Crystal Structure Descriptions, 2nd edition

In this appendix, most of the crystal structure types introduced in the main text are formally described by means of their chemical formulas, StrukturBericht symbols, space groups, lattice parameters, special atom positions, etc. In addition, examples of actual compounds with these structures are given, along with their lattice parameters. All lattice parameters are stated in nm.

Structure types are listed in the order in which they appear in the text, and are sequentially numbered. Most of the structural data in this appendix was extracted from the following sources:

- P. Villars, *Pearson's Handbook Desk Edition*, ASM International, Materials Park, OH (1997);
- R.W.G. Wyckoff, *Crystal Structures*, John Wiley, New York (1963);
- C.S. Hurlbut and C. Klein, *Manual of Mineralogy, 9th Edition*, John Wiley and Sons, New York (1977).

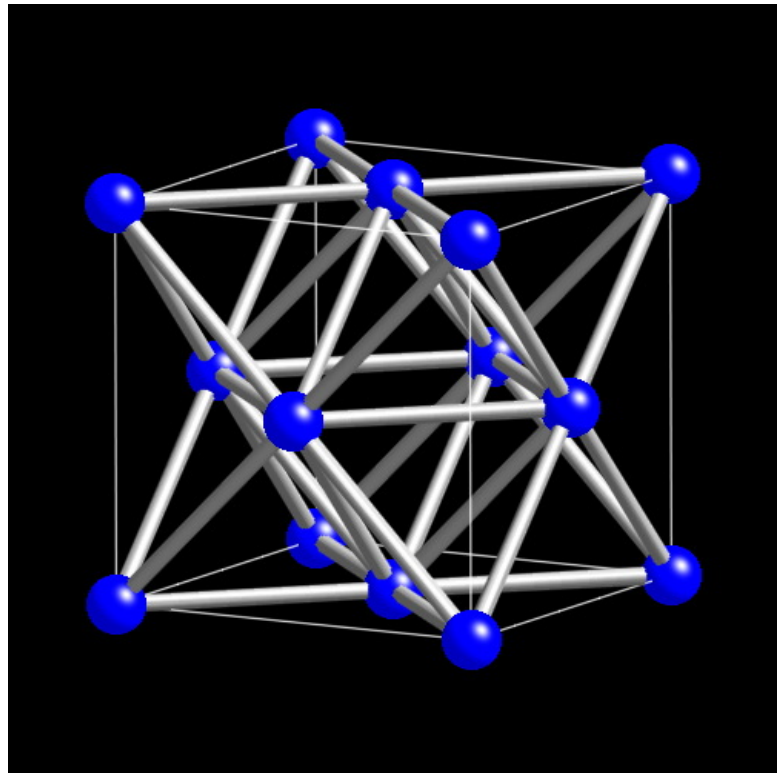
When consulting the tables on the following pages, one must be aware of the fact that many compounds can have multiple crystal structures; it is always a good idea to consult the original sources listed above (and others) to verify that the correct structure is obtained. In particular, the examples of structures of a given structure type will often include metastable structures, or high temperature/high pressure phases; we refer the reader to the original sources for those details. Furthermore, atom coordinates provided in this appendix have been used with the sole purpose of creating structure visualizations; this means that sites with partial occupancy will show up in a structure drawing as fully occupied sites. The reader who wishes to compute x-ray powder patterns for any of these structures should consult the original citations to make sure that all site occupancies are properly accounted for.

The compound names for intermetallics are listed in the same convention as in Pearson's lists, namely an alphabetical ranking of all the elements in the compound, except for the prototype chemical formulas, for which we follow the list by J. Lima de Faria (J. Lima de Faria, *Structural Classification and Notation*, Chapter 1 in *Intermetallic Compounds, Vol. 3*, edited by J.H. Westbrook and R.L. Fleischer, John Wiley and Sons, New York (2002)). For instance, BiF_3 is the prototype for the $D0_3$ structure, which has Mg_3Pr and $AlFe_3$ as example compounds; note that the elements are listed alphabetically, so that the AB_3 compound is sometimes written as B_3A. The only exception will be when the conventional prototype name is not in alphabetical order, for instance ZnS, in which case we do not change the order to SZn.

The present version of this structures appendix was completed on June 16, 2013; updates containing corrections will be posted as needed.

Table A.0. Alphabetical list of all prototype structures described in this appendix, along with the page number on which the complete description can be found. Note that for compounds, constituent elements are ranked alphabetically. If you know the structure number, then the page number is obtained simply by adding 2.

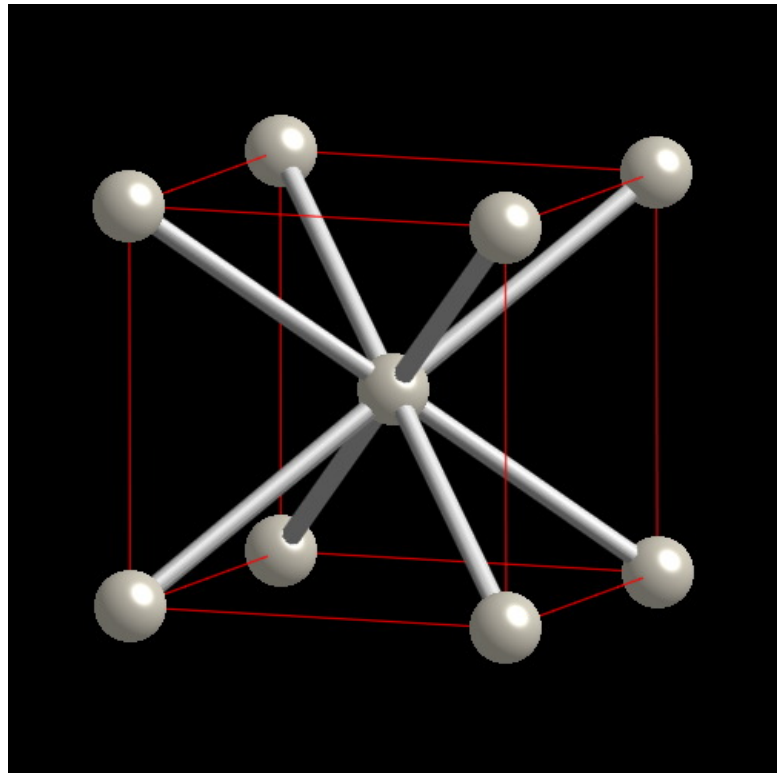
Structure 1 *Prototype:* Cu
SBS/PS: A1/cF4 *SG # 225:* **Fm$\bar{3}$m** (O_h^5)
Lattice complex: Cu @ $4a(0,0,0)$



Element	a	Element	a	Element	a	Element	a
Cu	0.3615	Ag	0.4086	Au	0.4078	Al	0.4049
Ni	0.3524	Pd	0.3891	Pt	0.3924	Pb	0.4950

Table A.1. Representative elements for Structure 1. Pearson's tables list 485 intermetallic compounds (mostly solid solutions) with this structure type.

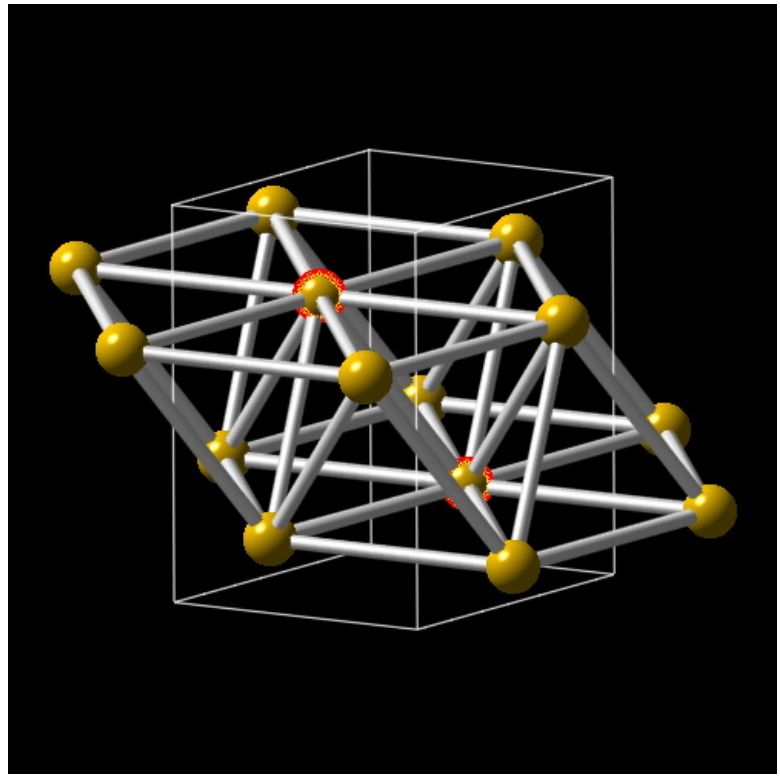
Structure 2 *Prototype:* W
SBS/PS: A2/cI2 *SG # 229:* **Im$\bar{3}$m** (O_h^9)
Lattice complex: W @ $2a(0,0,0)$



Element	a	Element	a		
W	3.1650	Fe	2.8664	Cr	2.8846
Mo	3.1469	Ta	3.3026	Ba	5.0190

Table A.2. Representative elements for Structure 2. Pearson's tables list 333 intermetallic compounds (mostly solid solutions) with this structure type.

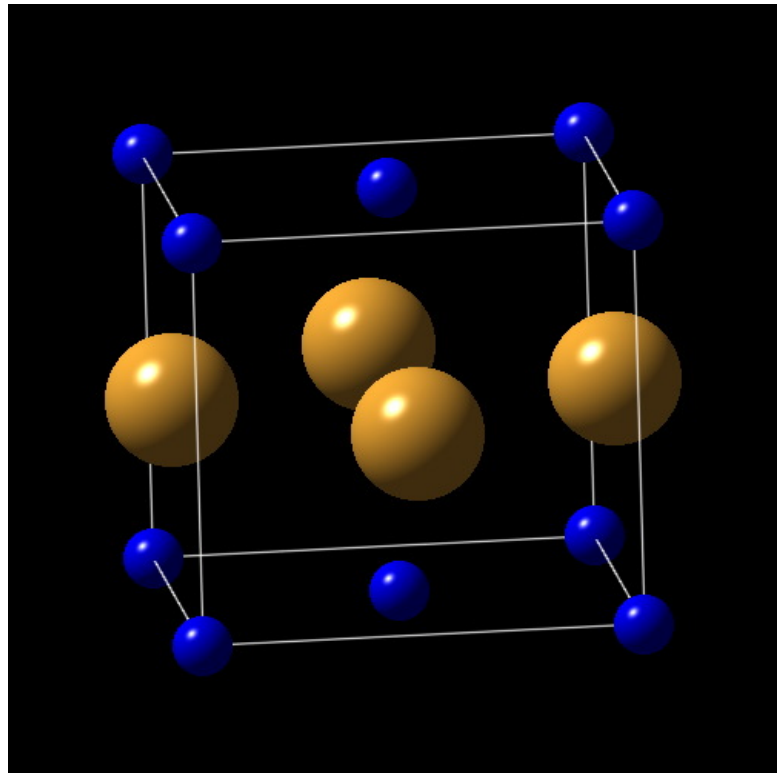
Structure 3 *Prototype:* Mg
SBS/PS: A3/hP2 *SG # 194:* **P6$_3$/mmc** (D^4_{6h})
Lattice complex: Mg @ $2d(\frac{2}{3}, \frac{1}{3}, \frac{1}{4})$



Compound	a	c	$\frac{c}{a}$	Compound	a	c	$\frac{c}{a}$
Mg	0.3209	0.5210	1.623	Be	0.2286	0.3583	1.568
Zn	0.2665	0.4947	1.856	Cd	0.2979	0.5617	1.885
Ti	0.2950	0.4679	1.586	Zr	0.3232	0.5148	1.593
Ru	0.2706	0.4282	1.582	Os	0.2735	0.4319	1.579
Re	0.2761	0.4458	1.615	Sm			

Table A.3. Representative elements for Structure 3. Pearson's tables list 120 intermetallic compounds (mostly solid solutions) with this structure type.

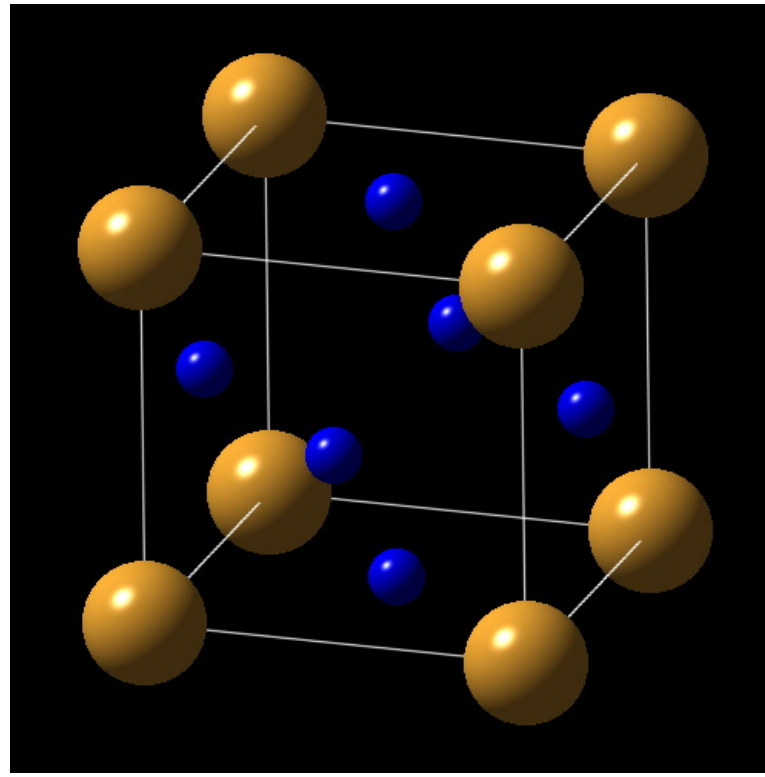
Structure 4 *Prototype:* AuCu
SBS/PS: $\mathsf{L1}_0$/tP4 (or tP4 with centered cell) *SG # 123:* **P4/mmm** (D_{4h}^1)
Lattice complex: Au @ $2e(0,\frac{1}{2},\frac{1}{2})$; Cu @ $1a(0,0,0)$ and $1c(\frac{1}{2},\frac{1}{2},0)$



Compound	a	c	$\frac{c}{a}$	Compound	a	c	$\frac{c}{a}$
AuCu	0.3963	0.3671	0.926	AgTi	0.4104	0.4077	0.993
AlTi	0.3984	0.4065	1.020	CoPt	0.3806	0.3684	0.968
CrPd	0.3879	0.3802	0.980	FePd	0.3852	0.3723	0.966
MnNi	0.3690	0.3490	0.945	PtZn	0.4026	0.3474	0.863

Table A.4. Representative compounds for Structure 4. Pearson's tables list 97 intermetallic compounds with this structure type.

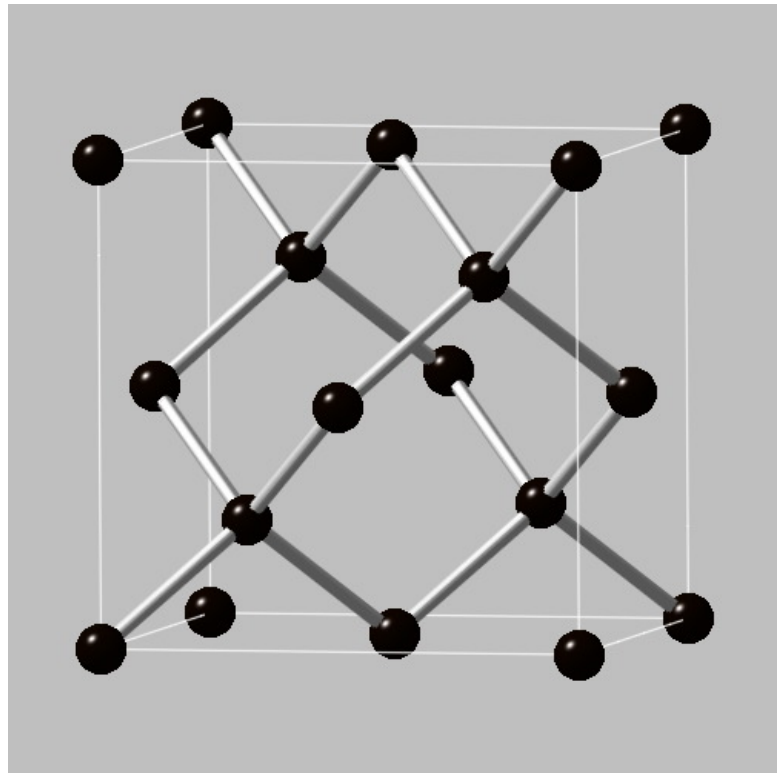
Structure 5 *Prototype:* $AuCu_3$
SBS/PS: $L1_2$/cP4 *SG # 221:* **Pm$\bar{3}$m** (O_h^1)
Lattice complex: Au @ $1a(0,0,0)$; Cu @ $3c(0,\frac{1}{2},\frac{1}{2})$



Compound	a	Compound	a	Compound	a	Compound	a
$AuCu_3$	0.3749	$AgPt_3$	0.3900	$AlNi_3$	0.3572	$TiZn_3$	0.3932
$AlPt_3$	0.3876	Al_3Er	0.4215	Al_3U	0.4287	Pd_3Y	0.4074

Table A.5. Representative compounds for Structure 5. Pearson's tables list 436 intermetallic compounds with this structure type.

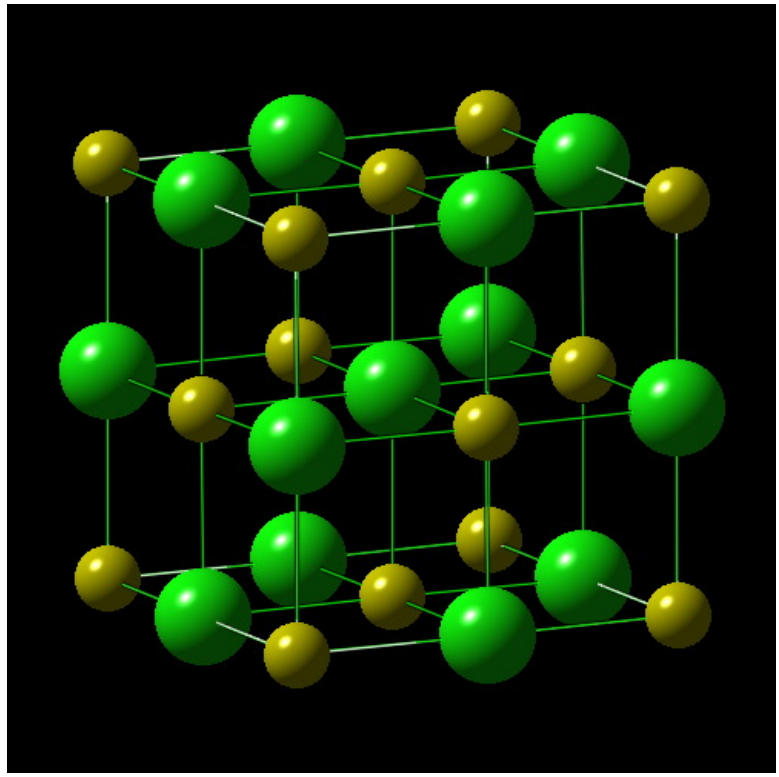
Structure 6 *Prototype:* C (diamond)
SBS/PS: A4/cF8 *SG # 227:* **Fd$\bar{3}$m** (O_h^7)
Lattice complex: C @ $8a(0,0,0)$



Element	a	Element	a
C	0.356	Si	0.5431
Ge	0.5657	α-Sn	0.6491

Table A.6. Representative elements for Structure 6. Pearson's tables list 16 intermetallic compounds with this structure type.

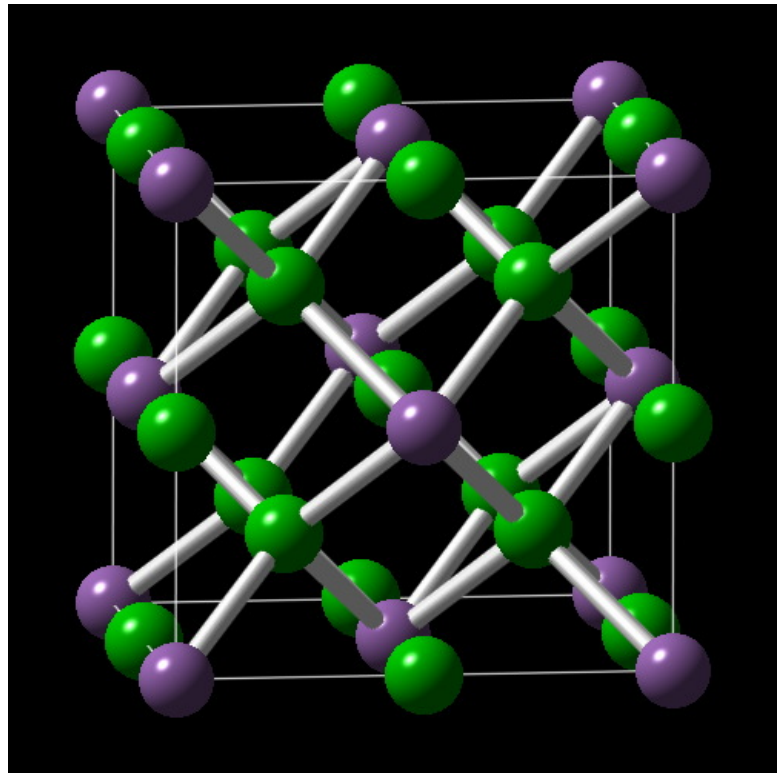
Structure 7 *Prototype:* NaCl (rock salt)
SBS/PS: B1/cF8 *SG # 225:* **Fm$\bar{3}$m** (O_h^5)
Lattice complex: Na @ $4a(0,0,0)$; Cl @ $4b(\frac{1}{2},\frac{1}{2},\frac{1}{2})$



Compound	a	Compound	a	Compound	a
NaCl	0.5640	MgO	0.4213	FeO	0.4307
MgS	0.5200	BaSe	0.6600	CaTe	0.6356
LiF	0.4027	BrNa	0.5977	TiN	0.4240

Table A.7. Representative compounds for Structure 7. Pearson's tables list 799 intermetallic compounds with this structure type.

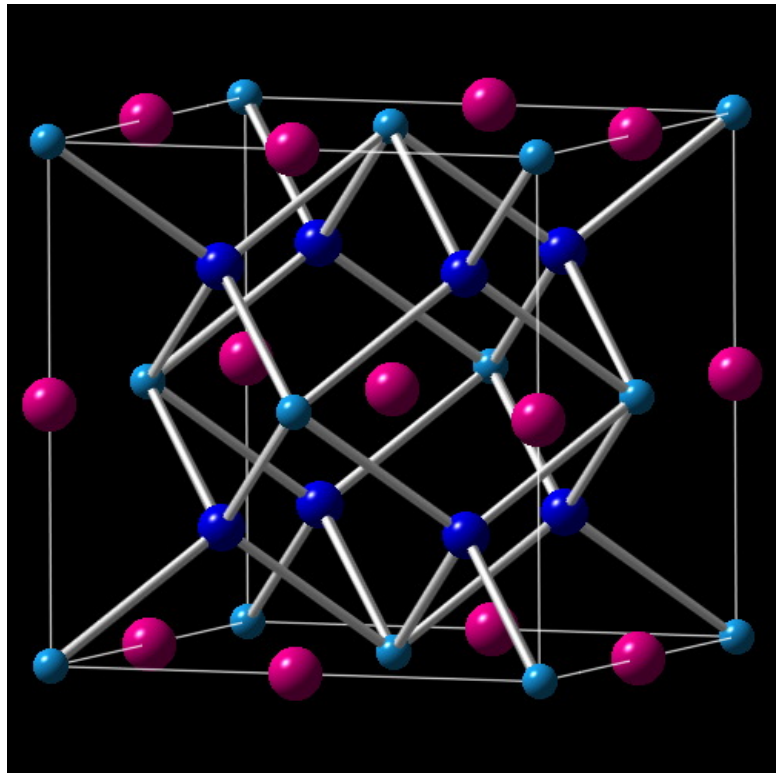
Structure 8 *Prototype:* BiF_3
SBS/PS: $D0_3$/cF16 *SG # 225:* $\mathbf{Fm\bar{3}m}$ (O_h^5)
Lattice complex: Bi @ $4a(0,0,0)$; F @ $4b(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ and $8c(\frac{1}{4},\frac{1}{4},\frac{1}{4})$



Compound	a	Compound	a	Compound	a
BiF_3	0.5865	$BiLi_3$	0.6722	Cd_3Pr	0.7200
$CeMg_3$	0.7438	Cu_3Sb	0.6010	Fe_3Si	0.5662
Mg_3Pr	0.7430	$AlFe_3$	0.5780	Mn_3Si	0.5722

Table A.8. Representative compounds for Structure 8. Pearson's tables consider both $D0_3$ and $L2_1$ structure types under the BiF_3 prototype, and list 394 intermetallic compounds with this structure type.

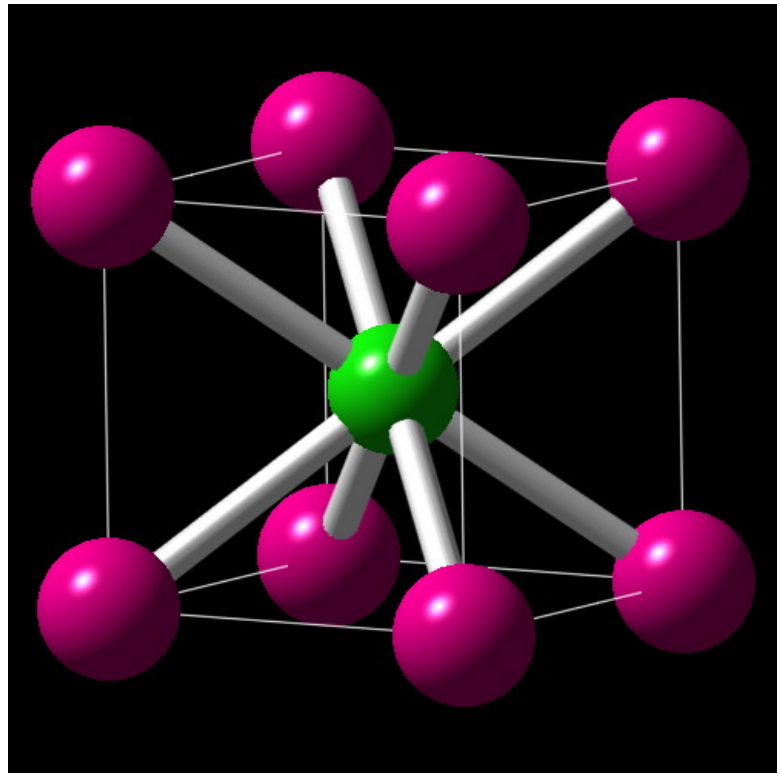
Structure 9 *Prototype:* $AlCu_2Mn$ (Heusler)
SBS/PS: $L2_1/cF16$ *SG # 225:* $\mathbf{Fm\bar{3}m}$ (O_h^5)
Lattice complex: Cu @ $8c(\frac{1}{4},\frac{1}{4},\frac{1}{4})$; Al @ $4a(0,0,0)$; Mn @ $4b(\frac{1}{2},\frac{1}{2},\frac{1}{2})$



Compound	a	Compound	a	Compound	a
$AlCu_2Mn$	0.5949	Cu_2MnSb	0.6097	Cu_2FeSn	0.5930
$AlCu_2Hf$	0.6172	$AlNi_2Ti$	0.5850	$GaMnNi_2$	0.xxxx
Co_2MnSn	0.5989	$AlCo_2Nb$	0.5946	$AlCo_2Ta$	0.5927

Table A.9. Representative compounds for Structure 9. Pearson's tables consider both $D0_3$ and $L2_1$ structure types under the BiF_3 prototype, and list 394 intermetallic compounds with this structure type.

