 | 225,hf$^2$b | 245 |
| $U_4O_9$ β | *cI*828 | 220,e$^{15}$d$^2$c$^3$a | 486 |
| $U_4O_9$ β | *cI*832 | 220,e$^{14}$d$^3$c$^4$ba | 487 |
| $U_{0.92}Pd_3S_4$ | *cP*16 | 223,eca | 323 |
| $U_4Re_7Si_6$ | *cI*34 | 229,edca | 22 |
| $U_6Rh_2Se_{15.5}$ | *cI*98 | 229,khdcb | 34 |
| $U_4S_3$ | *cP*7 | 221,dca | 347 |
| $U_4(Si,Re)_{13}$ | *cI*34 | 229,edca | 22 |
| $VAl_{10}$ | *cF*176 | 227,gfdc | 110 |
| $VAl_{10.25}$ | *cF*184 | 227,gfdca | 111 |

| structure type | Pearson symbol | space group number, Wyckoff sequence | page |
|---|---|---|---|
| $VH_{0.5}$ | *cI*14 | 229,da | 17 |
| (VH) α | *cI*14 | 229,da | 17 |
| $(VO)[Cr(CN)_6]_{0.67}\cdot 3.33H_2O$ | *cF*276 | 225,$j^2e^2$dca | 283 |
| W | *cI*2 | 229,a | 15 |
| "W β" | *cP*8 | 223,ca | 321 |
| $W_4Co_2C$ | *cF*112 | 227,fedc | 90 |
| $W_2Cr_{21}C_6$ | *cF*116 | 225,hfeca | 246 |
| $W_3Fe_3C$ | *cF*112 | 227,fedc | 90 |
| $W_6Fe_6C$ | *cF*104 | 227,fecb | 87 |
| $W_3N_4$ | *cP*7 | 221,dca | 347 |
| $W_3O$ | *cP*8 | 223,ca | 322 |
| $WTh_8Zr_{18}O_{53}F_4$ | *cF*408 | 225,$k^2$ihgfecba | 292 |
| $XeF_6$ form IV | *cF*1600 | 226,$j^7igf^2$ | 194 |
| YAG | *cI*160 | 230,hdca | 4 |
| $Y_3Al_5O_{12}$ | *cI*160 | 230,hdca | 4 |
| $Y_3Au_3Sb_4$ | *cI*40 | 220,cba | 468 |
| $YB_{66}$ | *cF*1936 | 226,$j^7i^5$gf | 196 |
| $Y_{0.5}Bi_{1.5}O_3$ | *cF*112 | 225,$gf^2$ | 239 |
| $Y_{0.54}Bi_{1.46}O_3$ | *cF*112 | 225,hfec | 240 |
| $Y_3Co_4Ge_{13}$ | *cP*64 | 223,$k^2$eca | 332 |
| $YF_3$ | *cP*15 | 221,gdca | 357 |
| $Y_3Fe_{62}B_{14}$ | *cI*158 | 229,kj$f^2$edb | 40 |
| $Y_6Mn_{23}H_{8.3}$ | *cF*152 | 225,$f^3$edba | 260 |
| $Y_6Mn_{23}H_{18}$ | *cF*248 | 225,j$f^3$edba | 279 |
| $Y_6Mn_{23}H_{23}$ rt | *cF*344 | 225,kj$f^3$edba | 289 |
| $Y_4PdGa_{12}$ | *cI*34 | 229,edca | 23 |
| $Y_3TaNi_{6+x}Al_{26}$ | *cP*49 | 221,$ji^2$gdba | 374 |
| $Y_3TaO_7$ | *cF*92 | 225,gfca | 233 |
| $Y_{0.28}Zr_{0.72}O_{1.86}$ | *cF*84 | 225,gfa | 228 |
| $Y_{0.22}Zr_{0.78}O_{1.89}$ ht | *cF*88 | 225,gfc | 232 |
| $Yb_2FeS_4$ | *cF*72 | 227,edca | 75 |
| $Yb_{1.33}In_{1.33}S_4$ | *cF*72 | 227,edca | 77 |
| $Yb_{11}Ni_{60}C_6$ | *cI*154 | 229,kjf$e^2$db | 39 |
| $Yb_3Rh_4Sn_{13}$ | *cP*40 | 223,keca | 326 |
| $Yb_{7+x}Se_8$ | *cF*64 | 225,edcba | 219 |
| $YbZrF_7$ | *cP*42 | 221,lje | 372 |
| $YbZrF_7$ | *cP*48 | 221,lj$e^2$ | 374 |
| $Yb_{0.2}Zr_{0.8}O_{0.3}F_{3.2}$ | *cP*42 | 221,lje | 372 |
| Zintl phase | *cF*16 | 227,ba | 67 |
| $Zn_{56}Al_{88}Si_{104}O_{384}\cdot 8HAlO_4\cdot 8H$ | *cF*872 | 227,$i^2hg^3e^3$a | 164 |
| $Zn_6Al_{12}Si_{12}O_{48}\cdot xH_2O$ | *cP*178 | 221,$mlk^2ji^2hg^3$edb | 451 |
| $Zn_6Al_{12}Si_{12}O_{48}\cdot 2.7ZnO$ | *cP*95 | 221,mkih$g^2$ea | 392 |
| $Zn(CN)_2$ | *cP*10 | 224,ea | 312 |
| $Zn_3[Fe(CN)_6]_2\cdot xH_2O$ | *cF*152 | 225,$f^2e^3$cba | 259 |
| $ZrB_{12}$ | *cF*52 | 225,ia | 212 |