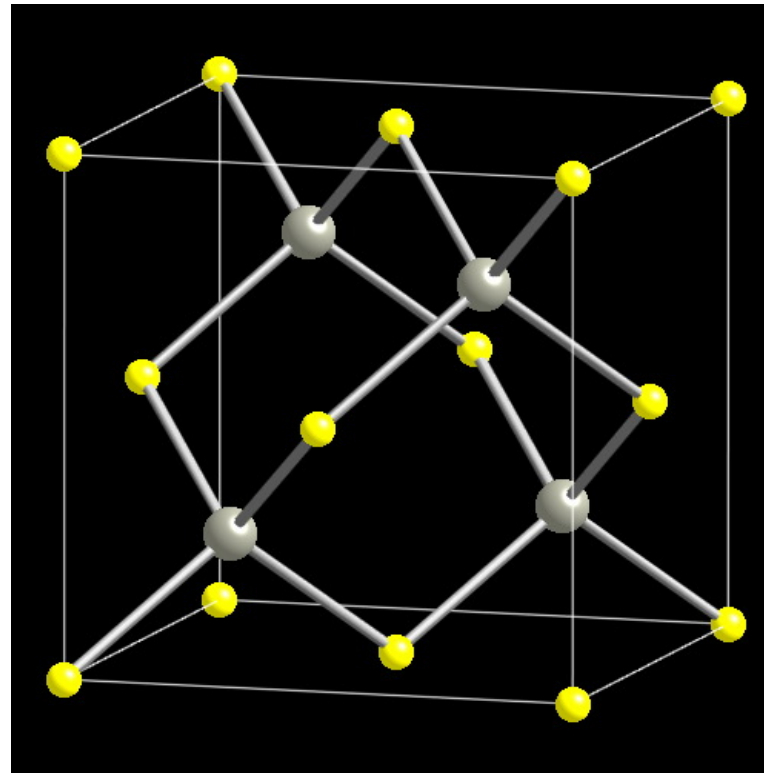
Structure 10 *Prototype:* CsCl
SBS/PS: B2/cP2 *SG # 221:* **Pm$\bar{3}$m** (O_h^1)
Lattice complex: Cs @ $1a(0,0,0)$; Cl @ $1b(\frac{1}{2},\frac{1}{2},\frac{1}{2})$



Compound	a	Compound	a	Compound	a	Compound	a
CsCl	0.4123	BrCs	0.4286	AlCo	0.2862	AgMg	0.3280
CoTi	0.2986	CuZn	0.2945	FeTi	0.2976	NiTi	0.2972

Table A.10. Representative compounds for Structure 10. Pearson's tables list 461 intermetallic compounds with this structure type.

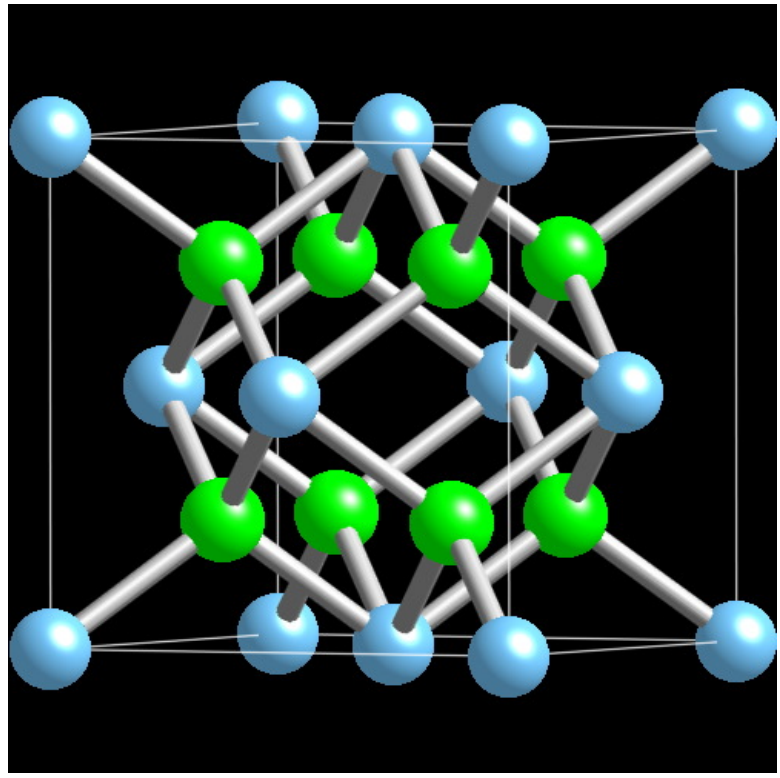
Structure 11 *Prototype:* ZnS (zinc-blende)
SBS/PS: B3/cF8 *SG # 216:* **F$\bar{4}$3m** (T_d^2)
Lattice complex: S @ $4a(0,0,0)$; Zn @ $4c(\frac{1}{4},\frac{1}{4},\frac{1}{4})$



Compound	a	Compound	a	Compound	a	Compound	a
ZnS	0.5406	AlP	0.5451	BeSe	0.5070	SeZn	0.5667
TeZn	0.6103	GaP	0.5448	AsGa	0.5653	GaSb	0.6095
InP	0.5869	CdTe	0.6481	AlAs	0.5662		

Table A.11. Representative compounds for Structure 11. Pearson's tables list 247 intermetallic compounds with this structure type.

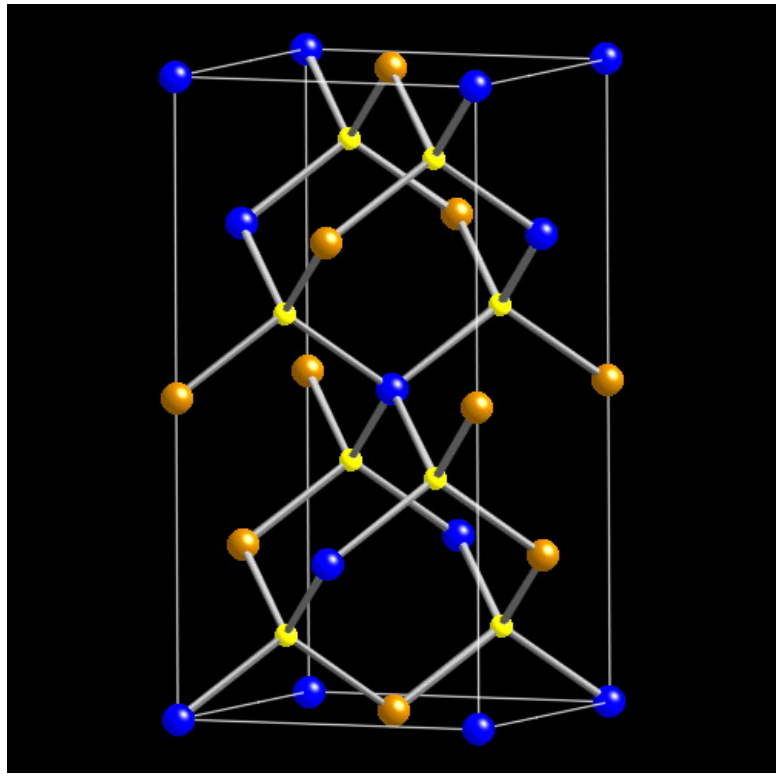
Structure 12 *Prototype:* CaF_2 (fluorite)
SBS/PS: C1/cF12 *SG # 225:* **Fm$\bar{3}$m** (O_h^5)
Lattice complex: Ca @ $4a(0,0,0)$; F @ $8c(\frac{1}{4},\frac{1}{4},\frac{1}{4})$



Compound	a	Compound	a	Compound	a
CaF_2	0.5463	F_2Sr	0.5800	$BaCl_2$	0.7311
O_2Pb	0.5349	O_2U	0.5372	Li_2O	0.4611
Na_2Se	0.6823	K_2S	0.7406	ORb_2	0.6740

Table A.12. Representative compounds for Structure 12. Pearson's tables list 137 intermetallic compounds with this structure type.

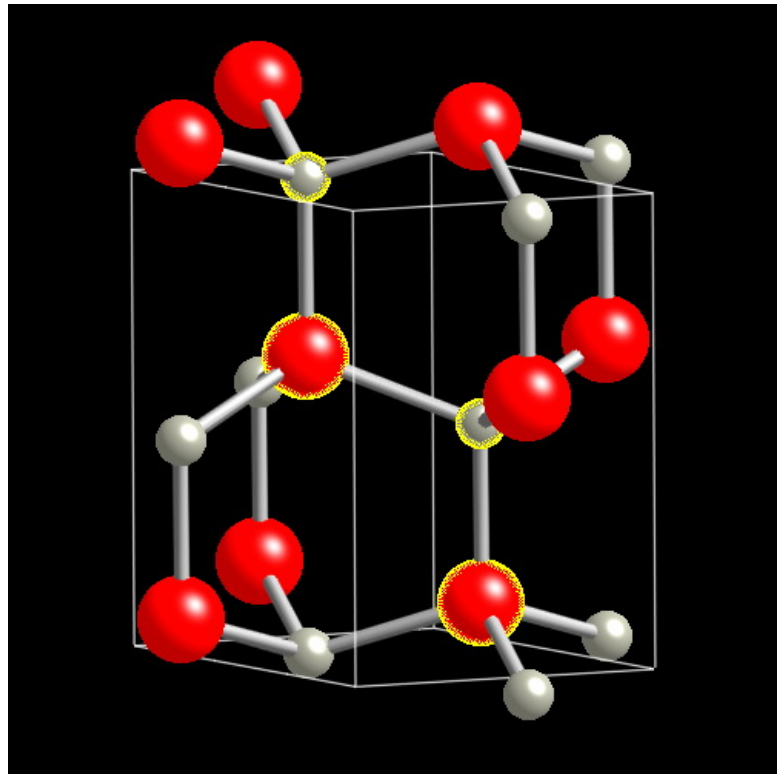
Structure 13 *Prototype:* $CuFeS_2$ (chalcopyrite)
SBS/PS: $E1_1$/tI16 *SG # 122:* $\mathbf{I\bar{4}2d}$ (D_{2d}^{12})
Lattice complex: Cu @ $4a(0,0,0)$; Fe @ $4b(0,0,\frac{1}{2})$; S @ $8d(x,\frac{1}{4},\frac{1}{8})$ with $x = \frac{1}{4}$



Compound	a	c	Compound	a	c
$CuFeS_2$	0.524	1.03	$AgAlTe_2$	0.6296	1.183
$AlCuSe_2$	0.5605	1.090	$CdGeP_2$	0.5738	1.0765

Table A.13. Representative compounds for Structure 13. Pearson's tables list 132 intermetallic compounds with this structure type.

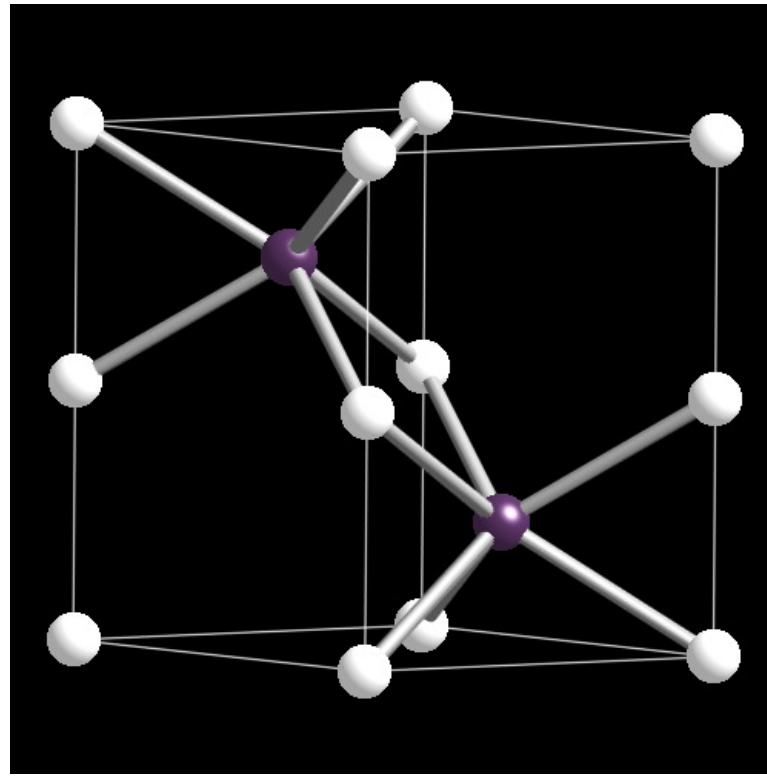
Structure 14 *Prototype:* ZnS(wurtzite)
SBS/PS: B4/hP4 *SG # 186:* **P6$_3$mc** (C_{6v}^4)
Lattice complex: Zn @ $2b(\frac{1}{3},\frac{2}{3},z)$ with $z=0$; S @ $2b(\frac{1}{3},\frac{2}{3}z)$ with $z=\frac{3}{8}$



Compound	a	c	Compound	a	c
ZnO	0.335	0.522	ZnS	0.381	0.623
BP	0.3562	0.590	GaN	0.3190	0.5189

Table A.14. Representative compounds for Structure 14. Pearson's tables list 86 intermetallic compounds with this structure type.

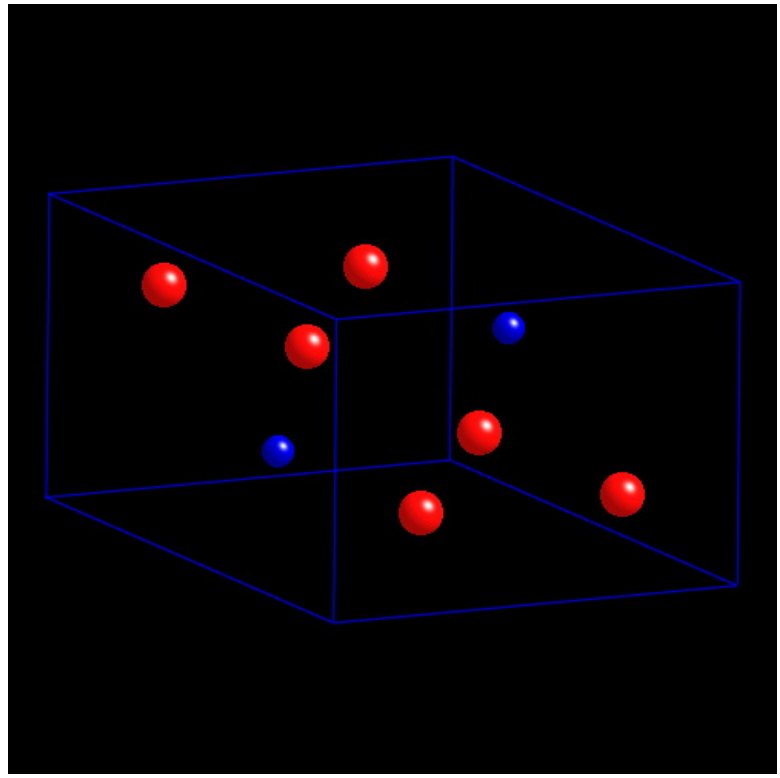
Structure 15 *Prototype:* NiAs
SBS/PS: $B8_1$/hP4 *SG # 194:* **$P6_3mmc$** (D^4_{6h})
Lattice complex: Ni @ $2a(0,0,0)$; As @ $2c(\frac{1}{3},\frac{2}{3},\frac{1}{4})$



Compound	a	c	Compound	a	c
NiAs	0.36	0.501	AuSe	0.412	0.539
NbSb	0.4270	0.5447	CrS	0.3419	0.5550

Table A.15. Representative compounds for Structure 15. Pearson's tables list 217 intermetallic compounds with this structure type.

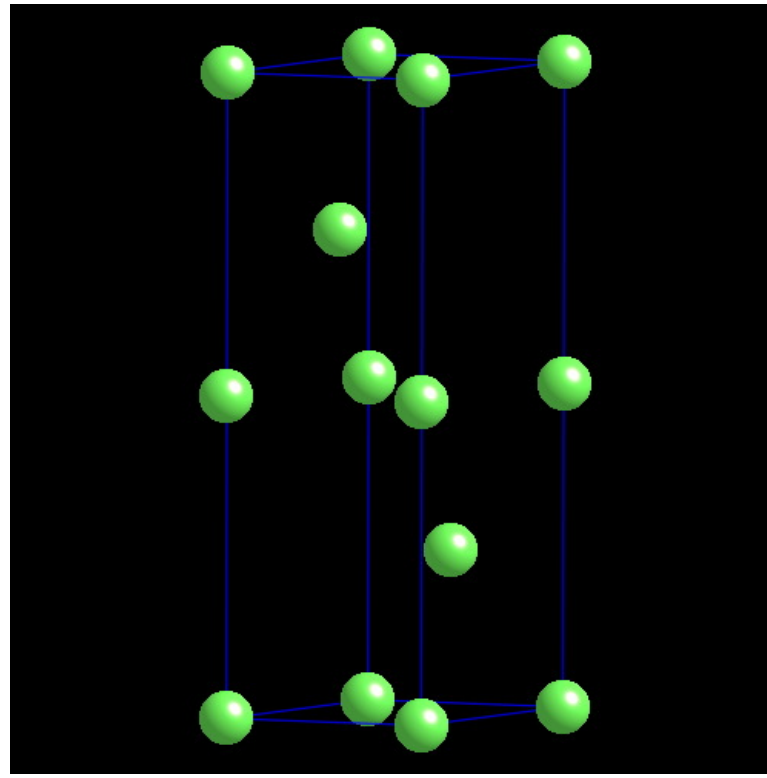
Structure 16 *Prototype:* Ni_3Sn
SBS/PS: $D0_{19}$/hP8 *SG # 194:* **P6$_3$mmc** (D^4_{6h})
Lattice complex: Ni @ $2c(\frac{1}{3},\frac{2}{3},\frac{1}{4})$; Sn @ $6h(x,2x,\frac{1}{4})$ with $x=\frac{5}{6}$



Compound	a	c	Compound	a	c
Ni_3Sn	0.5275	0.4234	Fe_3Ga	0.520	0.426
$InTi_3$	0.589	0.476	Al_3Sm	0.6380	0.4597

Table A.16. Representative compounds for Structure 16. Pearson's tables list 106 intermetallic compounds with this structure type.

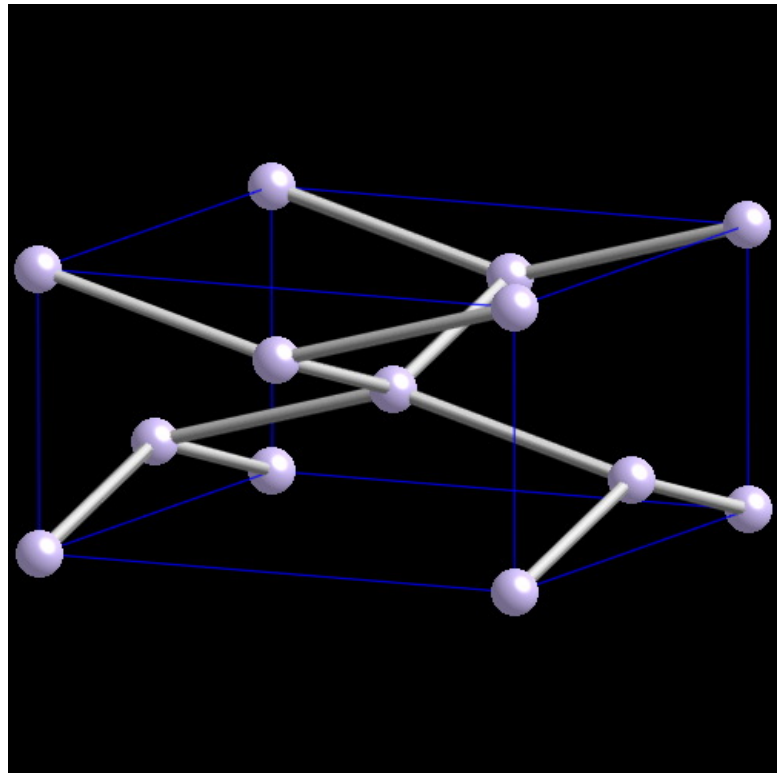
Structure 17 *Prototype:* α-La
SBS/PS: A3'/hP4 *SG # 194:* **P6$_3$mmc** (D^4_{6h})
Lattice complex: La @ $2a(0,0,0)$ and $2c(\frac{1}{3},\frac{2}{3},\frac{1}{4})$



Compound	a	c	Compound	a	c
α-La	0.377	1.21596	Nd	0.36562	1.18056
Gd	0.3402	1.1047	Sm	0.3565	1.11456

Table A.17. Representative compounds for Structure 17. Pearson's tables list 34 intermetallic compounds with this structure type.

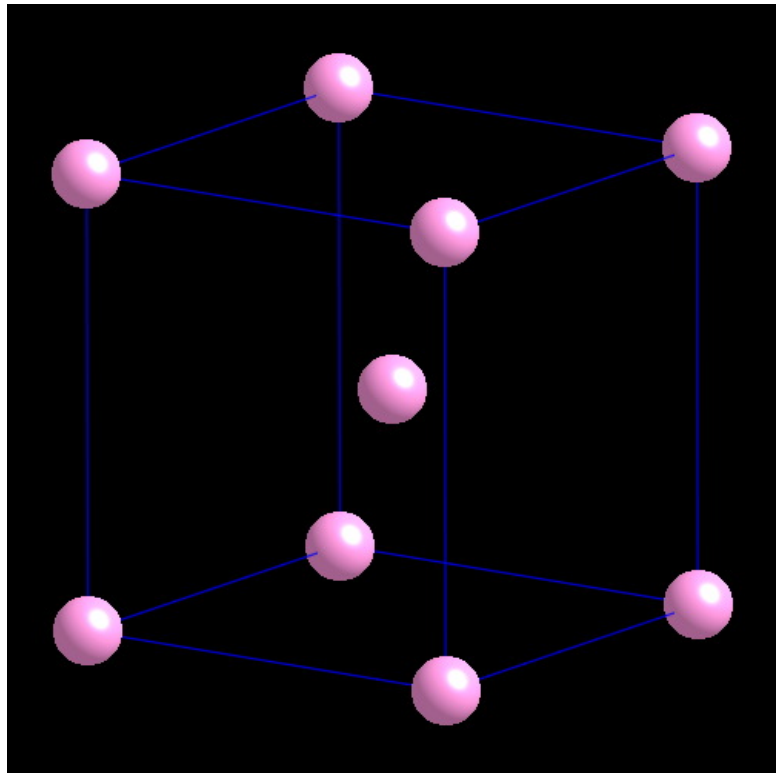
Structure 18 *Prototype:* β-Sn
SBS/PS: A5/tI4 *SG # 141:* $\mathbf{I4_1/amd}$ $(D_{4h}{}^{19})$
Lattice complex: Sn @ $4a(0,0,0)$ with origin (1) offset $(0, \frac{1}{4}, \frac{-1}{8})$ from the center of symmetry



Compound	a	c	Compound	a	c
β-Sn	0.58197	0.31750	Ge	0.49585	0.27463

Table A.18. Representative compounds for Structure 18. Pearson's tables list 20 intermetallic compounds with this structure type.

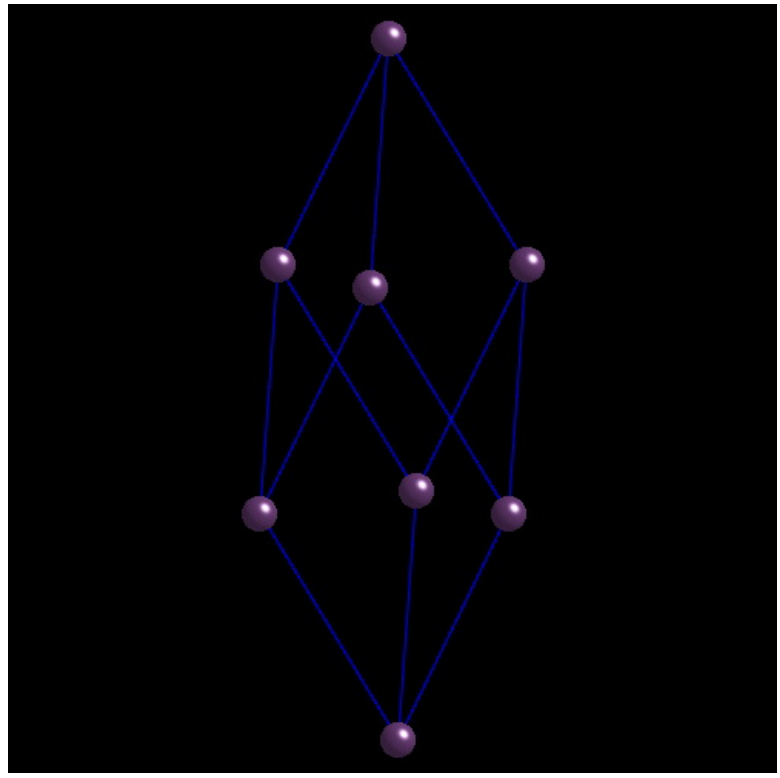
Structure 19 *Prototype:* In
SBS/PS: A6/tI2 *SG # 139:* **I4/mmm** $(D_{4h}{}^{17})$
Lattice complex: In @ $2a(0,0,0)$



Compound	a	c	Compound	a	c
In	0.4598	0.4947	Pa	0.3925	0.3238

Table A.19. Representative compounds for Structure 19. Pearson's tables list 28 intermetallic compounds with this structure type.

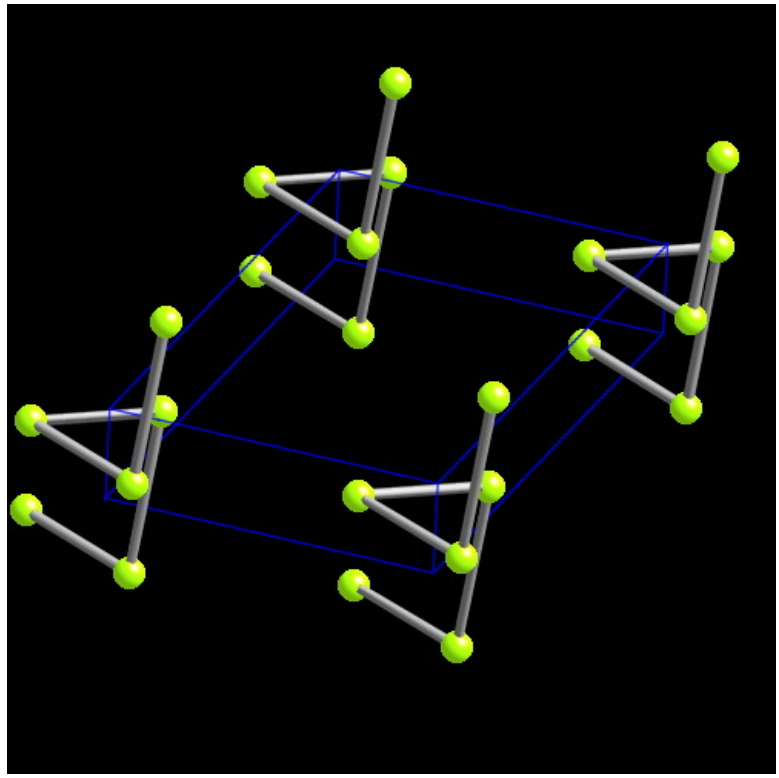
Structure 20 *Prototype:* As
SBS/PS: A7/hR2 *SG # 166:* **R$\bar{3}$m** $(D_{3d}{}^5)$
Lattice complex: As @ $6c(0,0,z)$ with $z = 0.2271$.



Compound	a	c	Compound	a	c
As	0.3760	1.0547	Bi	0.4546	1.1862

Table A.20. Representative compounds for Structure 20. Pearson's tables list 21 intermetallic compounds with this structure type.

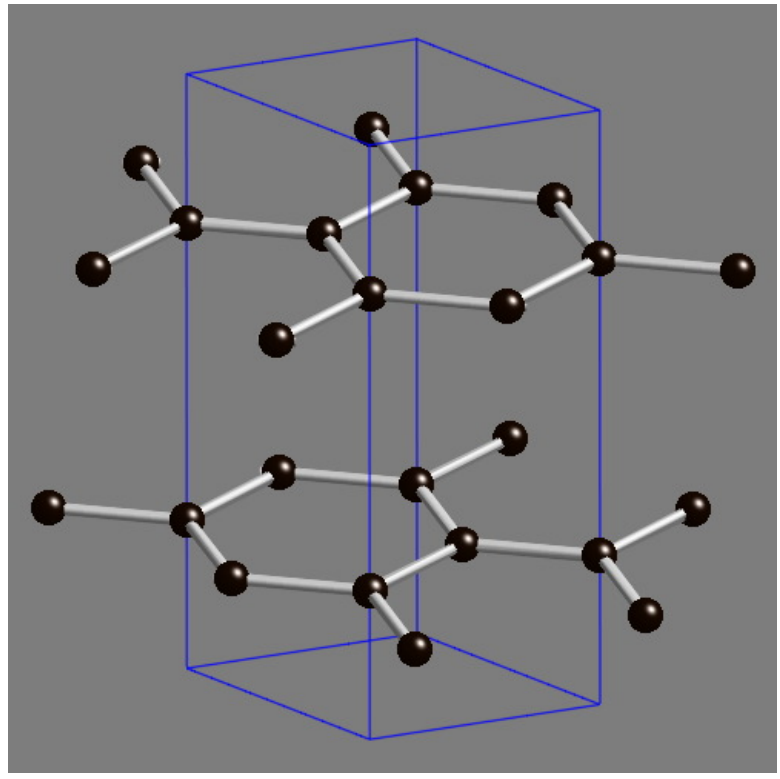
Structure 21 *Prototype:* γ-Se
SBS/PS: A8/hP3 *SG # 152:* **P3$_1$21** ($D_3{}^4$)
Lattice complex: Se @ $3a(0.7364, 0, \frac{1}{3})$



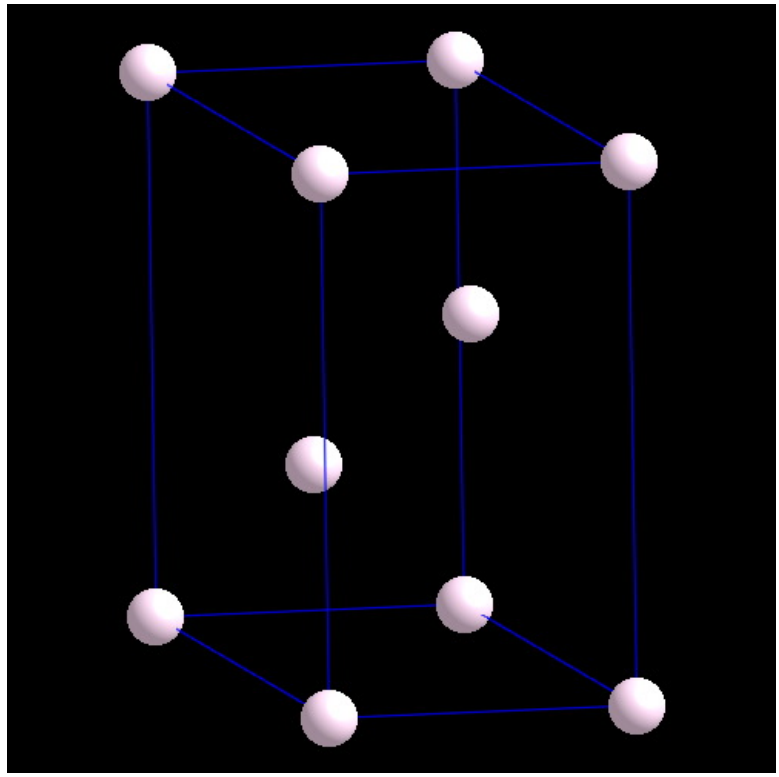
Compound	a	c	Compound	a	c
Se	0.4366	0.4959	Te	0.4527	0.5921

Table A.21. Representative compounds for Structure 21.

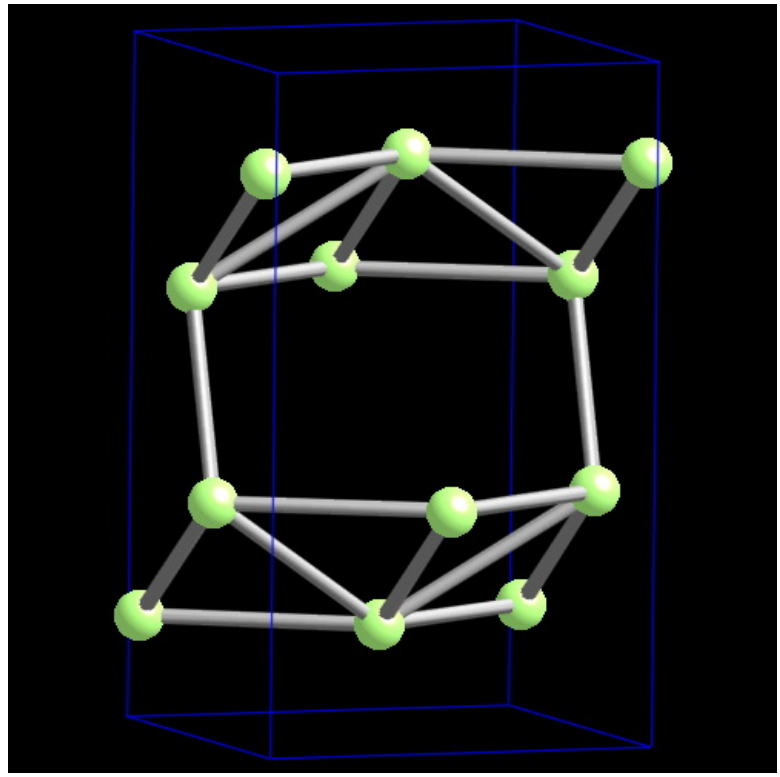
Structure 22 *Prototype:* C-graphite
SBS/PS: A9/hP4 *SG # 194:* **P6$_3$mmc** ($D_{6h}{}^4$)
Lattice parameters: $a = 0.2464, c = 0.6711$
Lattice complex: C @ $2b(0,0,\frac{1}{4})$, $2c(\frac{1}{3},\frac{2}{3},\frac{1}{4})$.



Structure 23 *Prototype:* α-Hg
SBS/PS: A10/hR1 *SG # 166:* $\mathbf{R\bar{3}m}$ $(D_{3d}{}^{5})$
Lattice parameters: $a = 0.3464, c = 0.6677$
Lattice complex: α-Hg @ $1a(0,0,0)$



Structure 24 *Prototype:* α-Ga
SBS/PS: A10/oC8 *SG # 64:* **Cmca** $(D_{2h}{}^{18})$
Lattice parameters: $a = 0.4517, b = 0.7645, c = 0.4511$
Lattice complex: Ga @ $8f(0, y, z)$ with $y = 0.1525$ and $z = 0.079$.

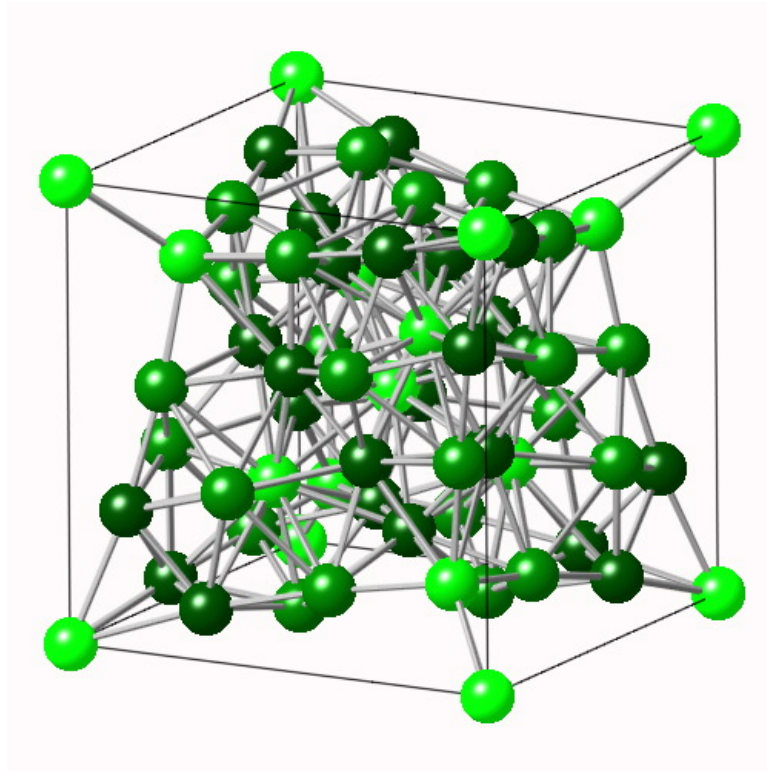


Structure 25 *Prototype:* α-Mn

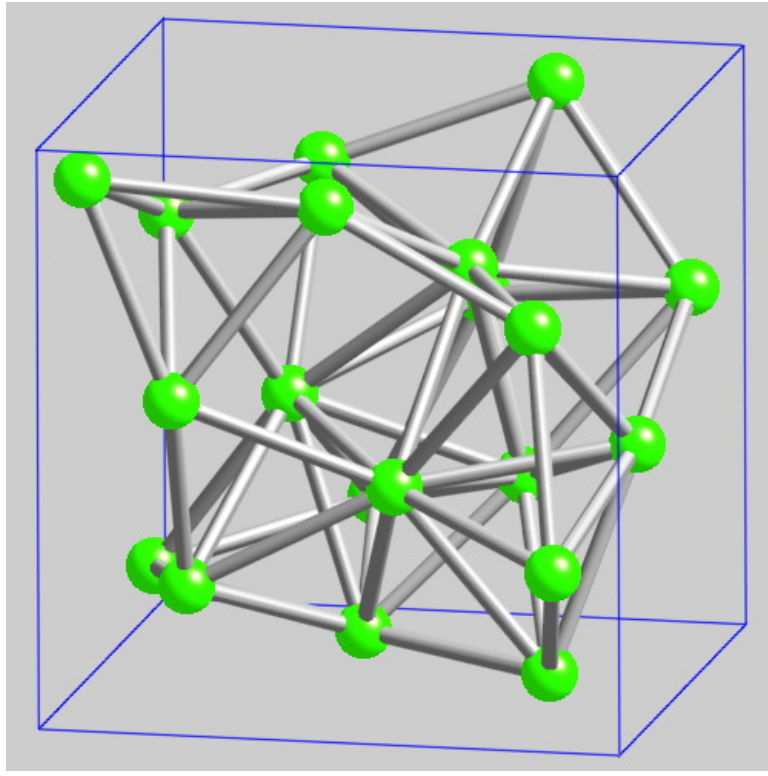
SBS/PS: A12/cI58 *SG # 217:* **I$\bar{4}$3m** $(T_d{}^3)$

Lattice parameters: $a = 0.8894$

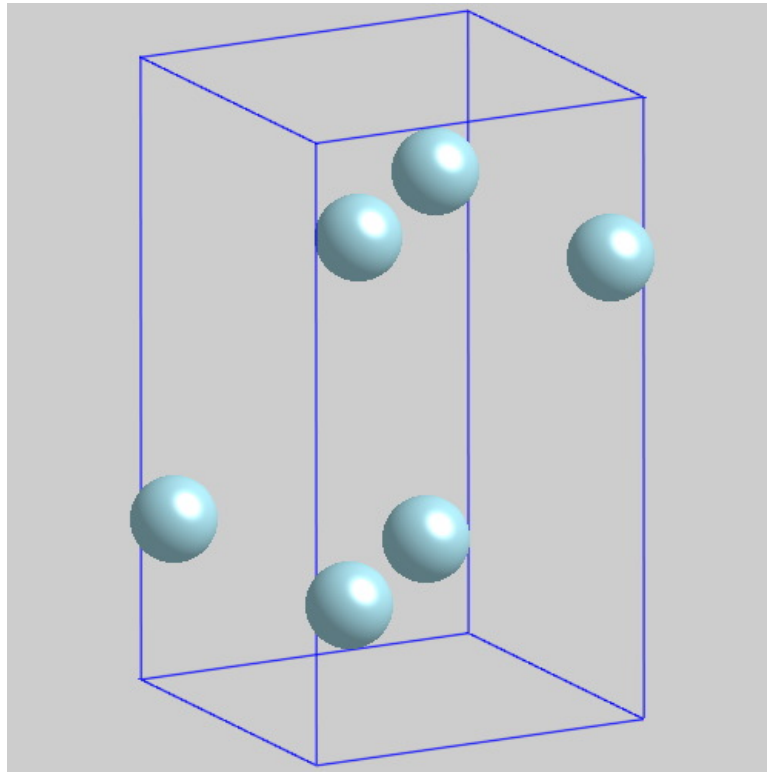
Lattice complex: Mn @ $2a(0,0,0)$, $8c(x,x,x)$ with $x = 0.317$, $24g(x,x,z)$ with (x,z)= $(0.356, 0.42)$ and $(0.089, 0.278)$.



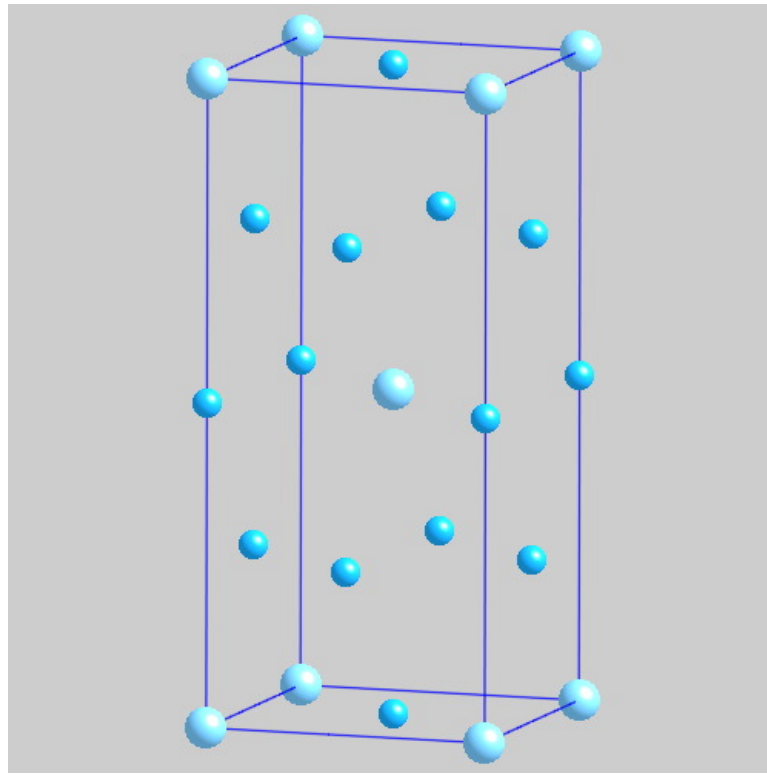
Structure 26 *Prototype:* β-Mn
SBS/PS: A13/cP20 *SG # 213:* **$P4_132$** (O^7)
Lattice parameters: $a = 0.6315$
Lattice complex: Mn @ $8c(x,x,x)$, $x = 0.0636$; and $12d(\frac{1}{8},y,y+\frac{1}{4})$ with $y = 0.2022$.



Structure 27 *Prototype:* α-U
SBS/PS: A20/oC4 *SG # 63:* **Cmcm** $(D_{2h}{}^{17})$
Lattice parameters: $a = 0.2854, b = 0.2854, c = 0.4955$
Lattice complex: U @ $4c(0, y, \frac{1}{4})$ with $y = 0.1025$



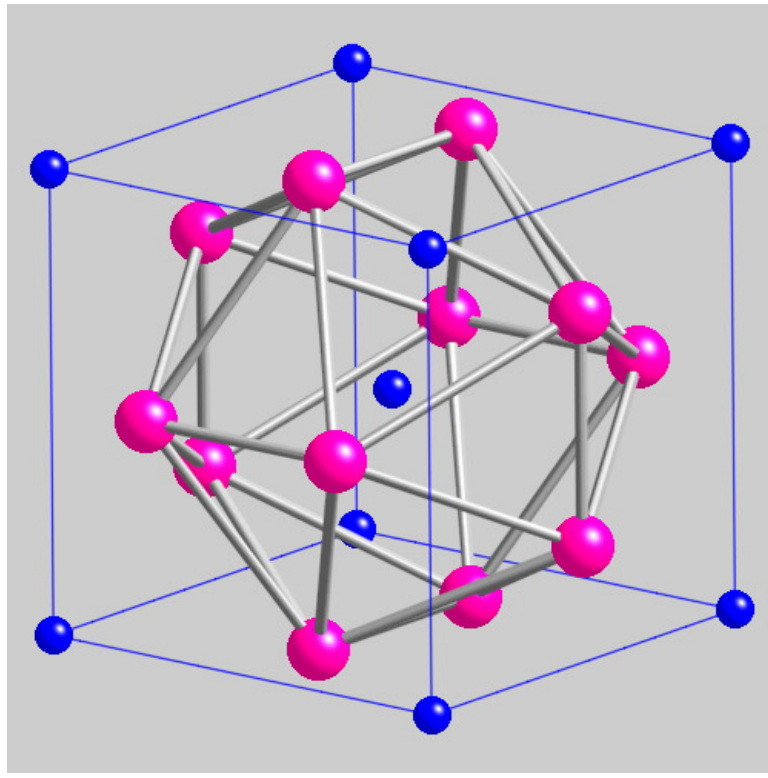
Structure 28 *Prototype:* Al_3Ti
SBS/PS: $D0_{22}$/tI8 *SG # 139:* **I4/mmm** (D_{4h}^{17})
Lattice complex: Ti @ $2a(0,0,0)$; Al @ $2b(0,0,\frac{1}{2})$ and $4d(0,\frac{1}{2},\frac{1}{4})$



Compound	a	c	Compound	a	c
Al_3Ti	0.3836	0.8579	Al_3Ta	0.3837	0.8550
Al_3Hf	0.3928	0.8888	Ga_3Ta	0.3836	0.8579
Pt_3V	0.3839	0.7796	Pd_3V	0.3850	0.7750

Table A.22. Representative compounds for Structure 28. Pearson's tables list 44 intermetallic compounds with this structure type.

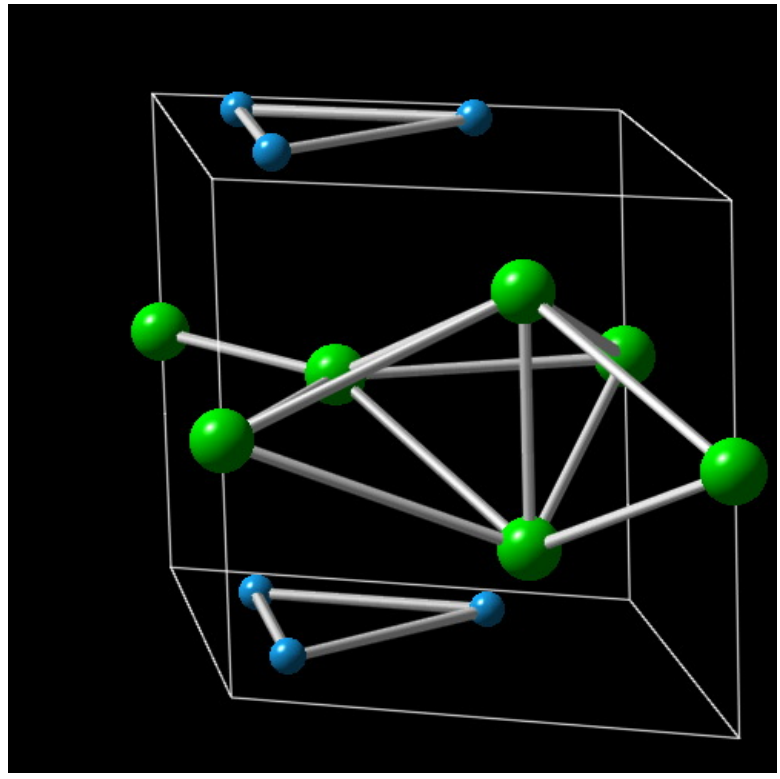
Structure 29 *Prototype:* Cr_3Si
SBS/PS: A15/cP8 *SG # 223:* **Pm$\bar{3}$n** (O_h^3)
Lattice complex: Si @ $2a(0,0,0)$; Cr @ $6c(\frac{1}{4},0,\frac{1}{2})$



Compound	a	Compound	a
Cr_3Si	0.4555	$AuZr_3$	0.5486
$GeMo_3$	0.4932	$IrTi_3$	0.50087
CoV_3	0.4676	Mo_3Os	0.49689
$BiNb_3$	0.5320	Re_7V_3	0.48783
Ti_4Tl	0.5256	$Nb_{38}Si_{24}V_{38}$	0.4915

Table A.23. Representative compounds for Structure 29. The compounds with stoichiometry deviating from the nominal A_3B composition typically have defect arrangements (vacancies) accommodating the deviation. Pearson's tables list 213 intermetallic compounds with this structure type.

Structure 30 *Prototype:* Al_3Zr_4
SBS/PS: —/hP7 *SG # 174:* $\mathbf{P\bar{6}}$ (C^1_{3h})
Lattice complex: Zr @ $1b(0,0,\frac{1}{2})$, $1f(\frac{2}{3},\frac{1}{3},\frac{1}{2})$ and $2h(\frac{1}{3},\frac{2}{3},\frac{1}{4})$; Al @ $3j(\frac{1}{3},\frac{!}{6},0)$



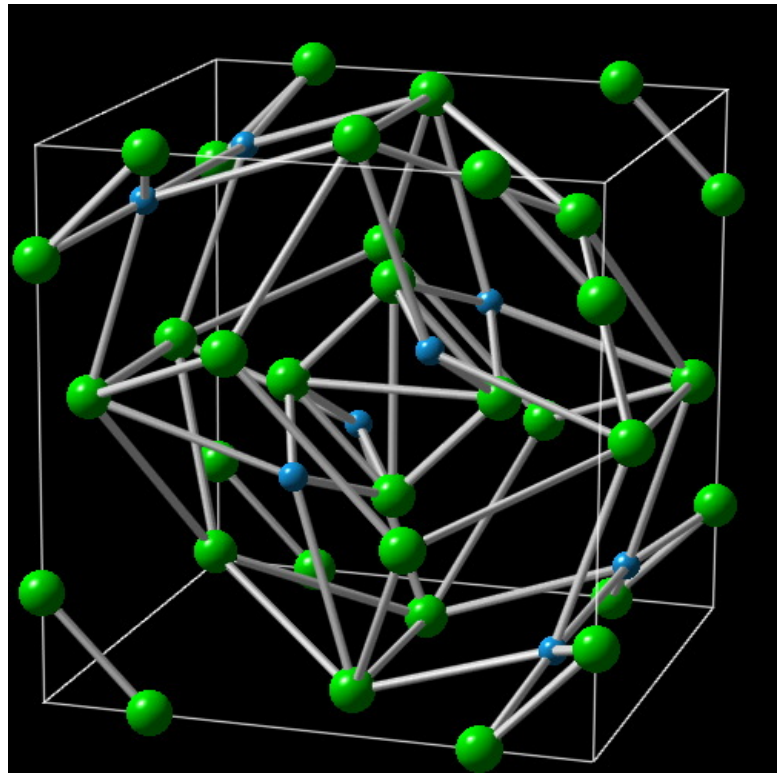
Compound	a	c	Compound	a	c
Al_3Zr_4	0.5433	0.5390	$Al_{40}Nb_{10}Zr_{50}$	0.5368	0.5333
Al_3Hf_4	0.5331	0.5414	$Al_{33}Cu_{10}Zr_{57}$	0.5375	0.5390

Table A.24. Representative compounds for Structure 30. Pearson's tables list 4 intermetallic compounds with this structure type.

Structure 31 *Prototype:* Al_2Zr_3

SBS/PS: —/tP20 *SG # 136:* $\mathbf{P4_2/mnm}$ (D_{4h}^{14})

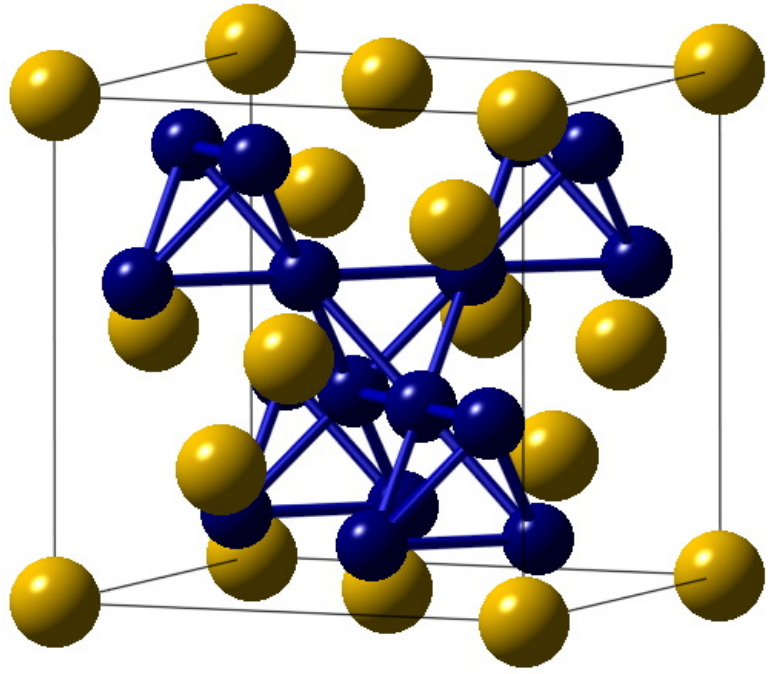
Lattice complex: Zr @ $4d(0,\frac{1}{2},\frac{1}{4})$, $4f(x,x,0)$ with $x = 0.34$ and $4g(x,\bar{x},0)$ with $x = 0.20$; Al @ $8j(x,x,z)$ with $x = \frac{1}{8}$ and $z = 0.21$.