| $Zr_6Cl_{15}N$ | *cI*352 | 230,$h^3$ga | 11 |
| $Zr_6CoCl_{15}$ | *cI*44 | 229,heba | 29 |
| $Zr_9Co_7In_{14}$ | *cF*120 | 225,ifecba | 252 |
| $ZrCr_2H_{3.1}$ ht | *cF*120 | 227,gcb | 98 |

| structure type | Pearson symbol | space group number, Wyckoff sequence | page |
|---|---|---|---|
| murdochite | *cF*60 | 225,edca | 216 |
| murdochite | *cF*64 | 225,fdba | 221 |
| natanite | *cP*32 | 224,kcb | 314 |
| palladseite | *cP*64 | 221,mjifeca | 380 |
| paulingite | *cI*2556 | 229,$l^{14}k^{12}j^{8}i^{2}h^{2}gf^{3}e^{3}$ | 61 |
| pentlandite | *cF*68 | 225,feca | 223 |
| perovskite | *cP*5 | 221,dba | 345 |
| perovskite $A_3A'B_2B'_2O_{12}$ | *cP*40 | 224,kdcba | 314 |
| perovskite $AA'B_2O_6$ | *cF*40 | 225,dcba | 206 |
| perovskite $AA'B_2O_6$ | *cF*296 | 225,lkba | 286 |
| perovskite $AA'_3B_4O_{12}$ | *cI*40 | 229,hcba | 27 |
| perovskite $A_8AB_6B'O_{24}$ | *cP*40 | 221,hgfedcba | 370 |
| perovskite $A_4AB_3O_{12}$ | *cI*40 | 229,edcba | 26 |
| perovskite $A_2BB'O_6$ | *cF*40 | 225,ecba | 207 |
| perovskite $A_4BB'_3O_{12}$ | *cI*40 | 229,edcba | 25 |
| perovskite $ABO_3$ cubic F | *cF*40 | 225,ecba | 207 |
| perovskite family | *cF*112 | 225,jcba | 241 |
| perovskite family | *cF*200 | 225,kjba | 272 |
| perovskite family | *cP*15 | 221,geb | 357 |
| pollucite | *cI*160 | 230,hgb | 5 |
| pyrochlore 2:2:6:1 | *cF*88 | 227,fdca | 82 |
| pyrochlore 2:2:7 | *cF*88 | 227,fdca | 81 |
| pyrochlore 2:6 | *cF*64 | 227,fc | 74 |
| pyrochlore 2:6:1 | *cF*72 | 227,fcb | 77 |
| pyrochlore family | *cF*88 | 227,fdca | 82 |
| pyrochlore family | *cF*96 | 227,fec | 86 |
| pyrochlore family | *cF*104 | 227,feda | 88 |
| pyrochlore family | *cF*112 | 227,fedc | 93 |
| pyrochlore family | *cF*112 | 227,fedc | 91 |
| pyrochlore family | *cF*112 | 227,fedc | 92 |
| pyrochlore family | *cF*120 | 227,fedca | 97 |
| pyrochlore family | *cF*128 | 227,$fe^2c$ | 99 |
| pyrochlore family | *cF*128 | 227,$fe^2d$ | 100 |
| pyrochlore family | *cF*128 | 227,$fe^2d$ | 101 |
| pyrochlore family | *cF*168 | 227,gfca | 108 |
| pyrochlore family | *cF*168 | 227,gfcb | 109 |
| pyrochlore family | *cF*168 | 227,hfca | 109 |
| pyrochlore family | *cF*184 | 227,gfdca | 113 |
| pyrochlore family | *cF*232 | 227,$gfe^2da$ | 118 |
| pyrochlore family | *cF*240 | 227,$gfe^2dc$ | 119 |
| pyrochlore family | *cF*240 | 227,$g^2ec$ | 118 |
| pyrochlore family | *cF*264 | 227,hgfcb | 120 |
| pyrochlore family | *cF*296 | 227,$g^2feda$ | 121 |
| pyrochlore family | *cF*304 | 227,$g^2fedc$ | 123 |
| pyrochlore family | *cF*320 | 227,igdc | 123 |
| pyrochlore-fluorite | *cF*96 | 227,fdcba | 83 |
| reineckate $NH_4$ | *cI*100 | 229,$h^3ecba$ | 35 |
| roaldite | *cP*5 | 221,dba | 346 |
| rock salt | *cF*8 | 225,ba | 198 |

| structure type | Pearson symbol | space group number, Wyckoff sequence | page |
|---|---|---|---|
| schorlomite | *cI*256 | 230,$h^2$dca | 8 |
| senarmontite | *cF*80 | 227,fe | 79 |
| sesquioxide X | *cI*26 | 229,ga | 20 |
| sesquisulfide C | *cI*28 | 220,ca | 467 |
| sodalite ASS ht | *cP*76 | 223,lidc | 335 |
| sodalite SACR ht | *cI*70 | 229,$h^2$dca | 33 |
| spinel | *cF*56 | 227,ecb | 72 |
| spinel family | *cF*72 | 227,edca | 76 |
| spinel family | *cF*72 | 227,edca | 77 |
| spinel family | *cF*104 | 227,fecb | 88 |
| spinel family | *cF*152 | 227,hecb | 106 |
| spinel family | *cF*200 | 227,hfecb | 115 |
| spinel family | *cF*704 | 219,$h^5e^6$ca | 494 |
| spinel inverse | *cF*56 | 227,ecb | 72 |
| sulphohalite | *cF*72 | 225,fecba | 226 |
| telluric acid cubic | *cF*224 | 228,hc | 63 |
| tschörtnerite | *cF*2476 | 225,$l^6k^7j^4hf^6$ea | 310 |
| tungsten bronze cubic | *cI*110 | 229,$k^2$cb | 35 |
| voltaite-(K) | *cF*1712 | 228,$h^8$gcba | 66 |
| voltaite-(Tl) | *cF*1424 | 228,$h^6$gfcba | 65 |
| wüstite | *cF*72 | 227,edca | 75 |
| wüstite | *cP*211 | 221,$m^2lkj^2i^2hg^3f^2e^2d$( | 458 |
| zeolite ANA-Cs | *cI*160 | 230,hgb | 5 |
| zeolite ANA(Ga)-Cs,Na | *cI*208 | 230,hgfb | 8 |
| zeolite ANA-K | *cI*160 | 230,hgb | 5 |
| zeolite ANA-Na hydrated | *cI*184 | 230,hgcb | 6 |
| zeolite ANA(Ti)-Cs | *cI*352 | 230,$h^3$gb | 12 |
| zeolite FAU dealuminated | *cF*576 | 227,ihg$^3$ | 130 |
| zeolite FAU dealuminated | *cF*608 | 227,ihg$^3$e | 132 |
| zeolite FAU dealuminated | *cF*640 | 227,ihg$^3$e$^2$ | 135 |
| zeolite FAU dealuminated | *cF*656 | 227,ihg$^3$e$^2$d | 140 |
| zeolite FAU dealuminated, residual water | *cF*616 | 227,ihg$^3$ea | 133 |
| zeolite FAU partly dealuminated | *cF*672 | 227,ihg$^3$e$^3$ | 141 |
| zeolite FAU-Ag | *cF*688 | 227,ihg$^3$e$^3$c | 143 |
| zeolite FAU-Ag | *cF*720 | 227,ihg$^3$e$^4$c | 150 |
| zeolite FAU-Ag | *cF*784 | 227,ihg$^4$e$^3$c | 157 |
| zeolite FAU-Ag | *cF*880 | 227,ihg$^5$e$^3$c | 165 |
| zeolite FAU-Ag hydrated | *cF*720 | 227,ihg$^3$e$^4$c | 149 |
| zeolite FAU-Ba(Na) hydrated | *cF*816 | 227,ihg$^4$e$^4$c | 161 |
| zeolite FAU-Ca | *cF*656 | 227,ihg$^3$e$^2$c | 138 |
| zeolite FAU-Ca hydrated | *cF*768 | 227,ihg$^4$e$^3$ | 156 |
| zeolite FAU-Ca hydrated | *cF*800 | 227,ihg$^4$e$^4$ | 160 |
| zeolite FAU-Ca,Na hydrated | *cF*672 | 227,ihg$^3$e$^3$ | 142 |
| zeolite FAU-$Ce^{3+}$,H residual water | *cF*688 | 227,ihg$^3$e$^3$c | 146 |
| zeolite FAU-$Ce^{3+}$,Na hydrated | *cF*704 | 227,ihg$^3$e$^4$ | 148 |
| zeolite FAU-$Ce^{3+}$,Na residual water | *cF*688 | 227,ihg$^3$e$^3$c | 147 |
| zeolite FAU-$Ce^{3+}$,Na,H | *cF*656 | 227,ihg$^3$e$^2$c | 139 |
| zeolite FAU-Cu | *cF*720 | 227,ihg$^4$ec | 152 |
| zeolite FAU-$Cu^{2+}$ hydrated | *cF*1256 | 227,$i^3hg^5e^3$a | 172 |

| structure type | Pearson symbol | space group number, Wyckoff sequence | page |