Compound	a	c	Compound	a	c
Al_2Zr_3	0.7630	0.6998	Al_2Dy_3	0.8281	0.7550
Ga_2Gd_3	0.8292	0.7530	Li_2Sr_3	0.9628	0.8550
Al_2Y_3	0.8239	0.7648	Ce_3Ga_2	0.83	0.764

Table A.25. Representative compounds for Structure 31. Pearson's tables list 17 intermetallic compounds with this structure type.

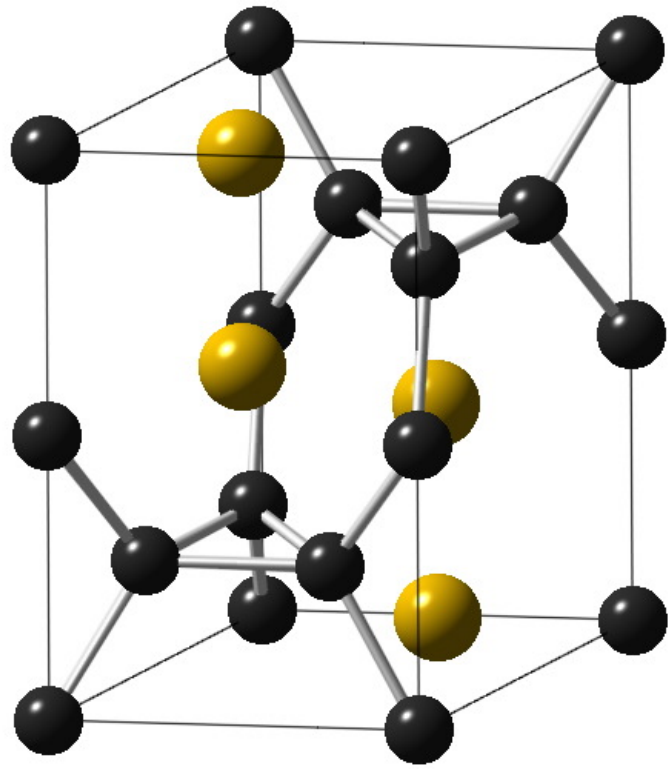
Structure 32 *Prototype:* Cu_2Mg (Laves Phase)
SBS/PS: C15/cF24 *SG # 227:* **Fd$\bar{3}$m** (O_h^7)
Lattice complex: Cu @ $16d(\frac{5}{8},\frac{5}{8},\frac{5}{8})$; Mg @ $8a(0,0,0)$



Compound	a	Compound	a	Compound	a
Cu_2Mg	0.7048	Be_2Ta	0.651	$CaNi_2$	0.7239
$DyMn_2$	0.756	$EuPt_2$	0.7714	Fe_2Tb	0.740
Li_2Pt	0.760	Mg_2Sn	0.6762	Mg_2Si	0.6352

Table A.26. Representative compounds for Structure 32. Pearson's tables list 1476 intermetallic compounds (many solid solutions) with this structure type.

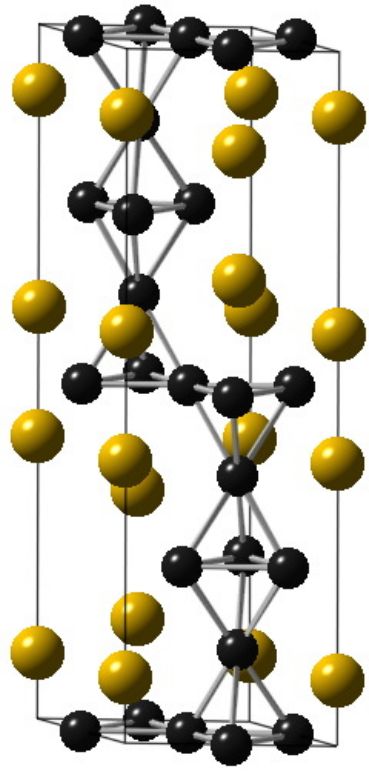
Structure 33 *Prototype:* $MgZn_2$ (Laves Phase)
SBS/PS: C14/hP12 *SG # 194:* $\mathbf{P6_3/mmc}$ (D^4_{6h})
Lattice complex: Mg @ $4f(\frac{1}{3},\frac{2}{3},z)$ with $z = 0.0629$; Zn @ $2a(0,0,0)$ and $6h(x,2x,\frac{1}{4})$ with $x = 0.8305$



Compound	a	c	Compound	a	c
$MgZn_2$	0.5221	0.8567	Al_2Hf	0.524	0.868
BeV_2	0.4385	0.7130	Cu_2Yb	0.5260	0.8567
Co_2Nb	0.4835	0.7860	Mn_3SiW_2	0.476	0.775

Table A.27. Representative compounds for Structure 33. Pearson's tables list 497 intermetallic compounds (many solid solutions) with this structure type.

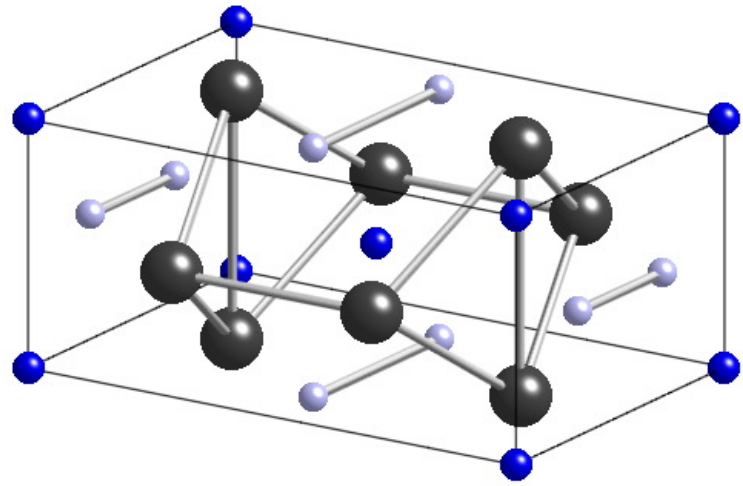
Structure 34 *Prototype:* $MgNi_2$ (Laves Phase)
SBS/PS: C36/hP24 *SG # 194:* $\mathbf{P6_3/mmc}$ (D^4_{6h})
Lattice complex: Mg @ $4e(0,0,z)$ with $z = 0.094$; $4f(\frac{1}{3},\frac{2}{3},z)$ with $z = 0.844$; Ni @ $4f(\frac{1}{3},\frac{2}{3},z)$ with $z = 0.125$; $6g(\frac{1}{2},0,0)$; $6h(\frac{1}{6},\frac{1}{3},\frac{1}{4})$



Compound	a	c	Compound	a	c
$MgNi_2$	0.4805	1.5770	$EuNi_2$	0.539	1.749
$HfZn_2$	0.519	1.689	Cr_2Ti	0.4932	1.601
$HfMn_2$	0.5016	1.637	Cr_2Zr	0.5100	1.661

Table A.28. Representative compounds for Structure 34. Pearson's tables list 40 intermetallic compounds (many solid solutions) with this structure type.

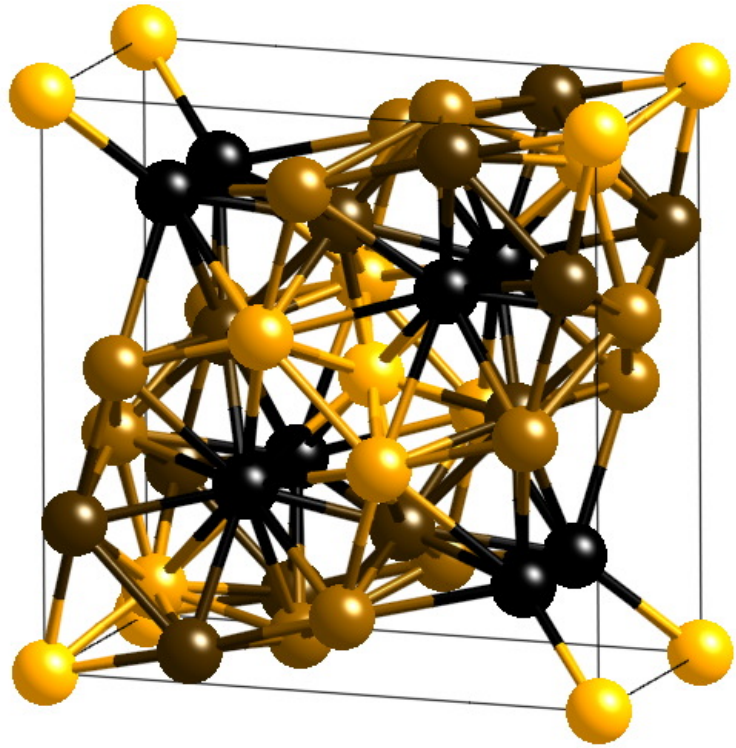
Structure 35 *Prototype:* B_2CoW_2
SBS/PS: —/oI10 *SG # 71:* **Immm** (D_{2h}^{25})
Lattice complex: Co @ $2a(0,0,0)$; W @ $4f(x,\frac{1}{2},0)$ with $x = 0.205$; B @ $4h(0,y,\frac{1}{2})$ with $y = 0.30$



Compound	*a*	*b*	*c*
B_2CoW_2	0.7075	0.4561	0.3177
$AlGd_2Ni_2$	0.8416	0.5408	0.4186
B_2NiW_2	0.7077	0.4559	0.3186
Cs_2PtTe_2	1.1387	0.9250	0.3994

Table A.29. Representative compounds for Structure 35. Pearson's tables list 27 intermetallic compounds with this structure type.

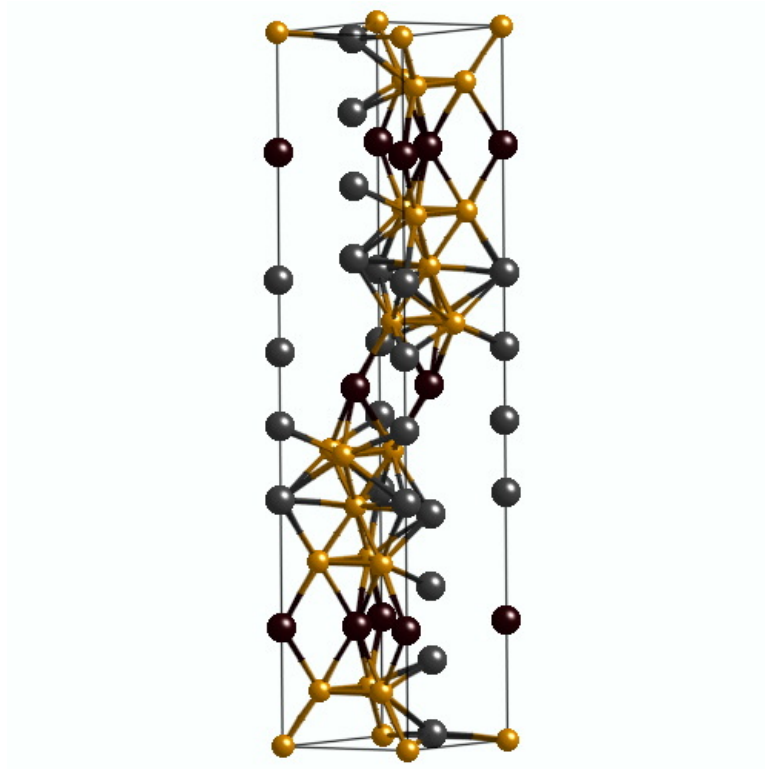
Structure 36 *Prototype:* CrFe (σ Phase)
SBS/PS: D8$_b$/tP30 *SG # 136:* $\mathbf{P4_2/mnm}$ (D_{4h}^{14})
Lattice complex: $M1$ (metal atom 1) @ $2a(0,0,0)$; $M2$ @ $4f(x,x,0)$ with $x = 0.3981$; $M3$ @ $8i(x,y,0)$ with $x = 0.4632$ and $y = 0.1316$; $M4$ @ $8i(x,y,0)$ with $x = 0.7376$ and $y = 0.0653$; $M5$ @ $4j(x,x,z)$ with $x = 0.1823$ and $z = 0.2524$



Compound	a	c	Compound	a	c
CrFe	0.87995	0.45442	FeV	0.894	0.462
FeMo	0.9218	0.4813	Mn_2Mo	0.910	0.474
$PdTa_3$	0.9978	0.5208	U	1.07589	0.56531

Table A.30. Representative compounds for Structure 36. Pearson's tables list 84 intermetallic compounds with this structure type.

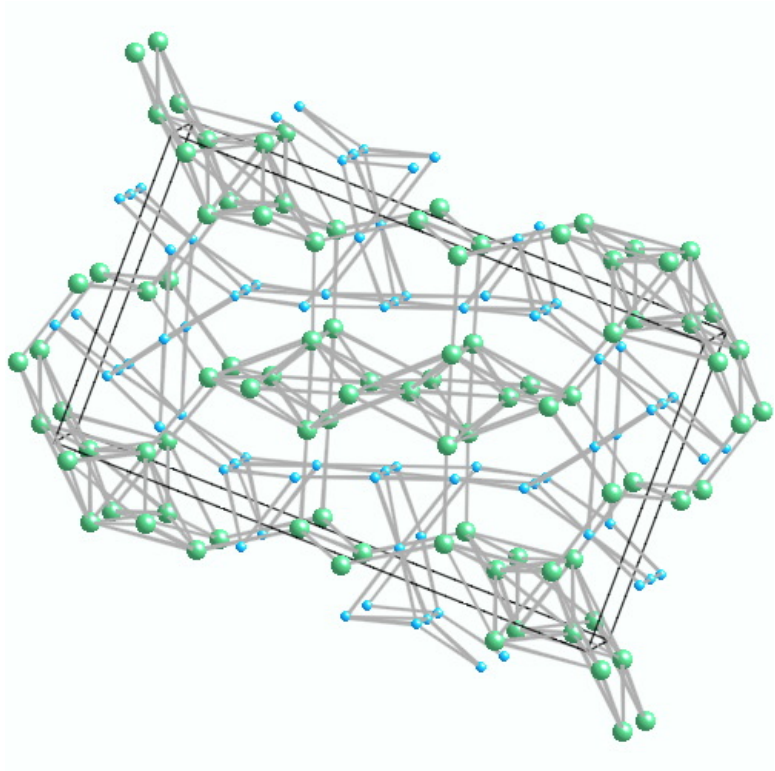
Structure 37 *Prototype:* W_6Fe_7 (μ Phase)
SBS/PS: $D8_5$/hR13 *SG # 166:* $\mathbf{R\bar{3}m}$ (D^5_{3d})
Lattice complex: hexagonal reference frame; Fe @ $3a(0,0,0)$ and $18h(x,\bar{x},z)$ with $x = 0.833$ and $z = 0.257$; W @ $6c(0,0,z)$ with $z = 0.167$, $z = 0.346$, $z = 0.448$



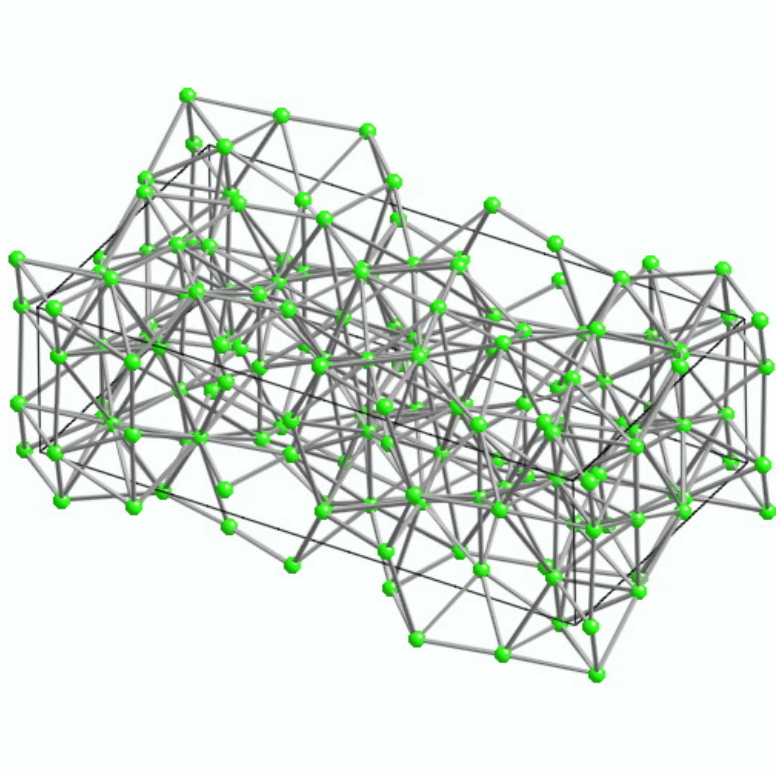
Compound	a	c	Compound	a	c
W_6Fe_7	0.4757	2.584	Co_7Nb_6	0.501	2.650
Mn_6Si_7	0.470	2.561	Ta_6Zn_7	0.5035	2.7528
$Al_3Nb_5Ni_2$	0.4993	2.7100	$CuNiTa_2$	0.495	2.700

Table A.31. Representative compounds for Structure 37. Pearson's tables list 36 intermetallic compounds with this structure type.

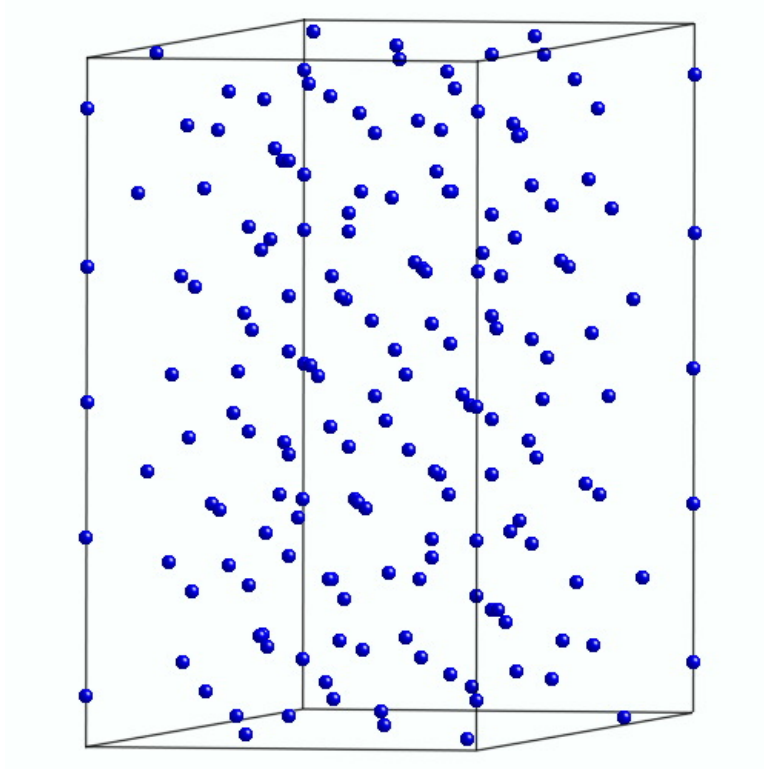
Structure 38 *Prototype:* $Al_3Nb_{10}Ni_9$ (M Phase)
SBS/PS: —/oP52 *SG # 62:* **Pnma** (D_{2h}^{16})
Lattice parameters: $a = 0.9393, b = 0.4933, c = 1.6266$ nm
Lattice complex: Nb @ $4c(x, \frac{1}{4}, z)$ with (x,z) equal to $(0.0593, 0.8506)$, $(0.2996, 0.6016)$, $(0.5242, 0.4590)$, $(0.6164, 0.2932)$, $(0.0144, 0.5518)$, and $(0.8388, 0.7062)$;
Al and Ni are in solid solution on the following sites: $4c(x, \frac{1}{4}, z)$ with (x,z) equal to $(0.0714, 0.3775)$, $(0.3255, 0.3303)$, and $(0.8168, 0.4222)$, and $8d(x,y,z)$ with (x,y,z) equal to $(0.1118, 0.0048, 0.7049)$ and $(0.2550, 0.9969, 0.4550)$



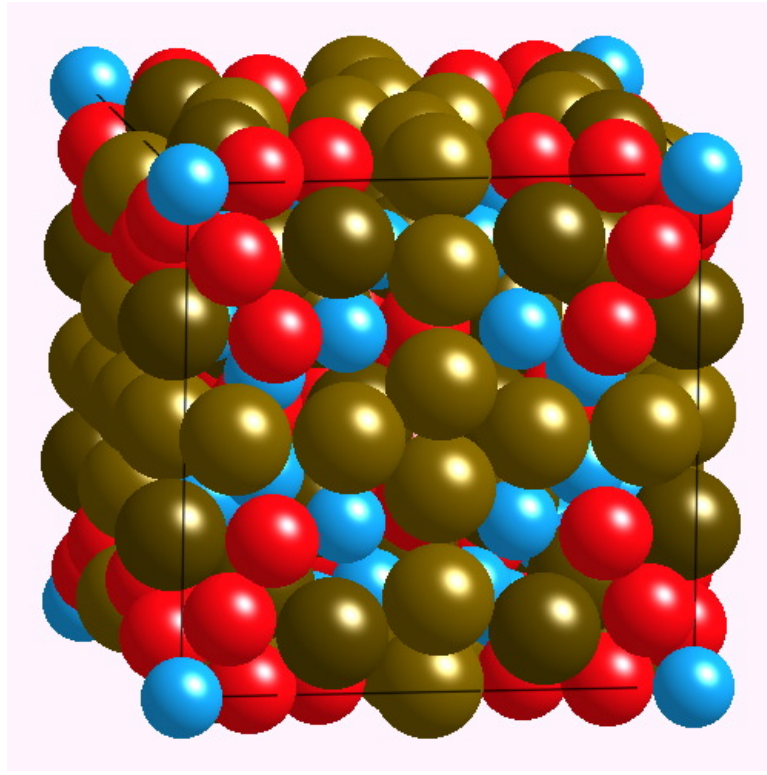
Structure 39 *Prototype:* $Cr_9Mo_{21}Ni_{20}$ (P Phase)
SBS/PS: —/oP56 *SG # 62:* **Pnma** (D_{2h}^{16})
Lattice parameters: $a = 1.6983, b = 0.4752, c = 0.9070$ nm
Lattice complex: the metal atoms are distributed over the following sites: $4c(x, \frac{1}{4}, z)$ with (x, z) equal to $(0.1134, 0.0737)$, $(0.2547, 0.1363)$, $(0.1578, 0.3257)$, $(0.1819, 0.6058)$, $(0.3253, 0.6650)$, $(0.4536, 0.4746)$, $(0.4047, 0.1988)$, $(0.0780, 0.8152)$, $(0.3650, 0.9383)$, and $(0.0355, 0.5202)$; and $8d(x, y, z)$ with (x, y, z) equal to $(0.5375, 0.9986, 0.2504)$ and $(0.2883, 0.0008, 0.3868)$.



Structure 40 *Prototype:* $Co_5Cr_2Mo_3$ (R Phase)
SBS/PS: —/hR53 *SG # 148:* $\mathbf{R\bar{3}}$ (C_{3i}^2)
Lattice parameters: $a = 1.0903, c = 1.9342$ nm
Lattice complex: the metal atoms are distributed over the following sites: $3b(0,0,\frac{1}{2})$; $6c(0,0,z)$ with z equal to 0.3044 and 0.0735; $18f(x,y,z)$ with (x,y,z) equal to $(0.0509, 0.2790, 0.1000)$, $(0.0212, 0.1393, 0.1962)$, $(0.2250, 0.1969, 0.2685)$, $(0.1759, 0.1265, 0.3969)$, $(0.1132, 0.2687, 0.4652)$, $(0.0330, 0.2579, 0.3183)$, $(0.1596, 0.2470, 0.0020)$, and $(0.2671, 0.2218, 0.1222)$



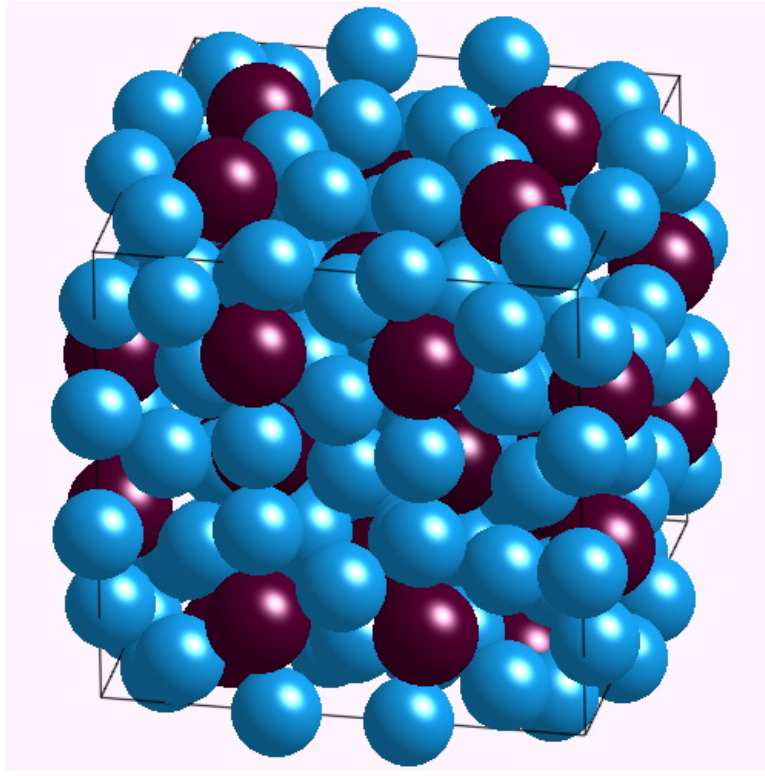
Structure 41 *Prototype:* $Mg_{32}(Al,Zn)_{49}$
SBS/PS: —/cI162 *SG # 204:* $\mathbf{Im\bar{3}}$ (T_h^5)
Lattice complex: Al,Zn @ $2a(0,0,0)$; $24g(0,y,z)$ with $y = 0.0908$ and $z = 0.1501$; $24g(0,y,z)$ with $y = 0.1748$ and $z = 0.3007$; $48h(x,y,z)$ with $y = 0.168$, $z = 0.1836$ and $z = 0.4031$; Mg @ $16f(x,x,x)$ with $x = 0.1836$; $24g(0,y,z)$ with $y = 0.2942$ and $z = 0.1194$; $12e(x,0,\frac{1}{2})$ with $x = 0.4002$; $12e(x,0,\frac{1}{2})$ with $x = 0.1797$.



Compound	a
$Mg_{32}(Al,Zn)_{49}$	1.416

Table A.32. Representative compound for Structure 41.