|---|---|---|---|
| zeolite FAU-$Cu^{2+}$ residual water | *cF*976 | 227,$i^2hg^3e^6c$ | 167 |
| zeolite FAU-$Cu^{2+}$,Na (HCl) hydrated | *cF*832 | 227,$ihg^5edc$ | 162 |
| zeolite FAU-$Cu^{2+}$,Na ($NH_3$) hydrated | *cF*784 | 227,$ihg^4fe^2$ | 158 |
| zeolite FAU-$Fe^{3+}$,Na residual water | *cF*688 | 227,$ihg^3e^3c$ | 145 |
| zeolite FAU(Ga)-Na | *cF*736 | 227,$ihg^4e^2$ | 153 |
| zeolite FAU(Ga)-Na | *cF*752 | 227,$ihg^4e^2c$ | 154 |
| zeolite FAU(Ga)-Na | *cF*848 | 227,$i^2hg^3e^2c$ | 163 |
| zeolite FAU-Gd,Na hydrated | *cF*960 | 227,$i^2hg^4e^3$ | 167 |
| zeolite FAU-H(Na) | *cF*592 | 227,$ihg^3c$ | 131 |
| zeolite FAU-H(Na,Ca) | *cF*608 | 227,$ihg^3e$ | 132 |
| zeolite FAU-In | *cF*1256 | 227,$i^4hg^3e^3a$ | 173 |
| zeolite FAU-K | *cF*1056 | 227,$ihg^6fe^4c$ | 168 |
| zeolite FAU-K,Na hydrated | *cF*880 | 227,$ihg^5e^3c$ | 166 |
| zeolite FAU-$La^{3+}$ hydrated | *cF*688 | 227,$ihg^3e^3d$ | 147 |
| zeolite FAU-$La^{3+}$ hydrated | *cF*736 | 227,$ihg^3e^5$ | 152 |
| zeolite FAU-$La^{3+}$ partly hydrated | *cF*648 | 227,$ihg^3e^2a$ | 136 |
| zeolite FAU-$La^{3+}$ partly hydrated | *cF*1176 | 227,$i^2hg^5e^6cb$ | 169 |
| zeolite FAU-$La^{3+}$ residual water | *cF*640 | 227,$ihg^3e^2$ | 135 |
| zeolite FAU-$La^{3+}$ residual water | *cF*704 | 227,$ihg^3e^4$ | 149 |
| zeolite FAU-$La^{3+}$ residual water | *cF*768 | 227,$ihg^4e^2dc$ | 155 |
| zeolite FAU-La,H | *cF*648 | 227,$ihg^3e^2a$ | 137 |
| zeolite FAU-La,Na | *cF*664 | 227,$ihg^3e^2ca$ | 140 |
| zeolite FAU-Li(H,Na,K) | *cF*640 | 227,$ihg^3e^2$ | 134 |
| zeolite FAU-Mn,Na partly hydrated | *cF*672 | 227,$ihg^3e^3$ | 142 |
| zeolite FAU-Mn,Na residual water | *cF*688 | 227,$ihg^3e^3c$ | 144 |
| zeolite FAU-$NH_4$,K hydrated | *cF*672 | 227,$ihg^3e^3$ | 142 |
| zeolite FAU-Na | *cF*624 | 227,$ihg^3ec$ | 134 |
| zeolite FAU-Na | *cF*656 | 227,$ihg^3e^2c$ | 138 |
| zeolite FAU-Na | *cF*752 | 227,$ihg^4e^2c$ | 154 |
| zeolite FAU-Na hydrated | *cF*800 | 227,$ihg^4e^4$ | 159 |
| zeolite FAU-Na hydrated | *cF*880 | 227,$ihg^5e^3c$ | 165 |
| zeolite FAU-Na hydrated | *cF*1856 | 227,$i^4hg^8fe^5c$ | 177 |
| zeolite FAU-Na hydrated | *cF*1872 | 227,$i^4hg^9e^4c$ | 178 |
| zeolite FAU-Na,Ca | *cF*624 | 227,$ihg^3ec$ | 134 |
| zeolite FAU-Na,Ca hydrated | *cF*640 | 227,$ihg^3e^2$ | 134 |
| zeolite FAU-Nd,Na hydrated | *cF*1160 | 227,$i^2hg^5fe^4da$ | 169 |
| zeolite FAU-Nd,Na hydrated | *cF*1248 | 227,$i^4hg^3e^3$ | 172 |
| zeolite FAU-Nd,Na hydrated | *cF*1360 | 227,$i^2hg^8e^3c$ | 174 |
| zeolite FAU-$Ni^{2+}$ | *cF*784 | 227,$ihg^4e^3c$ | 158 |
| zeolite FAU-$Ni^{2+}$ hydrated | *cF*848 | 227,$ihg^5e^2c$ | 164 |
| zeolite FAU-$Ni^{2+}$ residual water | *cF*752 | 227,$ihg^3e^5c$ | 154 |
| zeolite FAU-Pb hydrated | *cF*1568 | 227,$i^3hg^8e^4$ | 174 |
| zeolite FAU-Pb,Cs | *cF*1632 | 227,$i^5hg^4e^6$ | 175 |
| zeolite FAU-Pb,Na ($H_2S$) | *cF*688 | 227,$ihg^3e^3c$ | 145 |
| zeolite FAU-Pb,Na (PbS) | *cF*656 | 227,$ihg^3e^2c$ | 139 |
| zeolite FAU-Pd,H | *cF*688 | 227,$ihg^3e^3c$ | 144 |
| zeolite FAU-Rb,Na | *cF*720 | 227,$ihg^3e^4c$ | 151 |
| zeolite FAU-Rb,Na residual water | *cF*720 | 227,$ihg^3e^4c$ | 150 |
| zeolite FAU-Te,H | *cF*776 | 227,$ihg^4e^3a$ | 157 |

| structure type | Pearson symbol | space group number, Wyckoff sequence | page |
|---|---|---|---|
| zeolite FAU-Zn ($HAlO_4 \cdot H$) | *cF*872 | 227,$i^2hg^3e^3a$ | 164 |
| zeolite FAU-Zn,Na | *cF*768 | 227,$ihg^3e^6$ | 155 |
| zeolite KFI-Ba ($BaBr_2$) hydrated | *cI*364 | 229,$lk^2jihfe^2d$ | 50 |
| zeolite KFI-Ba ($BaCl_2$) hydrated | *cI*400 | 229,$lk^2jih^2fe^3d$ | 52 |
| zeolite KFI-Cs,H | *cI*348 | 229,$lk^2j^2ie$ | 50 |
| zeolite KFI-Cs,K | *cI*328 | 229,$lk^2jifed$ | 48 |
| zeolite KFI-Cs,K,H | *cI*312 | 229,$lk^2jied$ | 47 |
| zeolite KFI-K | *cI*336 | 229,$lk^2jifedc$ | 49 |
| zeolite KFI-Na | *cI*304 | 229,$lk^2jif$ | 46 |
| zeolite KFI-Na | *cI*324 | 229,$lk^2jifdc$ | 47 |
| zeolite KFI-Na ($BaCl_2$) hydrated | *cI*446 | 229,$lk^2j^3if^2edb$ | 57 |
| zeolite KFI-Na hydrated | *cI*288 | 229,$lk^2ji$ | 45 |
| zeolite LTA-$Ag_{12}$ | *cP*98 | 221,$mki^2hge$ | 396 |
| zeolite LTA-$Ag_{12}$ | *cP*106 | 221,$mki^2hg^2e$ | 404 |
| zeolite LTA-$Ag_{12}$ | *cP*122 | 221,$mkji^2h^2ge$ | 425 |
| zeolite LTA-$Ag_{12}$ ($AgNO_3$) | *cP*369 | 221,$n^2m^4lkj^2i^2hg^6fe^2$ | 464 |
| zeolite LTA-$Ag_{12}$ ($HCl,Cl_2$) | *cP*180 | 221,$mlk^3jihg^3$ | 451 |
| zeolite LTA-$Ag_{12}$ hydrated | *cP*118 | 221,$mlkihg^2e$ | 421 |
| zeolite LTA-$Ag_{12}$ hydrated | *cP*232 | 221,$nm^3l^2kihg^2$ | 462 |
| zeolite LTA-$Ag_{12}$ partly hydrated | *cP*174 | 221,$nmkjih^2g^3e$ | 450 |
| zeolite LTA-$Ag_{12}$ residual water | *cP*138 | 221,$mkji^2h^2g^3e$ | 434 |
| zeolite LTA-$Ag_{10}/Ag_2$ | *cP*86 | 221,mkihge | 387 |
| zeolite LTA-$Ag_{8.5}/Ag_{3.5}$ | *cP*110 | 221,$m^2kihge$ | 409 |
| zeolite LTA-$Ag_9Cs_3$ | *cP*89 | 221,mkihgec | 390 |
| zeolite LTA-$Ag_{8.75}H_{3.25}$ | *cF*856 | 226,$ji^5g^2eb$ | 185 |
| zeolite LTA-$Ag_{9.8}H_{2.2}$ ($Br_2$) | *cP*196 | 221,$m^2lk^3j^2hg^2$ | 455 |
| zeolite LTA-$Ag_{10.7}K_{1.3}$ | *cP*110 | 221,$mki^3hge$ | 410 |
| zeolite LTA-$Ag_{9.3}K_{2.7}$ | *cP*98 | 221,$mki^2hge$ | 395 |
| zeolite LTA-$Ag_3K_9$ hydrated | *cP*134 | 221,$mkji^2hg^4e$ | 432 |
| zeolite LTA-$Ag_{10}[NH_4]_2$ ($N_3H_3,N_3H_5,NH_3$) | *cP*172 | 221,$m^3ki^3hg^2e^2$ | 449 |
| zeolite LTA-$Ag_{6.5}Na_{5.5}$ | *cP*114 | 221,$mki^2hg^3e$ | 415 |
| zeolite LTA-$Ag_{7.6}Na_{4.4}$ | *cP*106 | 221,$mki^2hg^2e$ | 405 |
| zeolite LTA-$Ag_3Na_{6.6}Ba_{1.2}$ | *cP*108 | 221,$mki^2hg^3$ | 408 |
| zeolite LTA-$Ag_{3.6}Na_{7.4}H_{2.8}$ | *cP*172 | 221,$m^4ljihg^2$ | 449 |