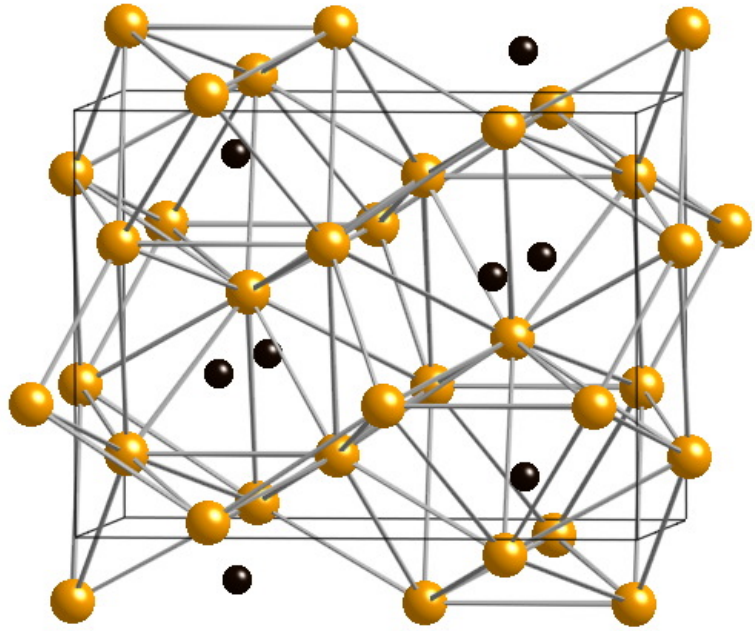
Structure 42 *Prototype:* α-Al-Mn-Si
SBS/PS: —/cP138 *SG # 200:* $\mathbf{Pm\bar{3}}$ (T_h^1)
Lattice complex: Mn @ $12j(y,z,0)$ with $y = 0.3271$, $z = 0.2006$; $12k(y,z,\frac{1}{2})$ with $y = 0.1797$, $z = 0.3085$; Al,Si @ $6e(x,0,0)$; with $x = 0.3638$; $6h(x,\frac{1}{2},\frac{1}{2})$ with $x = 0.1216$; $6f(x,0,\frac{1}{2})$ with $x = 0.2897$; $12j(y,z,0)$ with $y = 0.1636$ and $z = 0.0997$; $12k(y,z,\frac{1}{2})$ with $y = 0.3342$ and $z = 0.399$; $12j(y,z,0)$ with $y = 0.3319$, $z = 0.4037$; $12k(y,z,\frac{1}{2})$ with $y = 0.1205$, $z = 0.1175$; $24l(x,y,z)$ with $x = 0.1185$, $y = 0.1892$, $z = 0.298$; $24l(x,y,z)$ with $x = 0.3897$, $y = 0.3127$, $z = 0.1955$.



Compound	a
α-Al-Mn-Si	1.268

Table A.33. Representative compound for Structure 42.

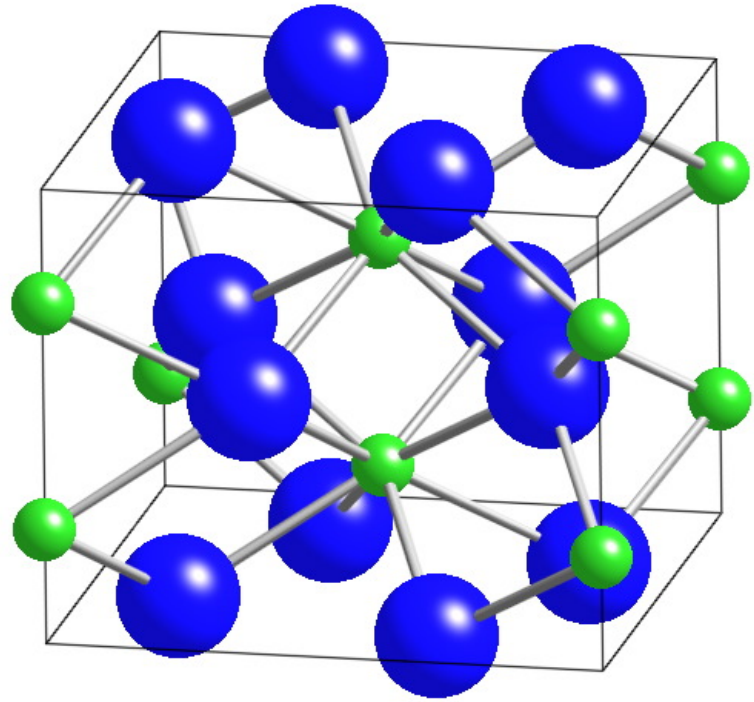
Structure 43 *Prototype:* Fe_3C
SBS/PS: —/oP16 *SG # 62:* **Pnma** (D_{2h}^{16})
Lattice complex: Fe @ $2c(x,\frac{1}{4},z)$ with $x = 0.044$ and $z = 0.837$; and $8d(x,y,z)$ with $x = 0.181$,$z = 0.063$, and $z = 0.337$; C @ $2c(x,\frac{1}{4},z)$ with $x = 0.881$ and $z = 0.431$.



Compound	*a*	*b*	*c*
Fe_3C	0.50787	0.67297	0.45144

Table A.34. Representative compound for Structure 43.

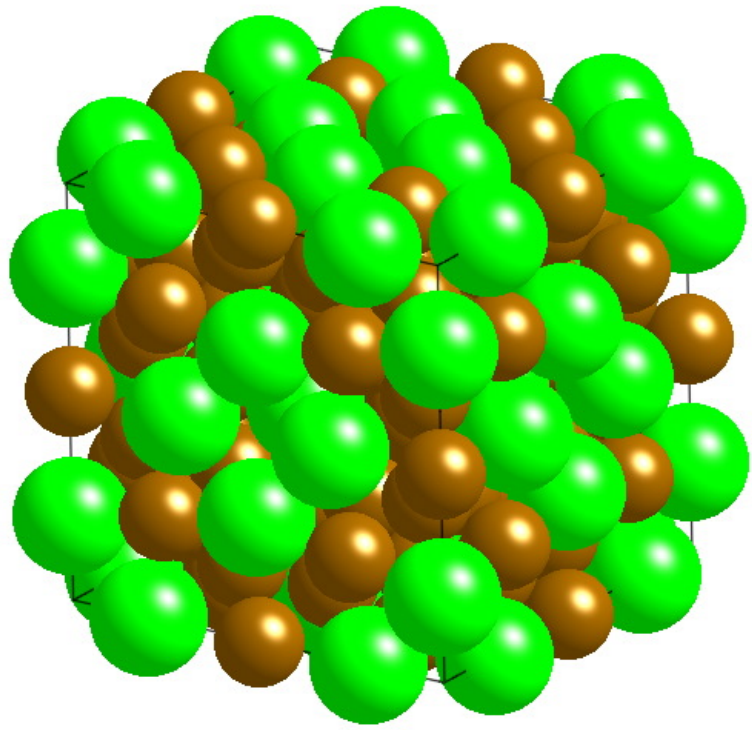
Structure 44 *Prototype:* Fe_2B
SBS/PS: —/tI12 *SG # 140:* **I4/mcm** (D_{4h}^{18})
Lattice complex: Fe @ $8h(x, \frac{1}{2}+x, 0)$ with $x = 0.1661$; and B @ $4a(0, 0, \frac{1}{4})$.



Compound	a	c
Fe_2B	0.5109	0.4249

Table A.35. Representative compound for Structure 44.

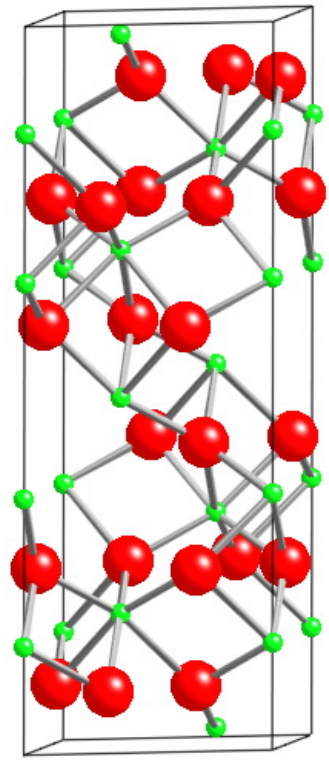
Structure 45 *Prototype:* $Fe_{23}Zr_6$
SBS/PS: —/cF116 *SG # 225:* **Fm$\bar{3}$m** (O_h^5)
Lattice complex: Fe @ $4b(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; and $24d(0,\frac{1}{4},\frac{1}{4})$; and $32f(x,x,x)$ with $x = 0.378$ and $x = 0.178$; Zr @ $24e(x,0,0)$ with $x = 0.203$.



Compound	a
$Mn_{23}Zr_6$	1.2523
$Fe_{23}Zr_6$	1.169

Table A.36. Representative compounds for Structure 45.

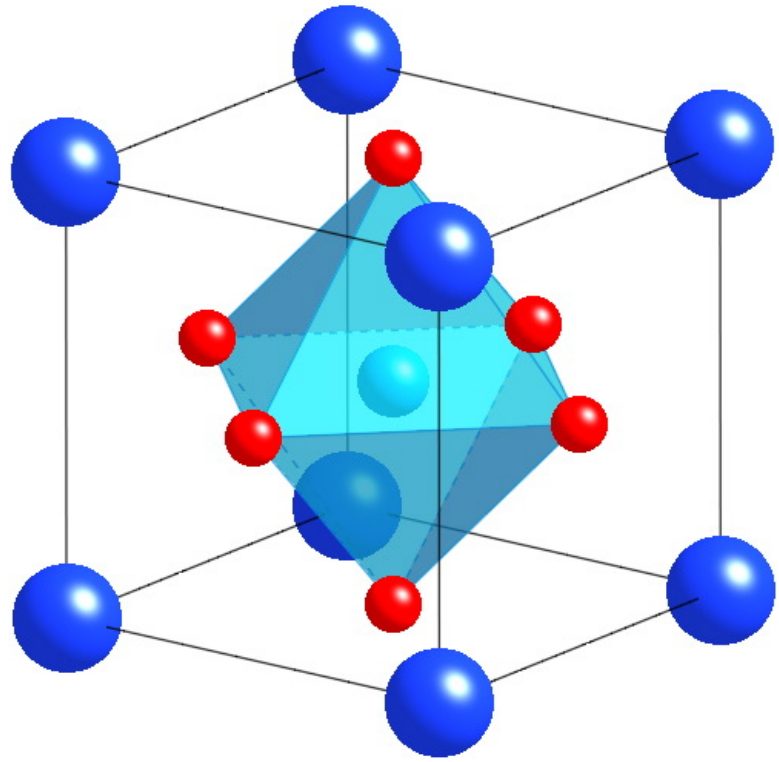
Structure 46 *Prototype:* Al_2O_3
SBS/PS: $D5_1$/hR30 *SG # 167:* $\mathbf{R\bar{3}c}$ $(D_{3d}{}^6)$
Lattice complex: Al@ $12c(0,0,z)$ with $z = 0.3521$; and O@ $18e(x,0,\frac{1}{4})$ with $x = 0.3065$;



Compound	a	c
Al_2O_3	0.47617	1.29947

Table A.37. Structural data for corundum: Structure 46.

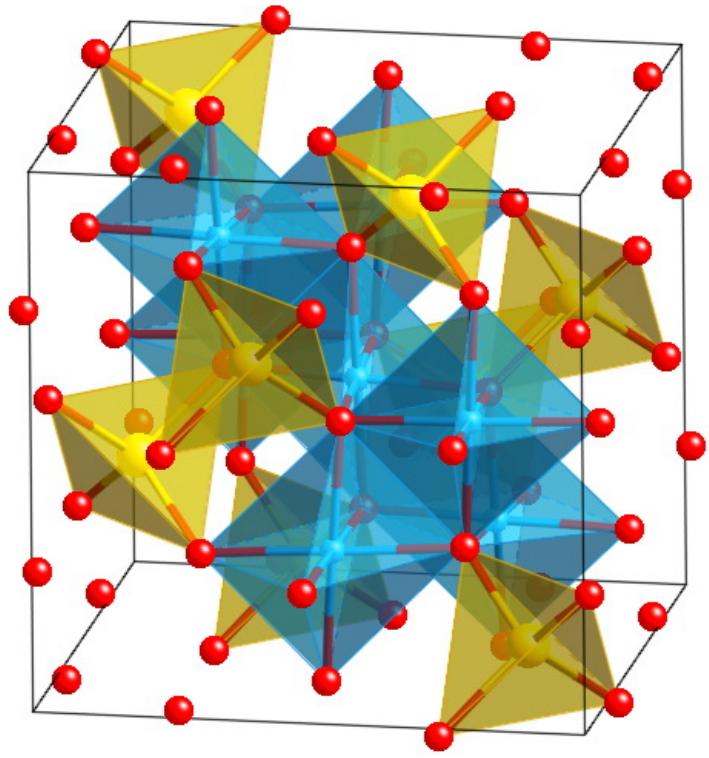
Structure 47 *Prototype:* $CaTiO_3$
SBS/PS: $E2_1/cP5$ *SG # 221:* **Pm$\bar{3}$m** $(O_h{}^1)$
Lattice complex: Ti@ $1b(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; and O@ $3d(\frac{1}{2},\frac{1}{2},0)$; and Ca@ $1a(0,0,0)$.



Compound	a
$CaTiO_3$	0.3795
$MgSiO_3$	0.348

Table A.38. Structural data for Structure 47.

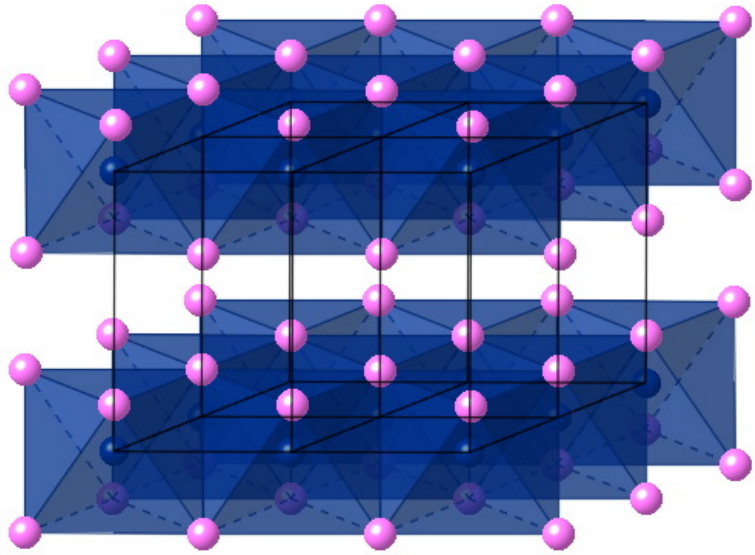
Structure 48 *Prototype:* $MgAl_2O_4$
SBS/PS: H1$_1$/cF56 *SG # 227:* **Fd3m** $(O_h{}^7)$
Lattice complex: Mg@ $8a(\frac{1}{8},\frac{1}{8},\frac{1}{8})$; and Al@ $16d(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; and O@ $32e(x,x,x)$ with $x = 0.262$.



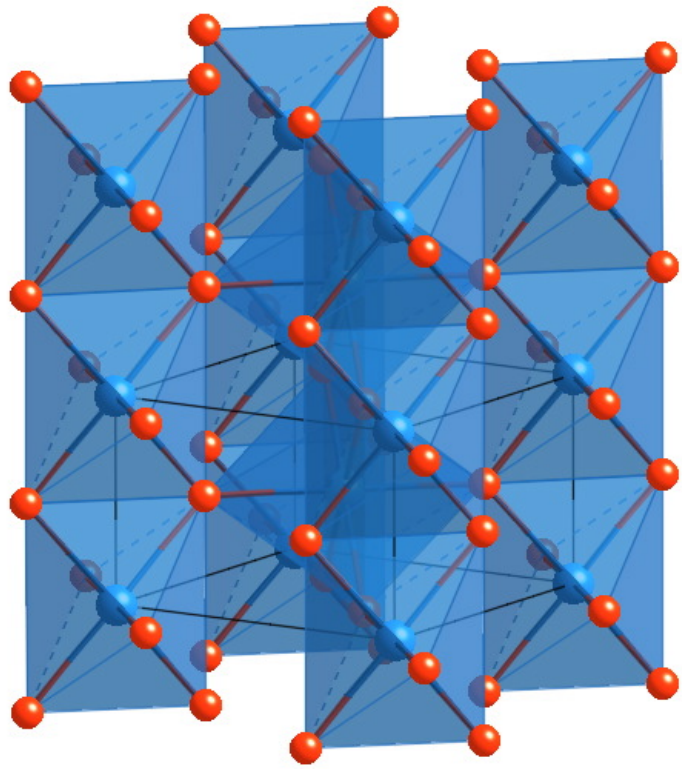
Compound	a	Compound	a
$MgAl_2O_4$	0.808	$ZnAl_2O_4$	0.812
Fe_3O_4	0.84	$(Zn,Mn,Fe)(Fe,Mn)_2O_4$	0.842
$FeCr_2O_4$	0.836		

Table A.39. Structural data for Structure 48.

Structure 49 *Prototype:* CdI_2
SBS/PS: C6/hP5 *SG # 164:* **P$\bar{3}$m1** $(D_{3d}{}^3)$
Lattice parameters: $a = 0.4224, c = 0.6859$
Lattice complex: Cd@ $1a(0,0,0)$; and I@ $2d(\frac{1}{3},\frac{2}{3},z)$ with $z = 0.2492$.



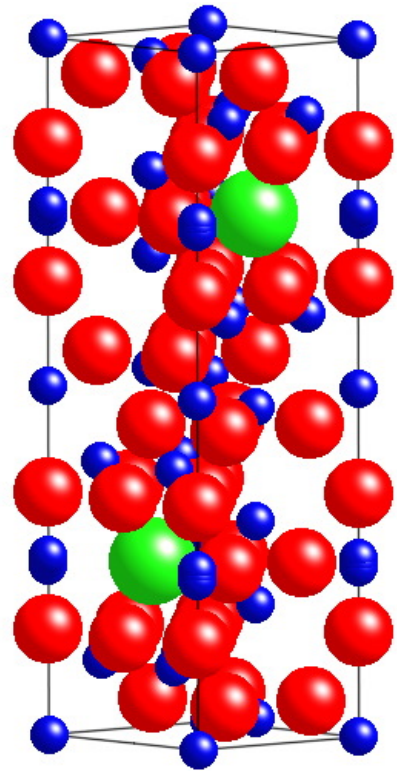
Structure 50 *Prototype:* TiO_2
SBS/PS: C4/tP6 *SG # 136:* $\mathbf{P4_2/mnm}$ $(D_{4h}{}^{14})$
Lattice complex: Ti@ $2a(0,0,0)$; and O@ $4f(x,x,0)$ with $x = 0.3053$



Compound	a	c
TiO_2	0.4537	0.2958

Table A.40. Structural data for Structure 50.

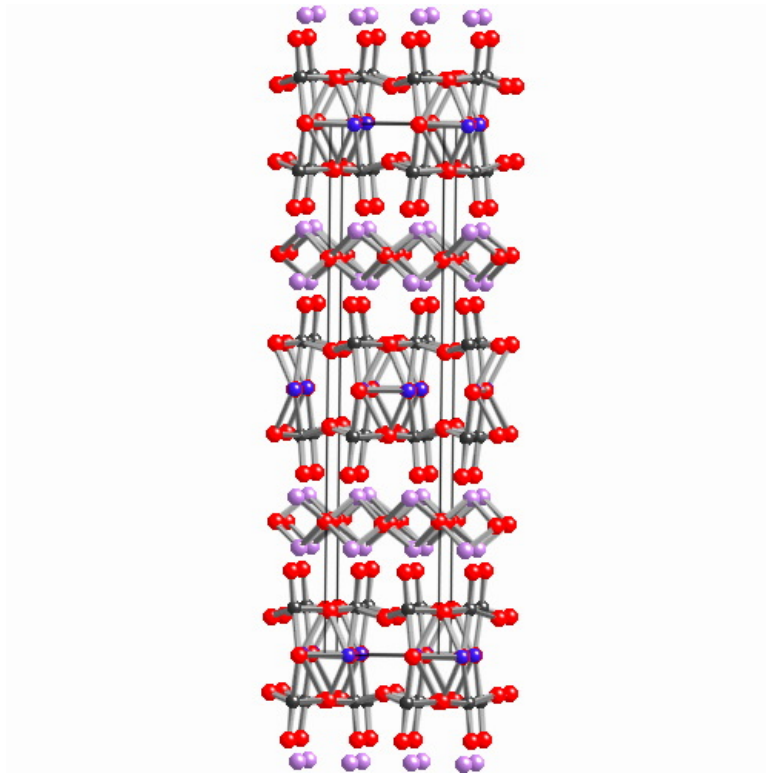
Structure 51 *Prototype:* $BaFe_{12}O_{19}$
SBS/PS: —/hP64 *SG # 194:* **P6$_3$/mmc** ($D_{6h}{}^4$)
Lattice complex: Ba@ $2d(\frac{2}{3},\frac{1}{3},\frac{1}{4})$; Fe@ $2a(0,0,0)$; $2b(0,0,\frac{1}{4})$; $4f(\frac{1}{3},\frac{2}{3},z)$ with $z = 0.0.028$; $12k(x,2x,z)$ with $x = 0.167$ and $z = -0.108$; O@ $4e(0,0,z)$ with $z = 0.150$; $4f(\frac{1}{3},\frac{2}{3},z)$ with $z = -0.05$; $6h(x,2x,\frac{1}{4})$ with $x = 0.5$; $12k(x,2x,z)$ with (x,z) = $(0.167,0.050)$ and $(0.5,0.150)$.



Compound	*a*	*c*
$BaFe_{12}O_{19}$	0.5892	2.3183
$Ba_{0.68}K_{0.31}Ti_{0.68}Fe_{5.93}$ $Mg_{0.69}(Cr,Mn,Ni)_{0.34}O_{19}$ (Haggertyite)	0.59369	2.32445

Table A.41. Structural data for Structure 51.

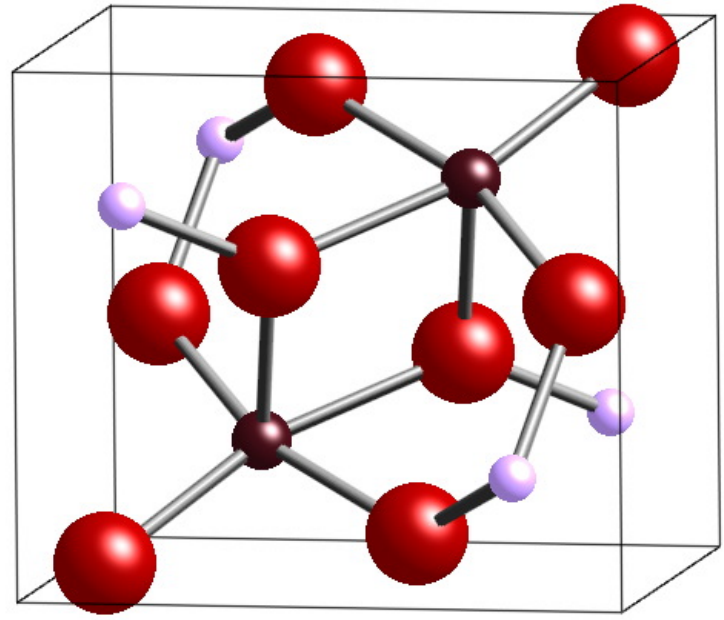
Structure 52 *Prototype:* $PbBi_2Nb_2O_9$
SBS/PS: —/oA56 *SG # 36:* **A2$_1$am** ($C_{2v}{}^{12}$)
Lattice complex: Pb@ $4a(\frac{1}{4},y,\frac{1}{2})$ with $y = 0.2693$; Bi@ $8b(x,y,z)$ with $y = 0.2662$, $y = 0.742$ and $z = 0.2013$; Nb@ $8b(x,y,z)$ with $x = 0.2776$, $y = 0.7435$ and $z = 0.4115$; O@ $4a(x,y,0)$ with $x = 0.3092$ and $y = 0.1936$; $8b(x,y,z)$ with (x,y,z) = $(0.3034, y = 0.2751, z = 0.1593)$, $(0.5236, 0.4977, 0.2473)$; $(0.5283, 0.027, 0.5715)$, and $(0.5967, 0.5457, 0.5846)$



Compound	*a*	*b*	*c*
$PbBi_2Nb_2O_9$	0.5503	0.5495	2.5531

Table A.42. Structural data for Structure 52.

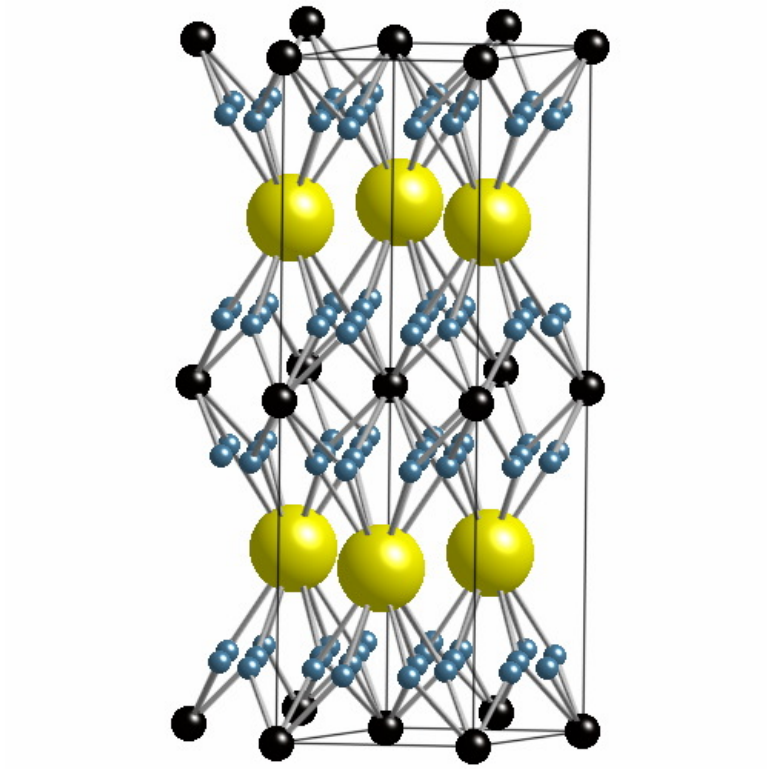
Structure 53 *Prototype:* $ZnWO_4$
SBS/PS: —/mP12 *SG # 13:* **P2/c** $(C_{2h}{}^4)$
Lattice complex: Zn@ $2f(\frac{1}{2},y,\frac{1}{4})$ with $y = 0.674$; W@ $2e(0,y,\frac{1}{4})$ with $y = 0.2662$; O@ $4g(x,y,z)$ with $(x,y,z) = (0.22,0.11,0.95)$ and $(0.26,0.38,0.39)$.



Compound	a	b	c	β
$ZnWO_4$	0.472	0.57	0.495	90.15°

Table A.43. Structural data for Structure 53.

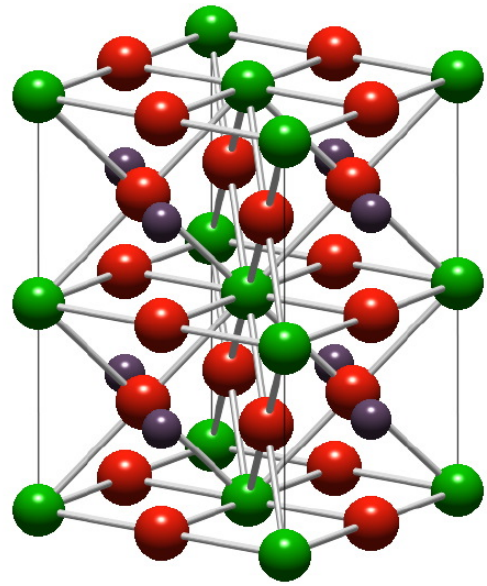
Structure 54 *Prototype:* Ti_2CS
SBS/PS: —/hP8 *SG # 194:* **P6$_3$/mmc** ($D_{6h}{}^4$)
Lattice complex: Ti@ $4e(0,0,z)$ with $z = 0.1$; C@ $2a(0,0,0)$; S@ $2d(\frac{1}{3},\frac{2}{3},\frac{3}{4})$.