| zeolite LTA-$Ag_{2.7}Na_6H_{3.3}/Ag_{3.2}$ | *cP*132 | 221,$mlkjihg^3$ | 430 |
| zeolite LTA-$AgRb_{11}/Ag_{2.4}$ | *cP*109 | 221,$mljihg^2ed$ | 409 |
| zeolite LTA-$Ag_8Tl_4$ | *cP*114 | 221,$mki^2hg^3e$ | 415 |
| zeolite LTA-$Ag_{5.5}Tl_{5.5}/Ag$ | *cP*138 | 221,$mlki^2hg^3e$ | 434 |
| zeolite LTA-$Ag_6Tl_5H/Ag$ | *cP*126 | 221,$mk^2ihg^3e$ | 427 |
| zeolite LTA-$Ag_8Tl_3H/Ag$ | *cP*106 | 221,$mki^2hg^2e$ | 404 |
| zeolite LTA-$Ag_9Tl_2H/Ag$ | *cP*122 | 221,$m^2ki^2hge$ | 424 |
| zeolite LTA-$Ca_6$ | *cF*896 | 226,$j^2i^4g^2$ | 187 |
| zeolite LTA-$Ca_6$ | *cF*992 | 226,$j^3i^3g^2$ | 191 |
| zeolite LTA-$Ca_6$ | *cF*1000 | 226,$j^3i^3g^2b$ | 191 |
| zeolite LTA-$Ca_6$ | *cP*108 | 221,$mki^2hg^3$ | 407 |
| zeolite LTA-$Ca_6$ | *cP*140 | 221,$m^2kihg^5ca$ | 436 |
| zeolite LTA-$Ca_6$ ($Br_2$) | *cP*136 | 221,$ml^2kihg^2$ | 433 |
| zeolite LTA-$Ca_{3.98}Cs_{4.04}$ | *cP*107 | 221,$mkihg^4c$ | 406 |
| zeolite LTA-$Ca_{5.13}Cs_{1.74}$ | *cP*83 | 221,mkihgc | 386 |

| structure type | Pearson symbol | space group number, Wyckoff sequence | page |
|---|---|---|---|
| zeolite LTA-$Ca_4Na_4$ | *cP*80 | 221,mkihg | 384 |
| zeolite LTA-$Ca_4Na_4$ | *cP*88 | 221,mkihg$^2$ | 388 |
| zeolite LTA-$Ca_4Na_4$ | *cP*97 | 221,mkihg$^3$a | 394 |
| zeolite LTA-$Ca_4Na_4$ | *cP*103 | 221,mki$^2$hg$^2$c | 398 |
| zeolite LTA-$Ca_5Na_2$ | *cF*704 | 226,ji$^4$g$^2$ | 181 |
| zeolite LTA-$Ca_{5.3}Na_{0.4}$ | *cP*97 | 221,mkihg$^3$a | 394 |
| zeolite LTA-$Ca_4Na_4$ ($AlO_x[OH]_{4-x}$) | *cP*89 | 221,mkihg$^2$a | 389 |
| zeolite LTA-$Ca_4Na_4$ ($AlO_x[OH]_{4-x}$) hydrated | *cP*106 | 221,mkihg$^4$ba | 406 |
| zeolite LTA-$Ca_4Na_4$ ($Br_2$) | *cP*136 | 221,ml$^2$kihg$^2$ | 433 |
| zeolite LTA-$Ca_5Na_2$ (CO) | *cF*1032 | 226,j$^2$i$^4$g$^4$b | 192 |
| zeolite LTA-$Ca_4Na_4$ ($I_2$) | *cP*128 | 221,ml$^2$kihg | 429 |
| zeolite LTA-$Ca_4Na_4$ hydrated | *cP*104 | 221,mkihg$^4$ | 401 |
| zeolite LTA-$Ca_4Na_4$ hydrated | *cP*119 | 221,mkihg$^5$ea | 421 |
| zeolite LTA-$Cd_6$ | *cP*80 | 221,mkihg | 384 |
| zeolite LTA-$Cd_6$ | *cP*88 | 221,mkihg$^2$ | 388 |
| zeolite LTA-$Cd_6$ hydrated | *cP*192 | 221,m$^2$l$^2$kihg$^6$ | 454 |
| zeolite LTA-$Cd_6$ partly hydrated | *cP*152 | 221,m$^2$ki$^3$hg$^4$ | 444 |
| zeolite LTA-$Cd_6$ residual water | *cP*112 | 221,m$^2$kihg$^2$ | 412 |
| zeolite LTA-$Cd_6/Cd_5$ | *cP*134 | 221,m$^2$kihg$^4$f | 431 |
| zeolite LTA-$Cd_{9.5}Cl_4[OH]_3$ | *cP*163 | 221,m$^3$lkihg$^2$c | 447 |
| zeolite LTA-$Cd_{9.5}Cl_4[OH]_3$ hydrated | *cP*225 | 221,nm$^3$ljhg$^6$ed | 461 |
| zeolite LTA-$[Cd(H_2O)^{2+}]_3(Cd^{+})_3(Cd_2^{2+})_{1.5}$ residual water | *cP*160 | 221,m$^3$kihg$^5$ | 445 |
| zeolite LTA-$Cd_4Rb_4$ | *cP*91 | 221,mkihg$^2$c | 391 |
| zeolite LTA-$Cd_5Rb_2$ | *cP*91 | 221,mkihg$^2$c | 391 |
| zeolite LTA-$Co^{2+}{}_4Na_4$ (CO) | *cP*104 | 221,mkihg$^4$ | 400 |
| zeolite LTA-$Co^{2+}{}_{5.25}Na_{1.5}$ (CO) | *cF*968 | 226,ji$^4$g$^6$b | 189 |
| zeolite LTA-$Co^{2+}{}_4Na_4$ ($CS_2$) | *cP*196 | 221,nm$^2$lkj$^2$hg$^2$ | 455 |
| zeolite LTA-$Co^{2+}{}_4Na_4$ ($Cl_2$) | *cP*148 | 221,mlk$^2$jh$^2$g$^2$ | 442 |
| zeolite LTA-$Co^{2+}{}_4Na_4$ ($H_2S$) | *cP*134 | 221,m$^2$lkjhge | 431 |
| zeolite LTA-$Co^{2+}{}_{3.5}Na_5$ ($I_2$) | *cP*148 | 221,ml$^2$ki$^2$hg$^2$ | 441 |
| zeolite LTA-$Co^{2+}{}_4Na_4$ (NO) | *cP*140 | 221,m$^2$ki$^2$hg$^4$ | 435 |
| zeolite LTA-$Co^{2+}{}_4Na_4$ ($NO_2$) | *cP*144 | 221,m$^3$kihg$^3$ | 438 |
| zeolite LTA-$Co^{2+}{}_4Na_4$ ($S_8$) | *cP*144 | 221,m$^2$lkihg$^3$ | 438 |
| zeolite LTA-$Co^{2+}{}_4Na_4$ hydrated | *cP*391 | 221,n$^5$m$^3$kihg$^3$fa | 465 |
| zeolite LTA-$Co^{3+}{}_4Na_4[Br_3]_4$ ($Br_2$) | *cP*144 | 221,ml$^2$kihg$^3$ | 439 |
| zeolite LTA-$Cs_{12}$ (CsOH) | *cP*115 | 221,m$^2$kihg$^2$c | 415 |
| zeolite LTA-$Cs_{12}/Ag_{4.5}Cs$ | *cP*97 | 221,mkihg$^2$fc | 393 |
| zeolite LTA-$Cs_{11}Ca_{0.5}/Cs_{0.5}$ | *cP*111 | 221,mkjihg$^3$c | 410 |
| zeolite LTA-$Cs_{12}/Cs_{0.5}$ | *cP*103 | 221,mkjihg$^2$c | 400 |
| zeolite LTA-$Cs_7K_5$ | *cP*115 | 221,mkihg$^5$c | 417 |
| zeolite LTA-$Cs_3Na_9$ | *cP*95 | 221,mkjihgc | 393 |
| zeolite LTA-$Cs_7Na_5$ | *cP*99 | 221,mkihg$^3$c | 396 |
| zeolite LTA-$Cs_3Na_9$ hydrated | *cP*147 | 221,m$^2$lkihg$^3$c | 439 |
| zeolite LTA-$Cs_{8.5}Na_{3.5}/Cs_{0.5}$ | *cP*123 | 221,m$^2$kihg$^3$c | 426 |
| zeolite LTA-$Cs_9Na_3/Cs_2$ | *cP*119 | 221,mkjihg$^4$c | 422 |
| zeolite LTA-$Cs_3Na_8H$ (Ar) | *cP*115 | 221,mkji$^2$hg$^2$c | 417 |
| zeolite LTA-$Cs_3Na_8H$ (Kr) | *cP*111 | 221,mkjihg$^3$c | 411 |
| zeolite LTA-$Cs_3Na_8H$ (Xe) | *cP*104 | 221,mkjihg$^2$ca | 403 |
| zeolite LTA-$Cs_3Na_8H$ (Xe) | *cP*120 | 221,mkjihg$^4$ca | 424 |

| structure type | Pearson symbol | space group number, Wyckoff sequence | page |
|---|---|---|---|
| zeolite LTA-$Cs_9Tl_3$ | *cP*129 | 221,mlkihg$^3$fc | 430 |
| zeolite LTA-$Cu^{2+}{}_8$ $(OH)_4$ | *cP*112 | 221,mkji$^2$hg$^2$ | 414 |
| zeolite LTA-$(Cu^{2+})_5(Cu^+)_{1.25}(Cu_3{}^+)_{0.25}$ $(Cu_2OH^+)_{0.5}$ | *cP*115 | 221,mkjihg$^3$ea | 418 |
| zeolite LTA-$(Cu^{2+})_5Cu^+(Cu_2$ $OH^+)$ residual water | *cP*124 | 221,mkjihg$^5$ | 427 |
| zeolite LTA-$Eu^{2+}{}_{5.75}Na_{0.5}$ | *cP*103 | 221,mkjihg$^2$c | 399 |
| zeolite LTA-$Eu^{2+}{}_5Na$ hydrated | *cP*208 | 221,nm$^4$kihg$^2$ | 457 |
| zeolite LTA-$[Eu^{4+}Cl_2]_4Eu^{2+}{}_{1.5}Na$ | *cP*102 | 221,mkihg$^3$f | 397 |
| zeolite LTA-$(Eu^{4+}O)_{2.75}Eu^{2+}{}_{1.75}Na_3$ | *cP*120 | 221,mkji$^2$hg$^3$ | 423 |
| zeolite LTA-$Fe^{2+}{}_{2.7}Na_{6.6}$ hydrated | *cP*161 | 221,m$^3$lkihg$^2$a | 446 |
| zeolite LTA-$In_{8.75}$ $(S_2)$ | *cP*225 | 221,n$^2$m$^2$kihg$^4$a | 460 |