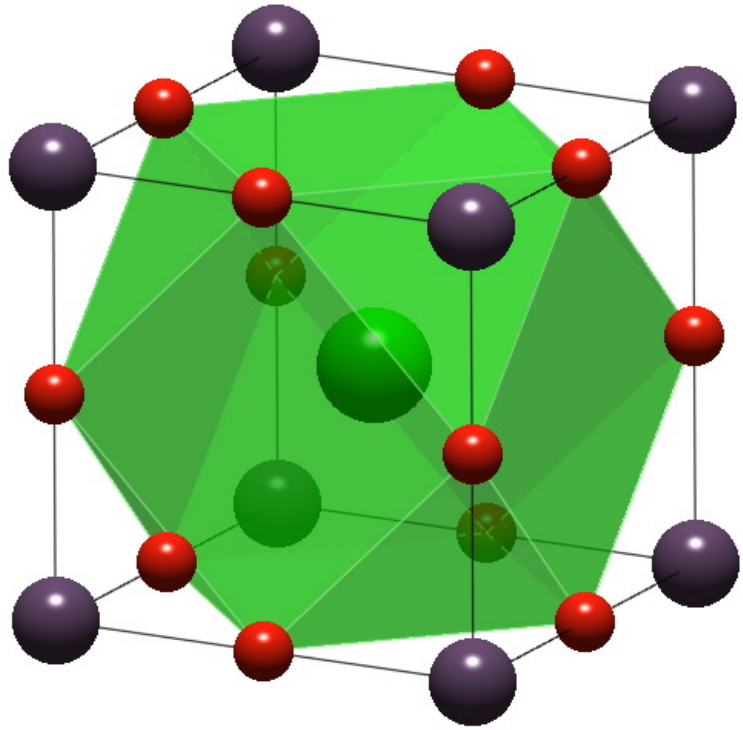
Compound	a	c
Ti_2CS	0.321	1.12

Table A.44. Structural data for Structure 54.

Structure 55 *Prototype:* $BaPb_{1-x}Bi_xO_3$ $(0.05 < x < 0.30)$
SBS/PS: —/tI5 *SG # 140:* **I4/mcm** $(D_{4h}{}^{18})$
Lattice parameters: $a = 0.605, c = 0.8621$
Lattice complex: Pb,Bi@ $4b(0, \frac{1}{2}\frac{1}{4})$; Ba@ $4c(0,0,0)$; O@ $4d(0, \frac{1}{2}, 0)$ and $8e(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$;



Structure 56 *Prototype:* $Ba_{1-x}K_xBiO_3$ $(0.37 < x < 0.5)$
SBS/PS: —/cP5 *SG # 221:* **Pm$\bar{3}$m** $(O_h{}^1)$
Lattice parameters: $a = 0.429$
Lattice complex: Bi@ $1a(0.5,0.5,0.5)$; Ba@ $1b(0,0,0)$; O@ $3d(0.5,0.5,0)$;

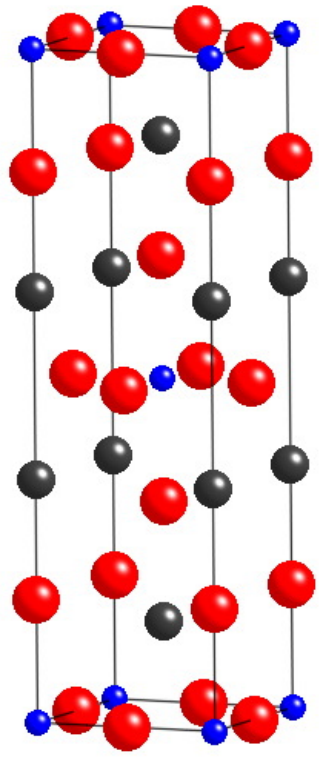


Structure 57 *Prototype:* La_2CuO_4

SBS/PS: —/tI5 *SG # 139:* **I4/mmm** $(D_{4h}{}^{17})$

Lattice parameters: $a = 0.3783, c = 1.32883$

Lattice complex: La@ $xx(0,0,z)$ with $z = 0.3606$; Cu@ $xx(0,0,0)$; O@ $xx(0,\frac{1}{2},0)$ and $xx(0,0,z)$ with $z = 0.1828$.

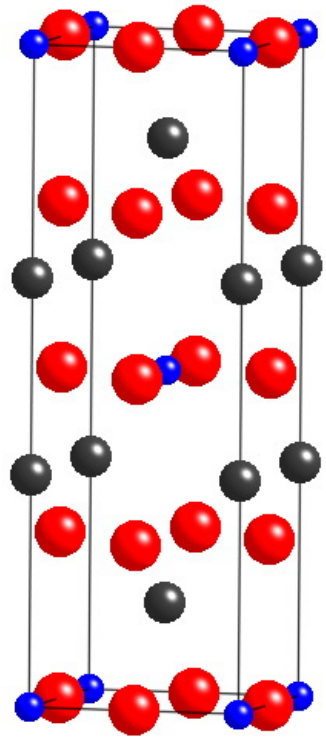


Structure 58 *Prototype:* Nd_2CuO_4

SBS/PS: —/tI5 *SG # 139:* **I4/mmm** $(D_{4h}{}^{17})$

Lattice parameters: $a = 0.395, c = 1.207$

Lattice complex: Nd@ $xx(0,0,z)$ with $z = 0.3513$; Cu@ $xx(0,0,0)$; O@ $xx(0,\frac{1}{2},0)$ and $xx(0,\frac{1}{2},\frac{1}{4})$.

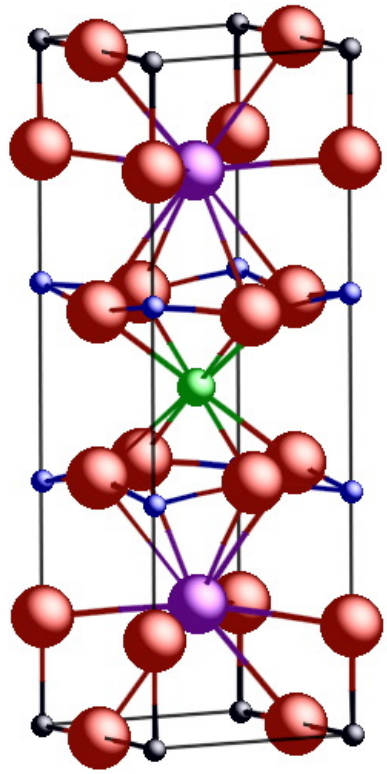


Structure 59 *Prototype:* $YBa_2Cu_3O_{7-x}$

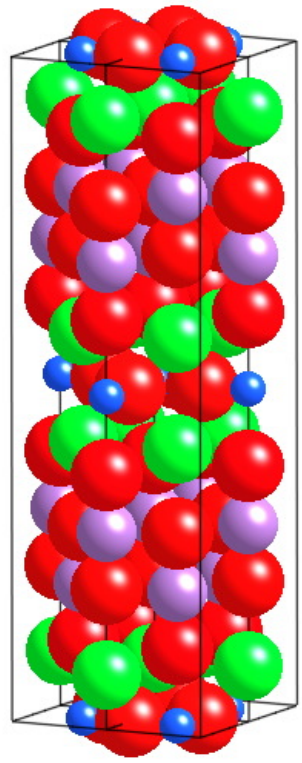
SBS/PS: —/tI5 *SG # 47:* **I4/mmm** $(D_{4h}{}^{17})$

Lattice parameters: $a = 0.38198, b = 0.38849, c = 1.16762$

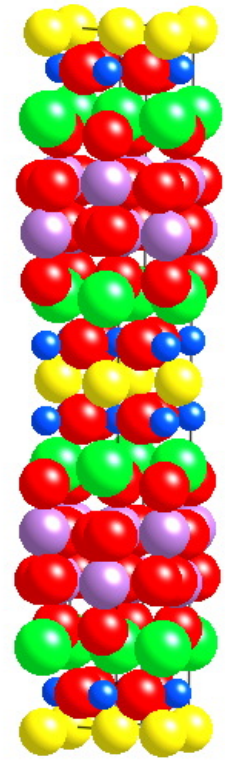
Lattice complex: Y@ $1h(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; Ba@ $2t(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.1843$; Cu@ $1a(0,0,0)$ and $2t(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.3556$; O@ $1e(0,\frac{1}{2},0)$, $2s(\frac{1}{2},0,z)$ with $z = 0.3779$ and $2r(0,\frac{1}{2},z)$ with $z = 0.379$.



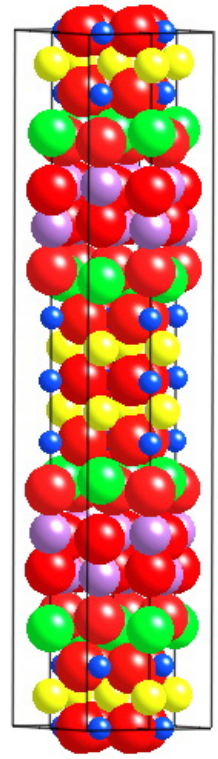
Structure 60 *Prototype:* $Bi_2Sr_2CuO_{6+x}$
SBS/PS: —/tI5 *SG # 139:* **I4/mmm** $(D_{4h}{}^{17})$
Lattice parameters: $a = 0.3886, c = 2.4662$
Lattice complex: Bi@ $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.202$; Sr@ $xx(0,0,z)$ with $z = 0.083$; Cu@ $xx(\frac{1}{2},\frac{1}{2},0)$; O@ $xx(0,\frac{1}{2},0)$; $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.116$ and $z = 0.288$.



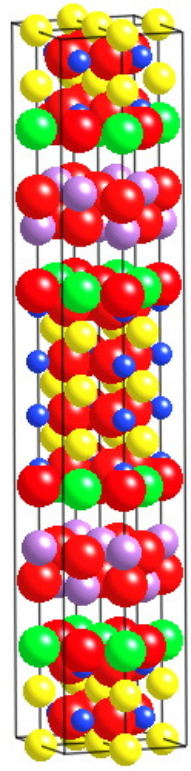
Structure 61 *Prototype:* $Bi_2Sr_2CaCu_2O_{8+x}$
SBS/PS: —/tI5 *SG # 139:* **I4/mmm** $(D_{4h}{}^{17})$
Lattice parameters: $a = 0.3828, c = 3.089$
Lattice complex: Bi@ $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.2136$; Ca@ $xx(0,0,0)$; Sr@ $xx(0,0,z)$ with $z = 0.1218$; Cu@ $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.054$; O@ $xx(0,\frac{1}{2},z)$ with $z = 0.0531$; $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.1461$; $xx(x,\frac{1}{2},z)$ with $x = 0.604$ and $z = 0.2815$.



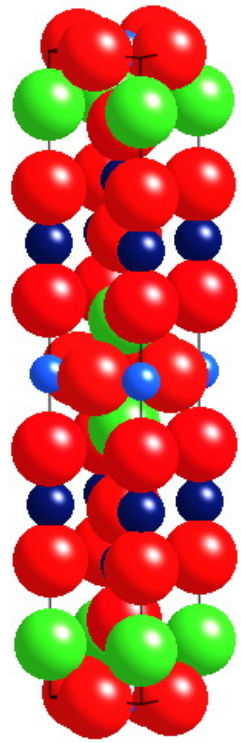
Structure 62 *Prototype:* $Bi_2Sr_2Ca_2Cu_3O_{10+x}$
SBS/PS: —/tI5 *SG # 139:* **I4/mmm** $(D_{4h}{}^{17})$
Lattice parameters: $a = 0.38503, c = 3.70$
Lattice complex: Bi@ $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.22$; Ca@ $xx(0,0,z)$ with $z = 0.046$; Sr@ $xx(0,0,z)$ with $z = 0.144$; Cu@ $xx(\frac{1}{2},\frac{1}{2},0)$; $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.089$; O@ $xx(\frac{1}{2},0,0)$; $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.158$ and $z = 0.2724$; $xx(\frac{1}{2},0,z)$ with $z = 0.087$.



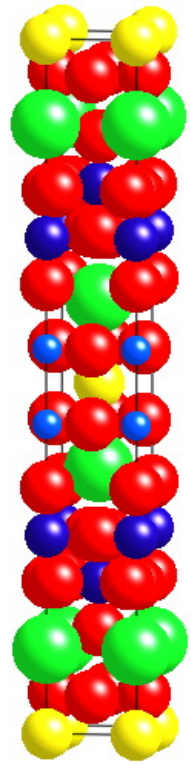
Structure 63 *Prototype:* $Bi_2Sr_2Ca_3Cu_4O_{12+x}$
SBS/PS: —/tI5 *SG # 139:* **I4/mmm** $(D_{4h}{}^{17})$
Lattice parameters: $a = 0.38503, c = 4.226$
Lattice complex: Bi@ $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.224$; Ca@ $xx(0,0,0)$; $xx(0,0,z)$ with $z = 0.076$; Sr@ $xx(0,0,z)$ with $z = 0.138$; Cu@ $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.038$ and $z = 0.136$; O@ $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.136$ and $z = 0.268$; $xx(\frac{1}{2},0,z)$ with $z = 0.0.038$ and $z = 0.114$.



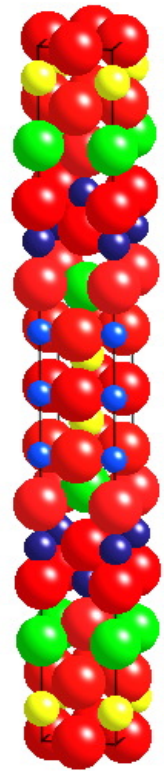
Structure 64 *Prototype:* $Tl_2Ba_2CuO_{6+x}$
SBS/PS: —/tI5 *SG # 139:* **I4/mmm** $(D_{4h}{}^{17})$
Lattice parameters: $a = 0.3866, c = 2.329$
Lattice complex: Tl@ $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.202$; Ba@ $xx(0,0,z)$ with $z = 0.083$; Cu@ $xx(\frac{1}{2},\frac{1}{2},0)$; O@ $xx(0,\frac{1}{2},0)$; $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.116$ and $z = 0.288$.



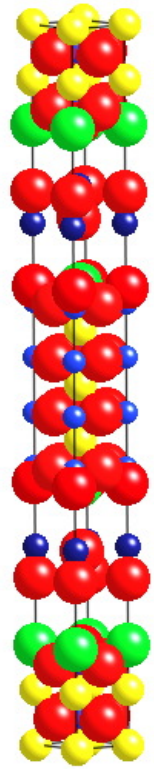
Structure 65 *Prototype:* $Tl_2Ba_2CaCu_2O_{8+x}$
SBS/PS: —/tI5 *SG # 139:* **I4/mmm** $(D_{4h}{}^{17})$
Lattice parameters: $a = 0.3855, c = 2.9318$
Lattice complex: Tl@ $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.2136$; Ca@ $xx(0,0,0)$; Ba@ $xx(0,0,z)$ with $z = 0.1218$; Cu@ $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.054$; O@ $xx(0,\frac{1}{2},z)$ with $z = 0.0531$; $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.1461$; $xx(x,\frac{1}{2},z)$ with $x = 0.604$ and $z = 0.2815$.



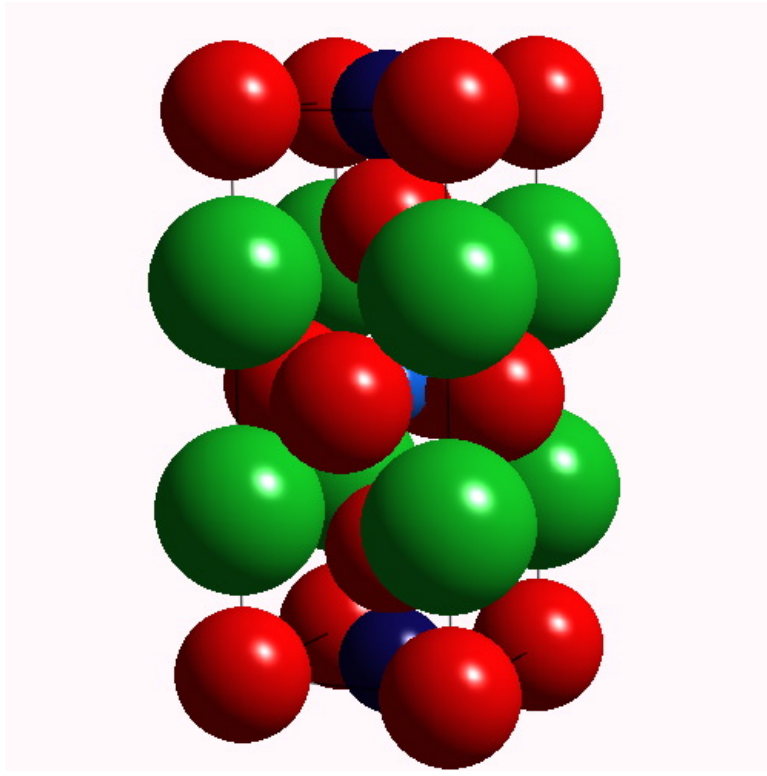
Structure 66 *Prototype:* $Tl_2Ba_2Ca_2Cu_3O_{10+x}$
SBS/PS: —/tI5 *SG # 139:* **I4/mmm** $(D_{4h}{}^{17})$
Lattice parameters: $a = 0.38503, c = 3.588$
Lattice complex: Tl@ $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.22$; Ca@ $xx(0,0,z)$ with $z = 0.046$; Ba@ $xx(0,0,z)$ with $z = 0.144$; Cu@ $xx(\frac{1}{2},\frac{1}{2},0)$; $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.089$; O@ $xx(\frac{1}{2},0,0)$; $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.158$ and $z = 0.2724$; $xx(\frac{1}{2},0,z)$ with $z = 0.087$.



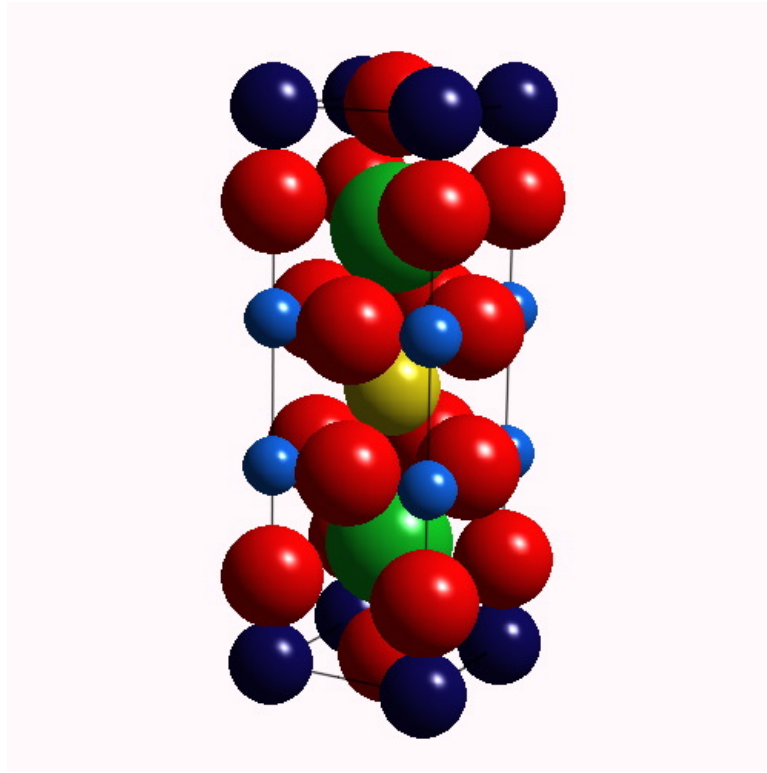
Structure 67 *Prototype:* $Tl_2Ba_2Ca_3Cu_4O_{12+x}$
SBS/PS: —/tI5 *SG # 139:* **I4/mmm** $(D_{4h}{}^{17})$
Lattice parameters: $a = 0.38503, c = 4.226$
Lattice complex: Tl@ $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.224$; Ca@ $xx(0,0,0)$; $xx(0,0,z)$ with $z = 0.076$; Ba@ $xx(0,0,z)$ with $z = 0.138$; Cu@ $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.038$ and $z = 0.136$; O@ $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.136$ and $z = 0.268$; $xx(\frac{1}{2},0,z)$ with $z = 0.0.038$ and $z = 0.114$.



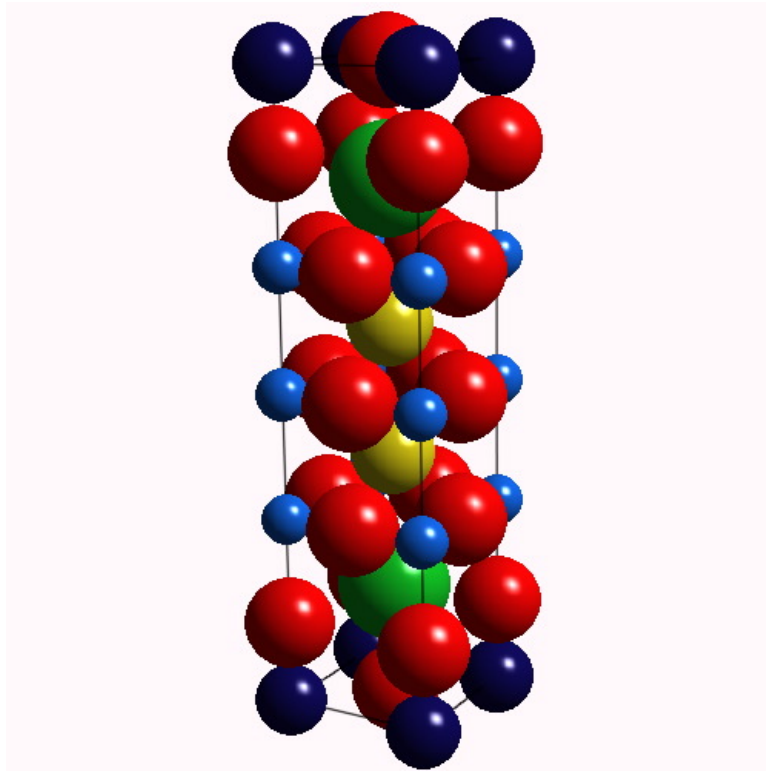
Structure 68 *Prototype:* $TlBa_2CuO_5$
SBS/PS: —/tI5 *SG # 123:* **P4/mmm** $(D_{4h}{}^{17})$
Lattice parameters: $a = 0.385, c = 0.954$
Lattice complex: Tl@ $xx(\frac{1}{2},\frac{1}{2},0)$; Ba@ $xx(0,0,z)$ with $z = 0.298$; Cu@ $xx(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; O@ $xx(0,0,0)$; $xx(0,\frac{1}{2},\frac{1}{2})$; $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.2078$.



Structure 69 *Prototype:* $TlBa_2CaCu_2O_7$
SBS/PS: —/tI5 *SG # 123:* **P4/mmm** $(D_{4h}{}^{17})$
Lattice parameters: $a = 0.38234, c = 1.2384$
Lattice complex: Tl@ $xx(0,0,0)$; Ba@ $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.2128$; Ca@ $xx(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; Cu@ $xx(0,0,z)$ with $z = 0.3675$; O@ $xx(\frac{1}{2},\frac{1}{2},0)$; $xx(0,0,z)$ with $z = 0.164$; $xx(\frac{1}{2},0,z)$ with $z = 0.3749$.



Structure 70 *Prototype:* $TlBa_2Ca_2Cu_3O_9$
SBS/PS: —/tI5 *SG # 123:* **P4/mmm** $(D_{4h}{}^{17})$
Lattice parameters: $a = 0.38429, c = 1.5871$
Lattice complex: Tl@ $xx(0,0,0)$; Ba@ $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.176$; Ca@ $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.397$; Cu@ $xx(0,0,\frac{1}{2})$; $xx(0,0,z)$ with $z = 0.302$; O@ $xx(\frac{1}{2},\frac{1}{2},0)$; $xx(0,\frac{1}{2},\frac{1}{2})$; $xx(0,\frac{1}{2},z)$ with $z = 0.304$; $xx(0,0,z)$ with $z = 0.132$.

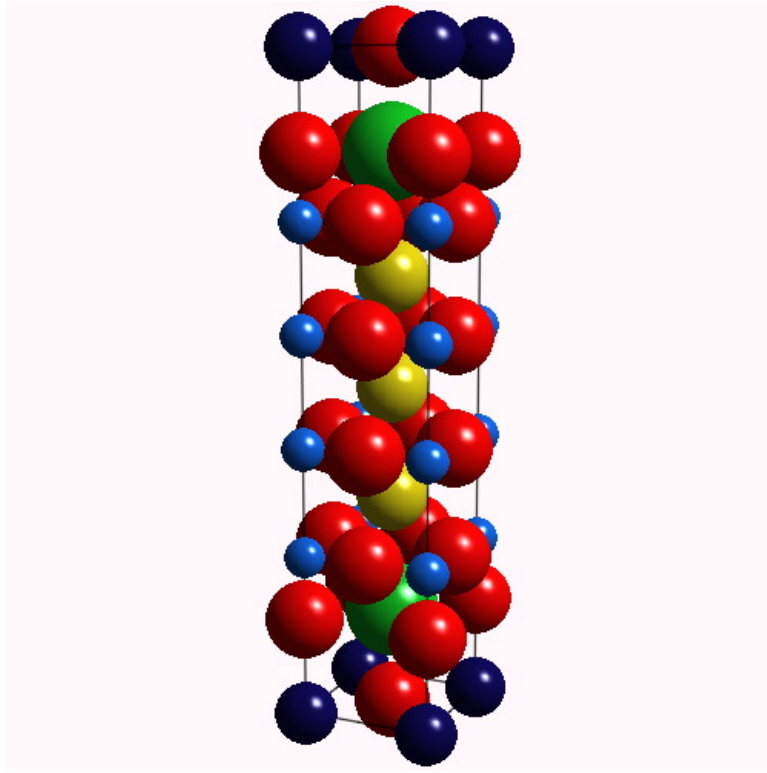


Structure 71 *Prototype:* $TlBa_2Ca_3Cu_4O_{11}$

SBS/PS: —/tI5 *SG # 139:* **I4/mmm** $(D_{4h}{}^{17})$

Lattice parameters: $a = 0.385, c = 1.915$

Lattice complex: Tl@ $xx(0,0,0)$; Ba@ $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.150$; Ca@ $xx(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.3315$; Cu@ $xx(0,0,z)$ with $z = 0.248$ and $z = 0.4151$; O@ $xx(\frac{1}{2},\frac{1}{2},0)$; $xx(0,0,z)$ with $z = 0.15$; $xx(\frac{1}{2},0,z)$ with $z = 0.248$ and $z = 0.4151$.