| zeolite LTA-$K_{11.5}$ | *cF*944 | 226,ji$^5$hg$^2$e | 189 |
| zeolite LTA-$K_{11.5}$ | *cP*118 | 221,mkji$^2$hg$^2$e | 420 |
| zeolite LTA-$K_{12}$ | *cP*116 | 221,mki$^2$hg$^4$ | 419 |
| zeolite LTA-$K_{12}$ hydrated | *cP*148 | 221,m$^3$ljihg$^2$ | 441 |
| zeolite LTA-$K_{12}/K_{0.5}$ | *cP*112 | 221,mkji$^2$hg$^2$ | 414 |
| zeolite LTA-$K_{12}/K_1$ | *cP*103 | 221,mkjihg$^2$c | 398 |
| zeolite LTA-$K_{12}/K_1$ | *cP*118 | 221,mkji$^2$hg$^2$e | 420 |
| zeolite LTA-$K_{12}/K_3$ | *cF*776 | 225,lk$^3$jhf$^4$e | 304 |
| zeolite LTA-$K_{12}/K_5$ | *cF*784 | 225,lk$^4$jhf$^2$ | 305 |
| zeolite LTA-$K_{7.5}Na_{4.5}$ | *cF*896 | 226,ji$^5$hg$^2$ | 187 |
| zeolite LTA-$Li_{12}$ | *cF*736 | 226,ji$^5$g | 181 |
| zeolite LTA-$Li_{12}$ $(LiNO_3)$ hydrated | *cP*225 | 221,m$^4$ljihg$^5$fe$^3$dba | 459 |
| zeolite LTA-$Li_{12}$ $(Li_2O)$ | *cF*760 | 226,ji$^5$gd | 182 |
| zeolite LTA-$Mg_2Na_8$ residual water | *cF*864 | 226,ji$^5$g$^3$ | 186 |
| zeolite LTA-$Mn^{2+}{}_{4.5}Na_3$ hydrated | *cP*151 | 221,ml$^2$kihg$^3$fa | 444 |
| zeolite LTA-$[NH_4]_{12}$ | *cF*992 | 226,j$^2$i$^4$hg$^2$ | 190 |
| zeolite LTA-$Na_{11.5}$ | *cP*104 | 221,mkji$^2$hg | 401 |
| zeolite LTA-$Na_{11.6}$ | *cF*832 | 226,ji$^5$hg | 183 |
| zeolite LTA-$Na_{12}$ | *cP*104 | 221,mlkihg | 403 |
| zeolite LTA-$Na_{12}$ | *cP*120 | 221,m$^2$lkih | 423 |
| zeolite LTA-$Na_{12}$ $(Br_2)$ | *cP*128 | 221,nmkihg | 429 |
| zeolite LTA-$Na_{12}$ $(H_2S)$ | *cP*160 | 221,m$^2$lkj$^2$ihg$^2$ | 445 |
| zeolite LTA-$Na_{11}$ $(NH_3)$ | *cP*150 | 221,m$^2$lkihg$^3$e | 443 |
| zeolite LTA-$Na_{12}$ $(NH_3)$ | *cP*116 | 221,m$^2$kjihg | 418 |
| zeolite LTA-$Na_{12}$ $(NaAlO_2)$ hydrated | *cP*72 | 221,mkih | 382 |
| zeolite LTA-$Na_{12}$ $(NaNO_3)$ hydrated | *cP*187 | 221,m$^3$lj$^2$i$^2$hg$^3$ea | 453 |
| zeolite LTA-$Na_{12}$ $(NaNO_3)$ hydrated | *cP*278 | 221,m$^4$lk$^2$jihg$^6$f$^2$e$^2$ba | 463 |
| zeolite LTA-$Na_{11}$ $(S_8)$ | *cP*140 | 221,m$^2$lkj$^2$hg | 436 |
| zeolite LTA-$Na_{12}$ (Xe) | *cP*201 | 221,nm$^3$kji$^2$hga | 457 |
| zeolite LTA-$Na_{12}$ hydrated | *cF*1600 | 226,j$^5$i$^5$hg | 193 |
| zeolite LTA-$Na_{12}$ hydrated | *cF*1864 | 226,j$^7$i$^4$g$^2$a | 194 |
| zeolite LTA-$Na_{12}$ hydrated | *cF*2120 | 226,j$^7$i$^5$hg$^3$a | 197 |
| zeolite LTA-$Na_{12}$ hydrated | *cP*92 | 221,mki$^2$hg | 392 |
| zeolite LTA-$Ni^{2+}Na_{10}$ hydrated | *cF*1312 | 226,j$^3$i$^5$g$^4$ | 192 |
| zeolite LTA-$Ni^{2+}{}_3Na_6$ hydrated | *cP*216 | 221,nm$^3$lkihg$^3$ | 459 |
| zeolite LTA-$Ni^{2+}{}_{3.5}Na_3H_2$ hydrated | *cP*269 | 221,nm$^4$lkj$^2$i$^2$hg$^2$b | 462 |
| zeolite LTA-$Pb_6$ | *cP*112 | 221,mk$^2$ihg$^2$ | 413 |
| zeolite LTA-$Pb_9(OH)_8$ residual water | *cP*280 | 221,n$^2$m$^4$kihg$^5$ | 464 |
| zeolite LTA-$Pb_9O(OH)_4$ residual water | *cP*188 | 221,m$^4$kjihg$^4$ | 453 |