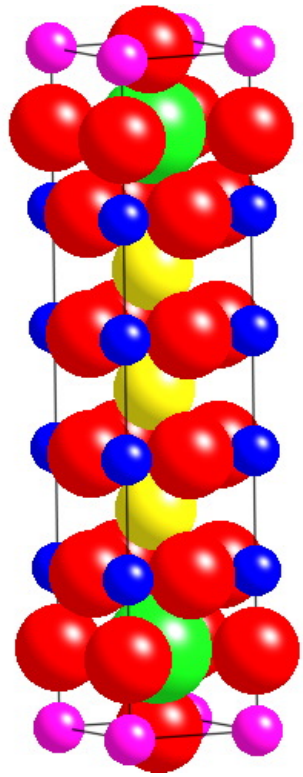


Structure 72 *Prototype:* $AgBa_2Ca_3Cu_4O_{10}$

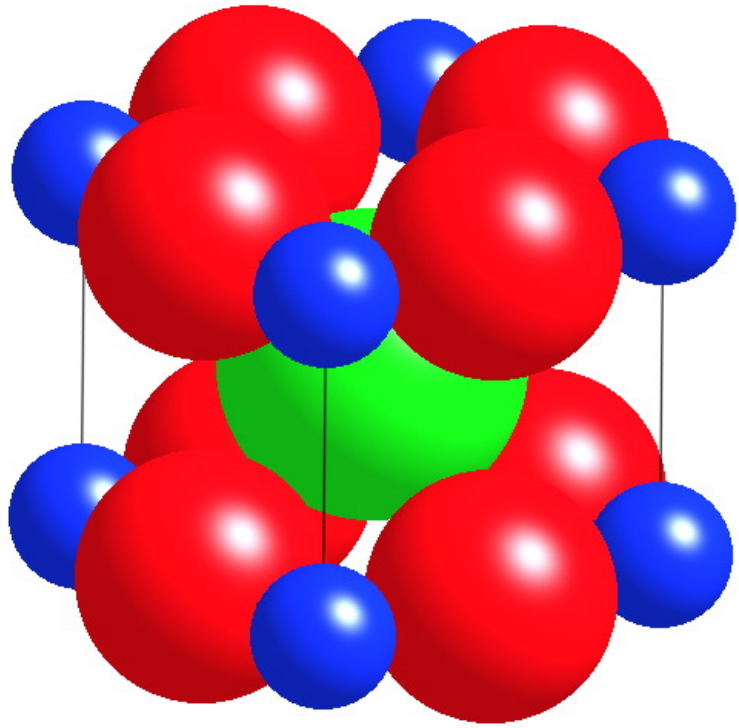
SBS/PS: —/tI5 *SG # 83:* **P4/m** $(D_{4h}{}^{17})$

Lattice parameters: $a = 0.386, c = 1.81$

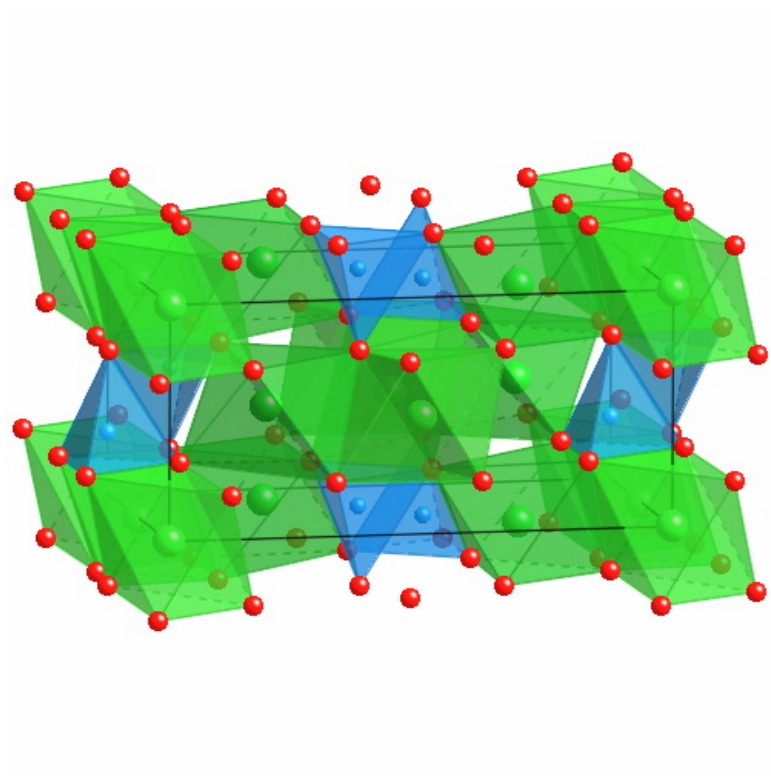
Lattice complex: Ag@ $xx(0,0,0)$; Ba@ $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.883$; Ca@ $xx(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.677$; Cu@ $xx(0,0,0)$; $xx(0,0,z)$ with $z = 0.5884$ and $z = 0.7650$; O@ $xx(\frac{1}{2},\frac{1}{2},0)$; $xx(0,\frac{1}{2},z)$ with $z = 0.5884$ and $z = 0.7650$; $xx(0,0,z)$ with $z = 0.8830$.



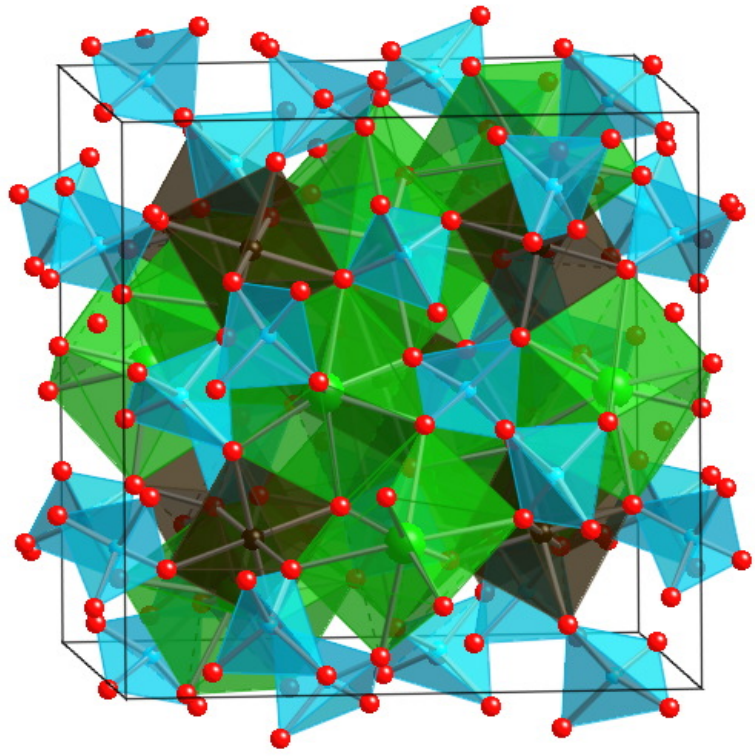
Structure 73 *Prototype:* (Ba,Sr)CuO_4
SBS/PS: —/tI5 *SG # 123:* **P4/mmm** $(D_{4h}{}^{17})$
Lattice parameters: $a = 0.393, c = 0.347$
Lattice complex: Ba,Sr@ $xx(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; Cu@ $xx(0,0,0)$; O@ $xx(0,\frac{1}{2},0)$.



Structure 74 *Prototype:* Forsterite: Mg_2SiO_4
SBS/PS: $S1_2$/oP28 *SG # 62:* **Pbnm** $(D_{2h}{}^{16})$
Lattice parameters: $a = 0.4762, b = 1.0225, c = 0.462$
Lattice complex: Mg@ $4a(0,0,0)$; and $4c(x,y,\frac{1}{4})$ with $x = 0.9896$ and $y = 0.2776$; O@ $4c(x,y,\frac{1}{4})$ with $x = 0.7667$ and $y = 0.0918$; $4c(x,y,\frac{1}{4})$ with $x = 0.2202$ and $y = 0.4477$; $8d(x,y,z)$ with $x = 0.2781$, $y = 0.1633$ and $z = 0.0337$; Si@ $4c(x,y,\frac{1}{4})$ with $x = 0.4226$ and $y = 0.5994$.



Structure 75 *Prototype:* Garnet: $Ca_3Fe_2Si_3O_{12}$
SBS/PS: —/cI160 *SG # 230:* **Ia$\bar{3}$** $(O_h{}^{10})$
Lattice parameters: $a = 1.203$
Lattice complex: Ca@ $24c(\frac{1}{8},0,\frac{1}{4})$; Fe@ $16a(0,0,0)$; O@ $96h(x,y,z)$ with $x = 0.0395$, $y = 0.0488$ and $z = 0.6556$; Si@ $24d(\frac{3}{8},0,\frac{1}{4})$.

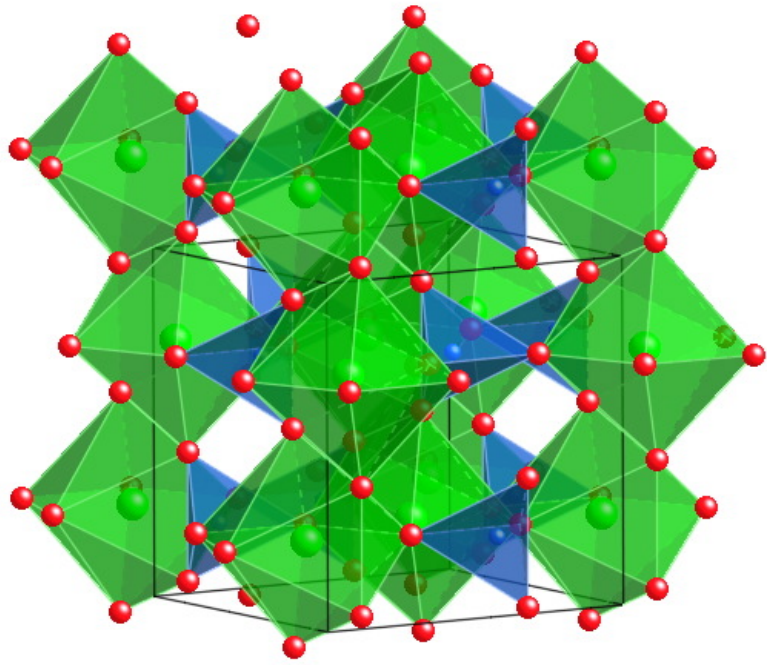


Structure 76 *Prototype:* Zircon $ZrSiO_4$

SBS/PS: —/tI24 *SG # 141:* $\mathbf{I4_1/amd}$ $(D_{4h}{}^{19})$

Lattice parameters: $a = 0.661, c = 0.6001$

Lattice complex: Zr@ $4a(0, \frac{3}{4}, \frac{1}{8})$; O@ $16h(0, y, z)$ with $y = 0.0646$ and $z = 0.1967$; Si@ $4b(0, \frac{1}{4}, \frac{3}{8})$.

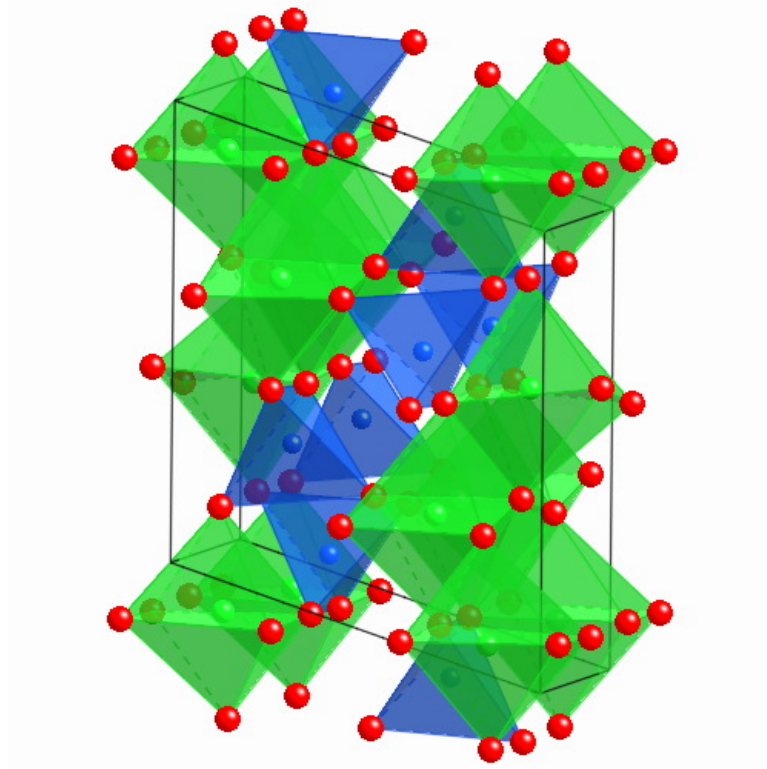


Structure 77 *Prototype:* Kyanite Al_2SiO_5

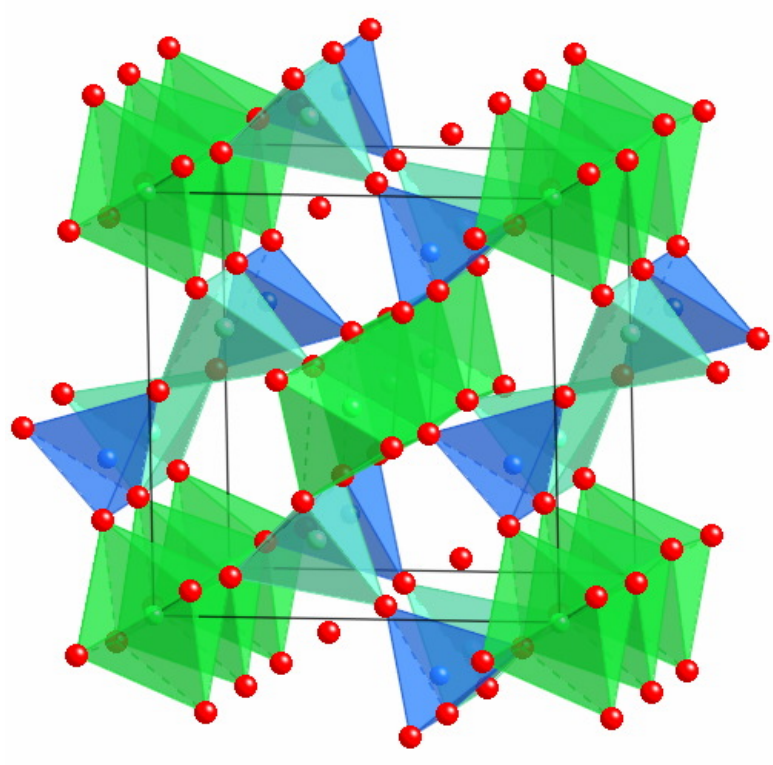
SBS/PS: —/tP16 *SG # 2:* $\mathbf{P\bar{1}}$ (C_i^1)

Lattice parameters: $a = 0.71262, b = 0.7852, c = 0.5724, \alpha = 89.99°, \beta = 101.11°, \gamma = 106.03°$

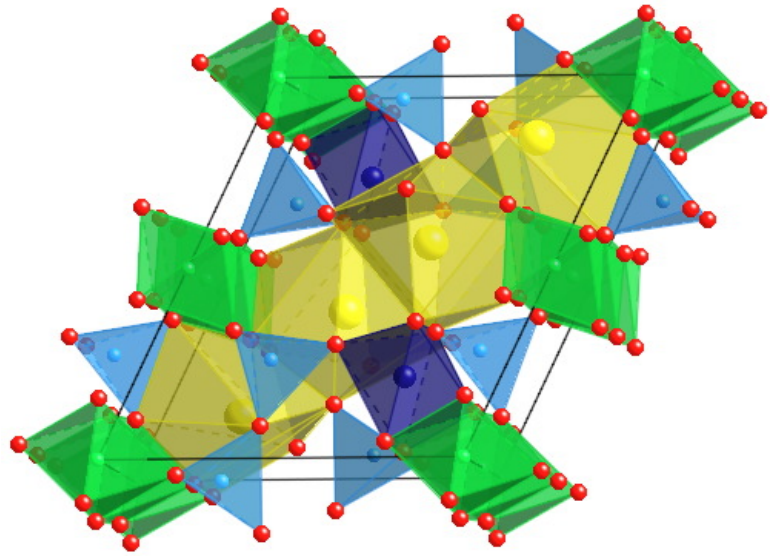
Lattice complex: Al@ $2i(x,y,z)$ with (x,y,z) = $(0.3254, 0.704, 0.4582)$, $(0.2974, 0.6989, 0.9505)$, $(0.0998, 0.3863, 0.6403)$, and $(0.112, 0.9175, 0.1649)$; O@ $2i(x,y,z)$ with (x,y,z) = $(0.1095, 0.1468, 0.1288)$, $(0.123, 0.6856, 0.1812)$, $(0.2747, 0.4545, 0.9547)$, $(0.2831, 0.9354, 0.9353)$, $(0.1084, 0.152, 0.6669)$, $(0.1219, 0.6307, 0.6389)$, $(0.2822, 0.4453, 0.4288)$, $(0.2915, 0.9467, 0.4459)$, $(0.5008, 0.2749, 0.244)$ and $(0.5015, 0.2312, 0.7553)$; Si@ $2i(x,y,z)$ with (x,y,z) = $(0.2962, 0.0649, 0.7066)$ and $(0.291, 0.3317, 0.1892)$.



Structure 78 *Prototype:* Sillimanite Al_2SiO_5
SBS/PS: —/oP32 *SG # 62:* **Pbnm** (*Orthorhombic*)
Lattice parameters: $a = 0.74883, b = 0.76808, c = 0.5774$
Lattice complex: Al@ $4a(0,0,0)$; and $4c(x,y,\frac{1}{4})$ with $x = 0.1417$ and $y = 0.3449$; O@ $4c(x,y,\frac{3}{4})$ with (x,y) = $(0.3605,0.4094)$, $(0.4763,0.0015)$ and $(0.3569,0.4341)$; $8d(x,y,z)$ with (x,y,z)= $(0.2747,0.4545,0.9547)$, $(0.2831,0.9354,0.9353)$ and
$(0.1252,0.223,0.5145)$; Si@ $4c(x,y,\frac{3}{4})$ with $x = 0.1533$ and $y = 0.3402$;



Structure 79 *Prototype:* Epidote $Ca_2(Al,Fe)Al_2Si_3O_{13}H$
SBS/PS: —/mP44 *SG # 11:* $\mathbf{P2_1/m}$ $(C_{2h}{}^2)$
Lattice parameters: $a = 0.8914, b = 0.564, c = 1.0162, \beta = 115.4°$
Lattice complex: Ca@ $2e(x, \frac{1}{4}, z)$ with (x,z) = $(0.2438, 0.849)$ and $(0.3968, 0.579)$; Al@ $2a(0,0,0)$; $2c(0,0,\frac{1}{2})$; Fe@ $2e(x, \frac{1}{4}, z)$ with $x = 0.2946$ and $z = 0.2245$; O@ $4f(x,y,z)$ with (x,y,z) = $(0.2339, 0.9923, 0.041)$, $(0.304, 0.9809, 0.3554)$ and $(0.7957, 0.0152, 0.3382)$; $2e(x, \frac{1}{4}, z)$ with (x,z) = $(0.0838, 0.4298)$, $(0.0528, 0.1294)$, $(0.5281, 0.3099)$ and $(0.6265, 0.099)$, $(0.9582, 0.8529)$, $(0.9317, 0.5922)$ and $(0.4836, 0.8175)$; Si@ $2e(x, \frac{1}{4}, z)$ with (x,z) = $(0.6604, 0.9527)$, $(0.8156, 0.6811)$ and $(0.6851, 0.2744)$.

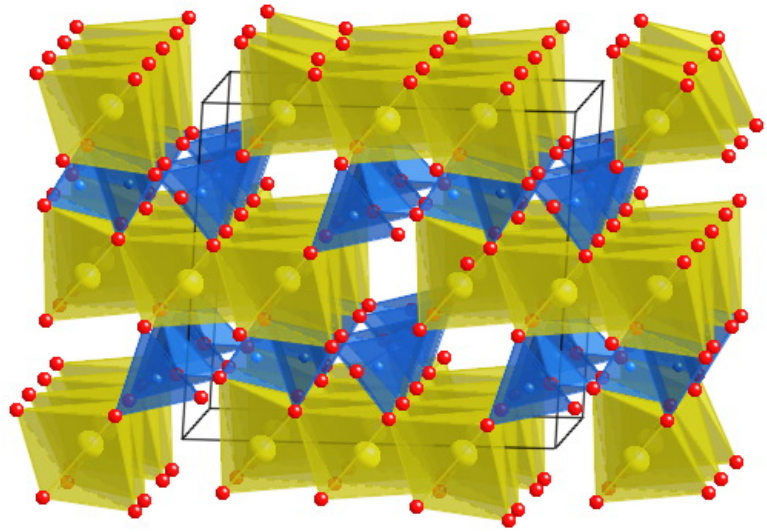


Structure 80 *Prototype:* Wollastonite-1T $CaSiO_3$

SBS/PS: —/tC40 *SG # 2:* $\mathbf{C\bar{1}}$ (*Triclinic*)

Lattice parameters: $a = 1.0121, b = 1.107, c = 0.7312, \alpha = 99.51^\circ, \beta = 100.51^\circ, \gamma = 83.43^\circ$

Lattice complex: Ca@ $2i(x,y,z)$ with (x,y,z) = $(0.0208, 0.7807, 0.0772)$, $(0.0171, 0.7806, 0.5709)$ and $(0.0144, 0.4885, 0.2504)$; O@ $2i(x,y,z)$ with $(0.1163, 0.5797, 0.0381)$, $(0.1169, 0.5814, 0.5611)$, $(0.1149, 0.3141, 0.7307)$, $(0.1239, 0.8584, 0.8745)$, $(0.123, 0.8577, 0.3669)$, $(0.1152, 0.2864, 0.2267)$, $(0.2211, 0.9963, 0.6785)$, $(0.182, 0.0886, 0.3704)$ and $(0.1872, 0.0907, 0.0121)$; Si@ $2i(x,y,z)$ with (x,y,z) = $(0.2265, 0.9583, 0.8877)$, $(0.2267, 0.9577, 0.4537)$, and $(0.2264, 0.1707, 0.2263)$.

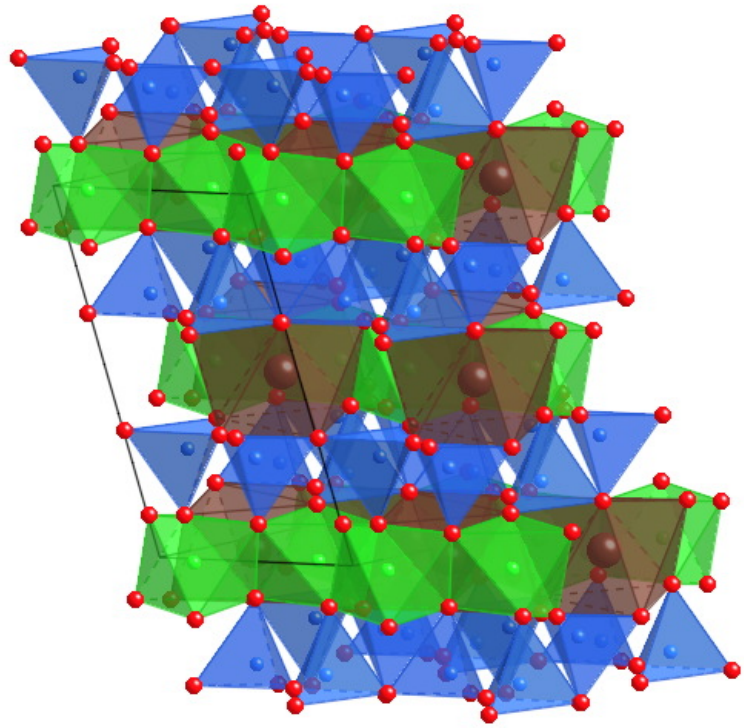


Structure 81 *Prototype:* Jadeite $NaAlSi_2O_6$

SBS/PS: —/hP40 *SG # 15:* **C2/c** $(C_{2h}{}^6)$

Lattice parameters: $a = 0.9418, b = 0.8562, c = 0.5219, \beta = 107.58^\circ$

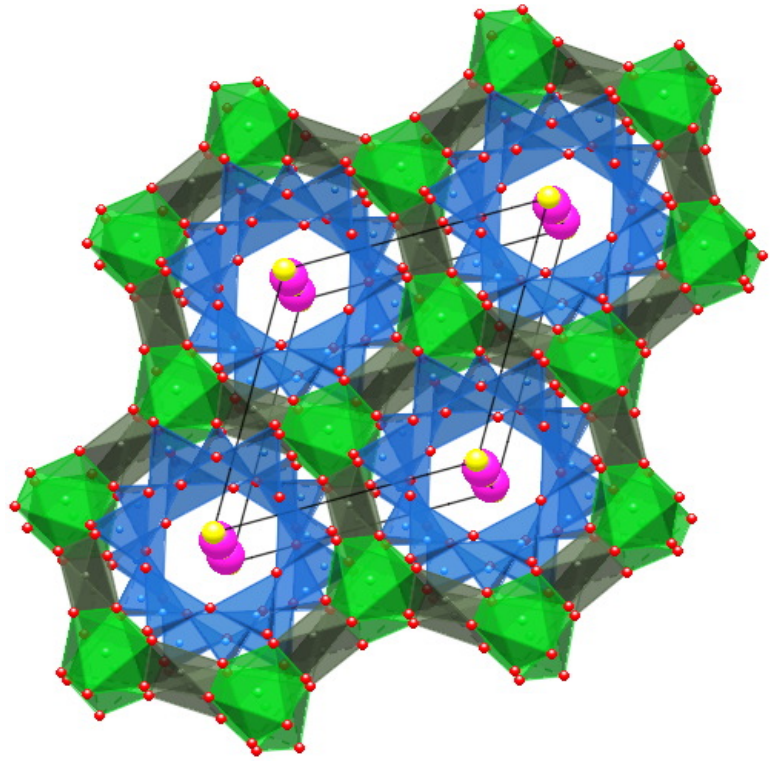
Lattice complex: Al@ $4e(0, y, \frac{1}{4})$ with $y = -0.094$; Na@ $4e(0, y, \frac{1}{4})$ with $y = 0.3009$; O@ $8f(x, y, z)$ with $(x, y, z) = (0.109, 0.0763, 0.1277)$, $(0.3608, 0.263, 0.2929)$, and $(0.3433, 0.007, 0.0058)$; Si@ $8f(x, y, z)$ with $x = 0.2906$, $y = 0.0934$ and $z = 0.2277$.



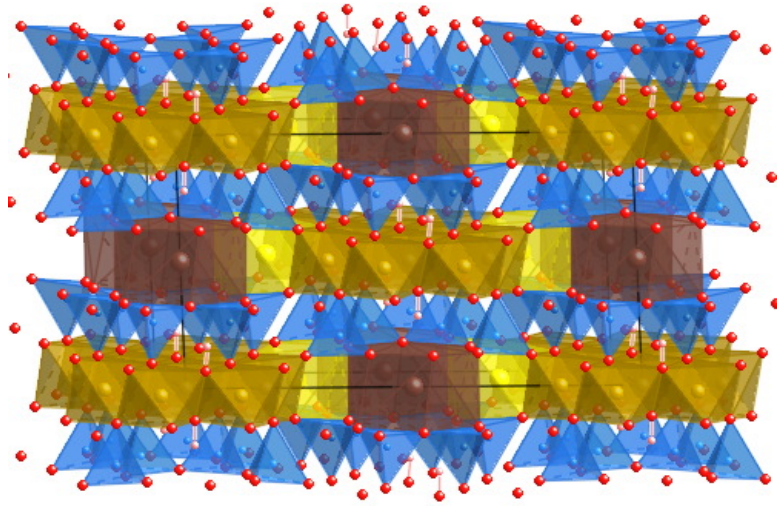
Structure 82 *Prototype:* Beryl $Be_3Al_2Si_6O_{18}$

SBS/PS: —/hP40 *SG # 192:* **P6/mmc** $(D_{6h}{}^2)$

Lattice complex: $a = 0.9212, c = 0.9236$ Al@ $4c(\frac{2}{3},\frac{1}{3},\frac{1}{4})$; Be@ $6f(\frac{1}{2},0,\frac{1}{4})$; Cs@ $2a(0,0,\frac{1}{4})$; Na@ $2b(0,0,0)$; O@ $12l(x,y,0)$ with $x = 0.3048$ and $y = 0.2352$; and $24m(x,y,z)$ with $x = 0.4983$, $y = 0.1473$ and $z = 0.1445$; Si@ $12l(x,y,0)$ with $x = 0.3892$ and $y = 0.1189$.



Structure 83 *Prototype:* Tremolite $Ca_2Mg_5(Si_8O_{22})(OH)_3$
SBS/PS: —/mC78 *SG # 12:* **C3/m** ($C_{2h}{}^3$)
Lattice complex: $a = 0.9863, b = 1.8048, c = 0.5285, \beta = 107.58^\circ$ Ca@ $4h(0, y, \frac{1}{2})$ with $y = 0.2779$; H@ $4i(x, 0, z)$ with $x = 0.2088$ and $z = 0.7628$; Mg@ $2a(0, 0, 0)$; $4h(0, y, \frac{1}{2})$ with $y = 0.0883$; $4g(0, y, 0)$ with $y = 0.177$; Na@ $2b(0, \frac{1}{2}, 0)$; O@ $8j(x, y, z)$ with (x, y, z) = $(0.1114, 0.0847, 0.2182)$, $(0.1187, 0.1707, 0.725)1$, $(0.3642, 0.2482, 0.7928)$, $(0.3467, 0.1339, 0.0998)$ and $(0.3437, 0.1181, 0.591)$; $4i(x, 0, z)$ with (x, z)= $(0.338, 0.2921)$ and $(0.1082, 0.7154)$; Si@ $8j(x, y, z)$ with (x, y, z) = $(0.2799, 0.0842, 0.2974)$ and $(0.2882, 0.1713, 0.8056)$.

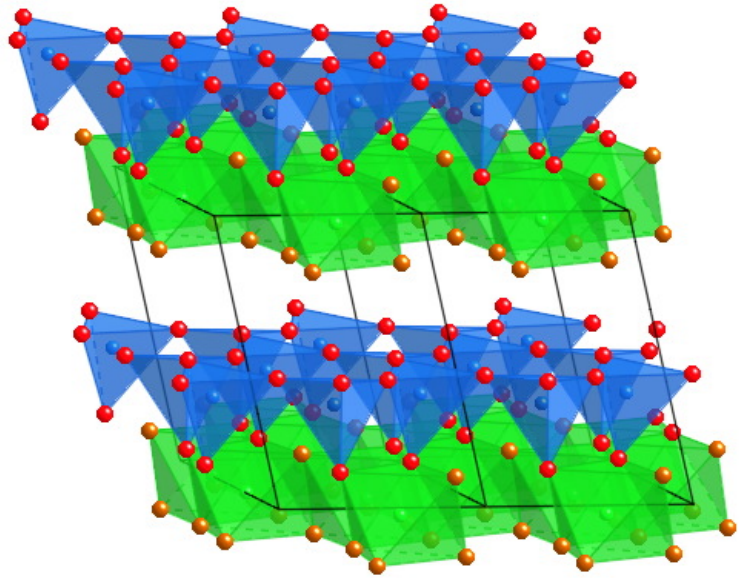


Structure 84 *Prototype:* Kaolinite $Al_2Si_2O_5(OH)_4$

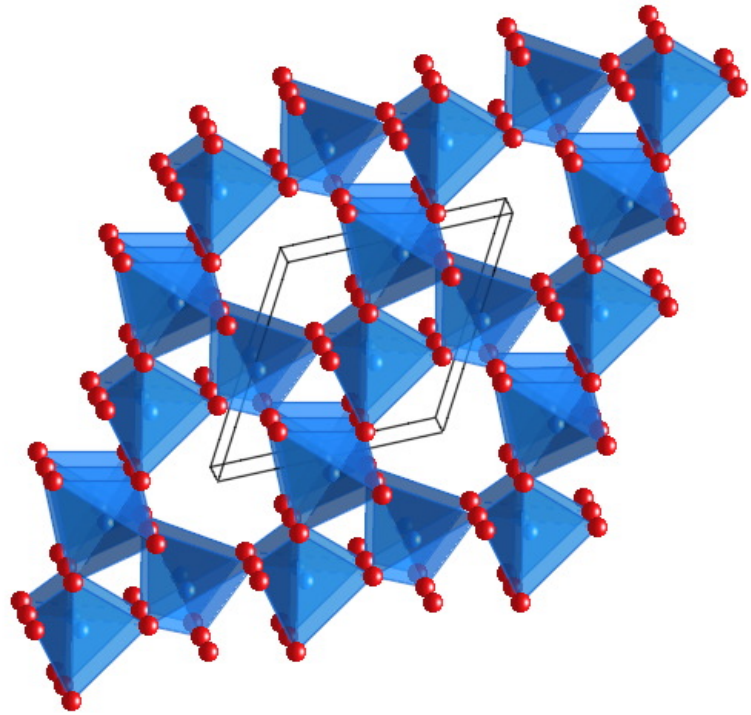
SBS/PS: —/tC26 *SG # 1:* **C1** (*Triclinic*)

Lattice parameters: $a = 0.514, b = 0.893, c = 0.737, \alpha = 91.8°, \beta = 104.5°, \gamma = 90°$

Lattice complex: All atoms in $1a(x,y,z)$ positions: Al$(0.502, 0.172, 0.003)$ and $(0.002, 0.33, 0.002)$; O$(0.754, 0.315, 0.155)$, $(0.69, 0.004, 0.157)$, $(0.791, 0.165, 0.482)$, $(0.612, -0.12, 0.455)$ and $(0.108, -0.058, 0.455)$; OH$(0.778, 0.18, -0.14)$, $(0.278, 0.32, -0.38)$, $(0.316, -0.008, -0.136)$ and $(0.248, 0.184, 0.155)$; Si$(0.8, 0.322, 0.382)$ and $(0.8, 0.0, 0.385)$.



Structure 85 *Prototype:* α-Quartz SiO_2
SBS/PS: C8/hP9 *SG # 154:* **$P3_221$** $(D_3{}^6)$
Lattice parameters: $a = 0.49137, c = 0.54047$
Lattice complex: O@ $6c(x,y,z)$ with $x = 0.4133$, $y =, 0.2672$ and $z = 0.1188$; Si@ $3a(x,0,0)$ with $x = 0.4697$; origin offset by $(0,0,\frac{-1}{3})$.

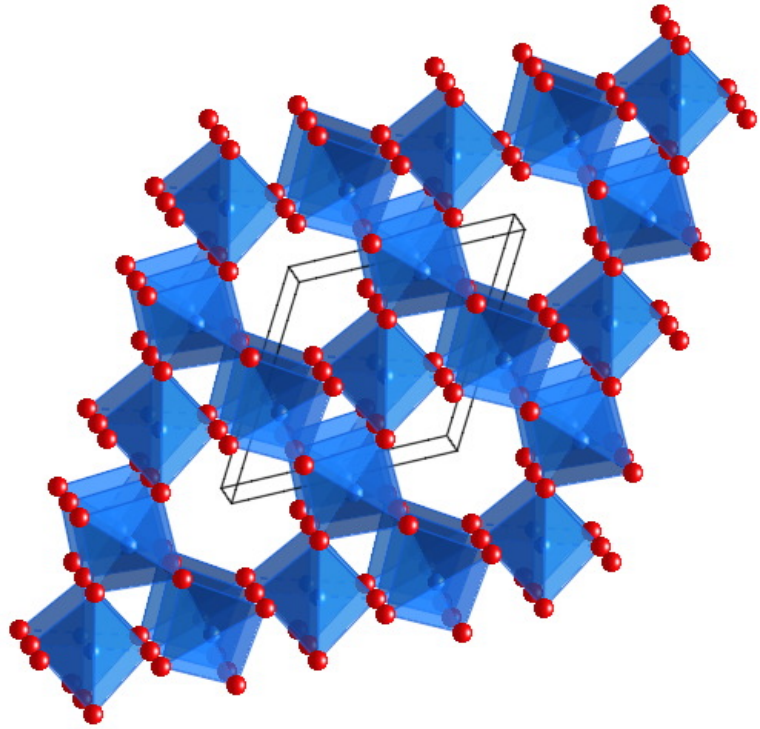


Structure 86 *Prototype:* β-Quartz SiO_2

SBS/PS: —/hP9 *SG # 171:* **P6$_2$** ($C_6{}^4$)

Lattice parameters: $a = 0.49965, c = 0.54546$

Lattice complex: O@ $6c(x,y,z)$ with $x = 0.4157$, $y = 0.2078$ and $z = 0.1667$; Si@ $3a(\frac{1}{2},0,0)$; origin offset by $(0,0,\frac{-1}{3})$.

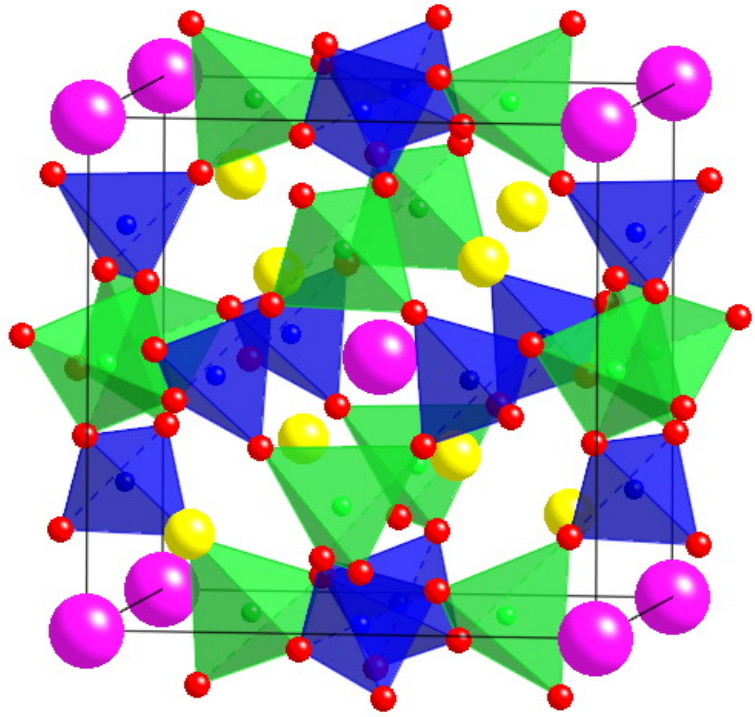


Structure 87 *Prototype:* $Na_4Al_3Si_3O_{12}Cl$

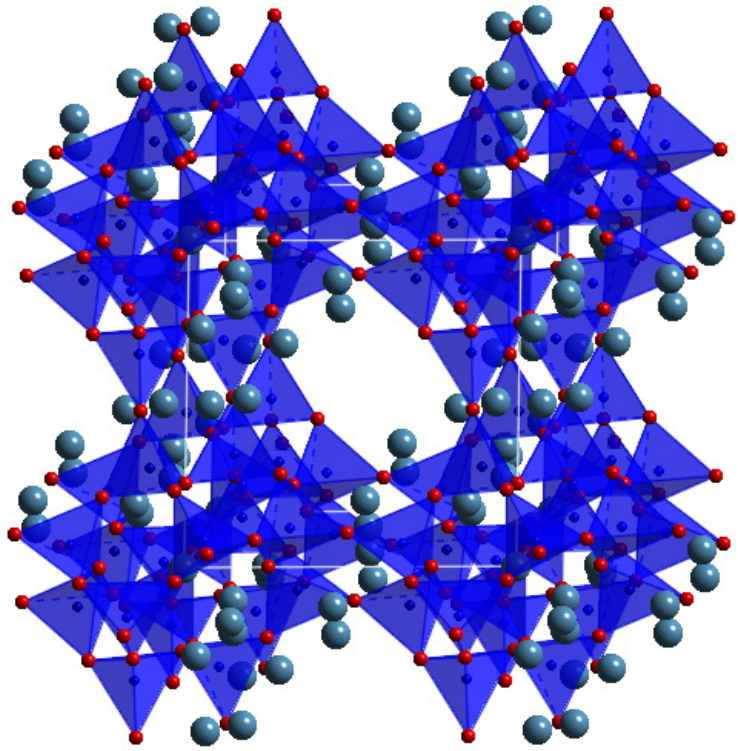
SBS/PS: —/cP9 *SG # 218:* **P$\bar{4}$3n** $(T_d{}^4)$

Lattice parameters: $a = 0.891$

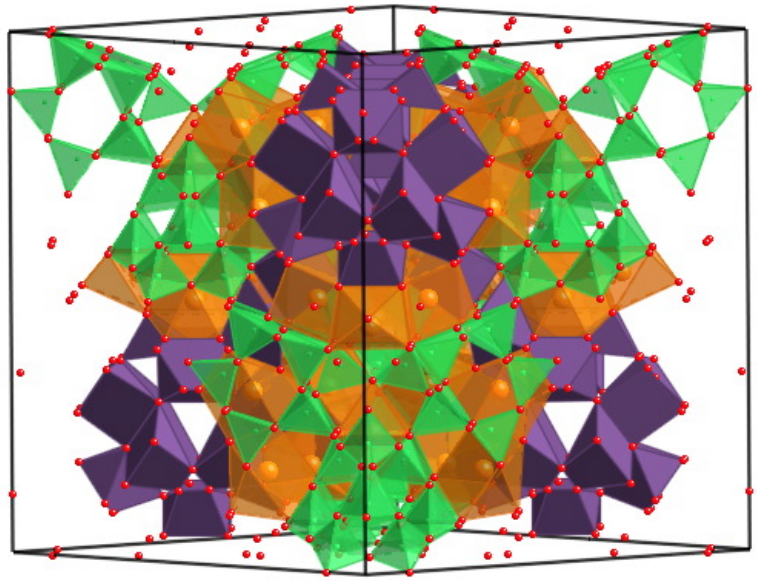
Lattice complex: Al@ $6c(\frac{1}{4},\frac{1}{2},0)$; Cl@ $2a(0,0,0)$; Na@ $8e(x,x,x)$;with $x = 0.175$; O@ $24i(x,y,z)$ with $x = 0.15$, $y = 0.135$ and $z = 0.44$; and Si@ $6c(\frac{1}{4},\frac{1}{2},0)$;



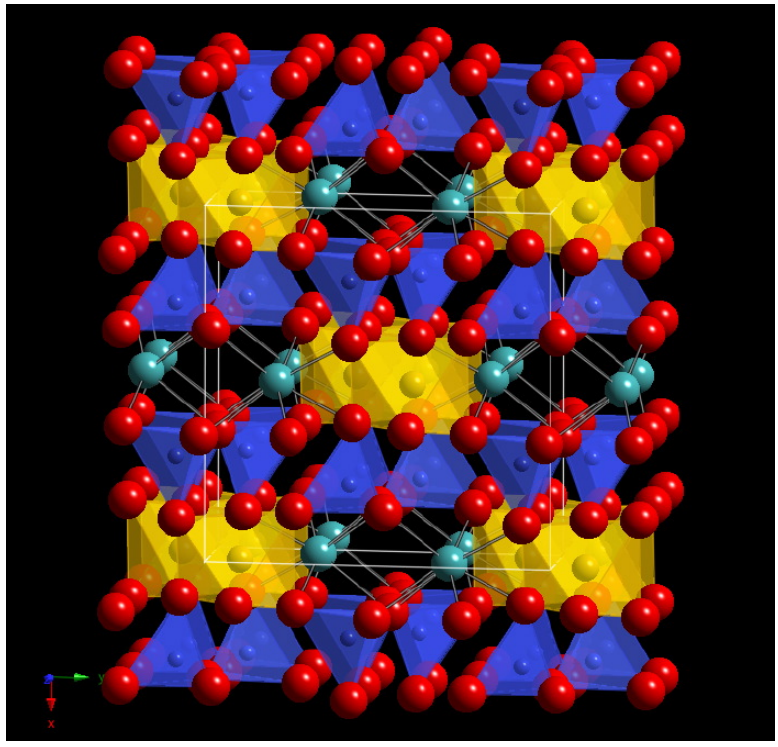
Structure 88 *Prototype:* $CaAl_2Si_4O_{12}\cdot 6H_2O$
SBS/PS: —/hR74 *SG # 166:* **R$\bar{3}$m** $(D_{3d}{}^5)$
Lattice parameters: $a = 0.937, \alpha = 92.02^\circ$
Lattice complex: (dehydrated form) Ca@ $1a(0,0,0)$ with 0.6 site occupancy, $2c(x,x,x)$ with $x = 0.169$ and 0.35 site occupancy, $12i(x,y,z)$ with $x = 0.09$, $y = 0.1609$ and $z = 0.47$ and 0.16 site occupancy; O@ $6f(x,\bar{x},0)$ with $x = 0.284$, $6g(x,\bar{x},0.5)$ with $x = 0.124$, $6h(x,x,z)$ with $x = 0.238$ and $z = 0.878$, $6c(0,0,z)$ with $z = 0.255$; Al,Si@ $12i(x,y,z)$ with $x = 0.095$, $y = 0.328$ and $z = 0.864$.



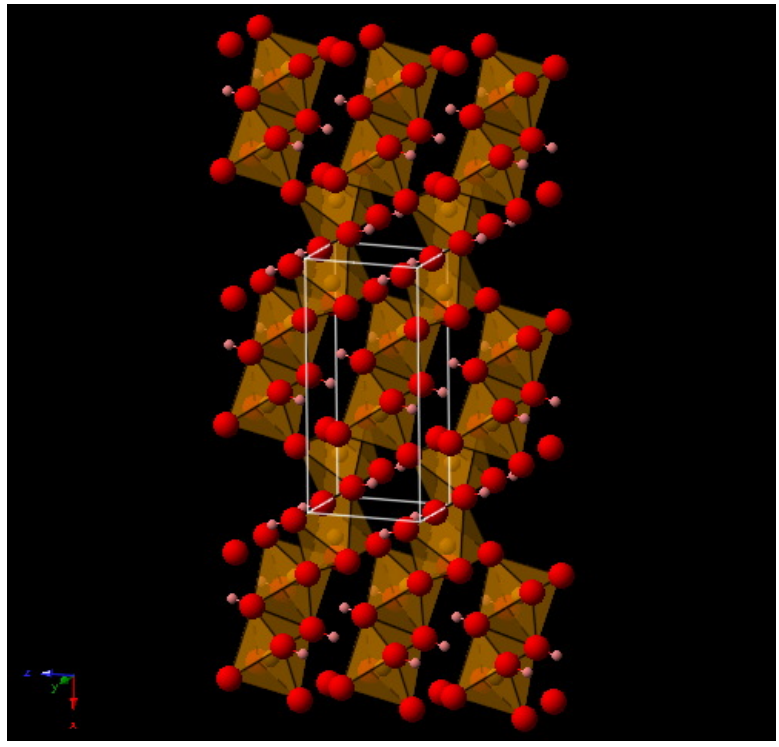
Structure 89 *Prototype:* Fullerenoid Oxide $Sr_{33}Bi_{24+\delta}Al_{48}O_{141+\frac{3\delta}{2}}$
SBS/PS: —/cF1784 *SG # 216:* **F$\bar{4}$3m** ($T_d{}^2$)
Lattice parameters: $a = 2.509$
Lattice complex: Bi@ $16e(x,x,x)$ with $x = 0.85$; $48h(x,x,z)$ with $(x,z) = (0.3,0.5932)$ and $(0.944475,0.74886;occ.0.7)$; Sr@ $4c(\frac{3}{4},\frac{1}{4},\frac{3}{4})$; and $48h(x,x,z)$ with $(x,z) = (0.82763,0.46345)$ and $(0.17534,0.99084)$; $16e(x,x,x)$ with $x = 0.92946$ and $x = 0.587$; Al@ $48h(x,x,z)$ with $(x,z) = (0.0468,0.1345)$, $(0.0895,0.2444)$, $(0.7942,0.1177)$ and $(0.4545,0.3661)$; O@ $16e(x,x,z)$ with $x = 0.8269$ and $z = 0.1731$; $24f(0,0,z)$ with $z = 0.1121$; $24g(\frac{3}{4},\frac{3}{4},z)$ with $z = 0.1476$; $48h(x,z,z)$ with $x = 0.0259$ and $y = 0.1083$, $48h(x,x,z)$ with $x = 0.0772$ and $z = 0.312$; $48h(x,y,z)$ with $(x,y,z) = (0.51,0.49,0.345;occ.0.5)$ and $(0.331,0.372,0.628;occ.1/3)$; $48h(x,y,x)$ with $(x,y) = (0.4047,0.4853)$ and $(0.796,0.890;occ.0.6)$; $96i(x,y,z)$ with $(x,y,z) = (0.0421,0.0585,0.2042;occ.0.5)$, $(0.1577,\ 0.0775,0.2356)$, $(0.9,0.826,0.9206;occ.0.5)$ and $(0.273,0.3597,0.5388)$.



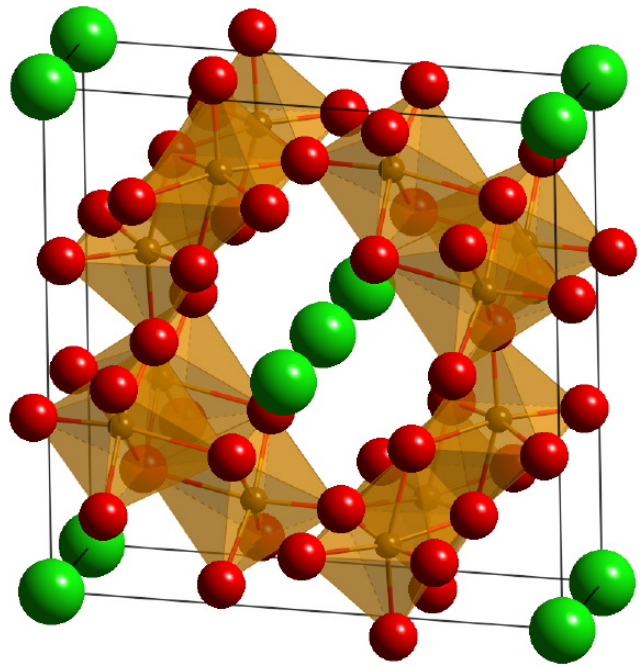
Structure 90 *Prototype:* Diopside $CaMgSi_2O_6$
SBS/PS: —/mP16 *SG # 15:* **C2/c** $(C_{2h}{}^6)$
Lattice parameters: $a = 0.9746, b = 0.8899, c = 0.5251, \beta = 105.63^\circ$
Lattice complex: Ca@ $4e(0, y, \frac{1}{4})$ with $y = 0.3015$; Mg@ $4e(0, y, \frac{1}{4})$ with $y = -.9082$; Si@ $8f(x, y, z)$ with $x = 0.2862, y = 0.0933, z = 0.2293$; O@ @ $8f(x, y, z)$ with $x = 0.1156, y = 0.0873, z = 0.1422$, $x = 0.3611, y = 0.25, z = -.318$, $x = 0.3503, y = 0.0176, z = 0.9953$.



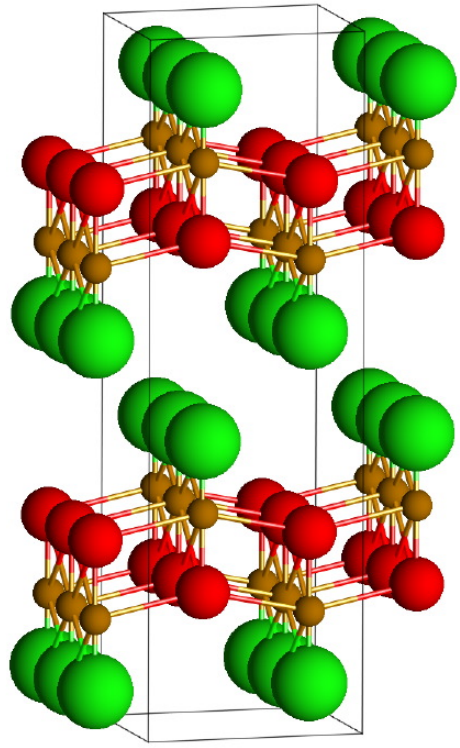
Structure 91 *Prototype:* Goethite α-FeO(OH)
SBS/PS: —/oP40 *SG # 62:* **Pnma** $(D_{2h}{}^{16})$
Lattice parameters: $a = 0.995, b = 0.301, c = 0.462$
Lattice complex: Fe@ $4c(x, \frac{1}{4}, z)$ with $x = 0.145, z = 0.955$; H@ $4c(x, \frac{1}{4}, z)$ with $x = 0.92, z = 0.62$; O@ $4c(x, \frac{1}{4}, z)$ with $x = 0.801, z = 0.288$, $x = 0.947, z = 0.802$.



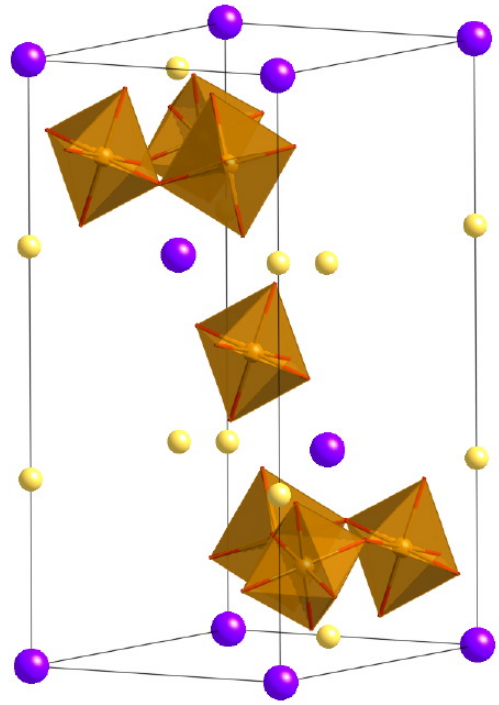
Structure 92 *Prototype:* Akaganeite β-FeO(OH,Cl)
SBS/PS: —/mP40 *SG # 12:* **I2/m** $(C_{2h}{}^3)$
Lattice parameters: $a = 1.06, b = 0.3034, c = 1.0513, \beta = 90.24^\circ$
Lattice complex: Fe@ $(0.858, 0.0, 0.341)$, $(0.339, 0.0, 0.141)$; Cl@ $(0, 0, 0)$; O@ $(0.663, 0.0, 0.29)$, $(0.657, 0.0, 0.03)$, $(0.293, 0.0, 0.357)$, $(0.039, 0.0, 0.332)$.



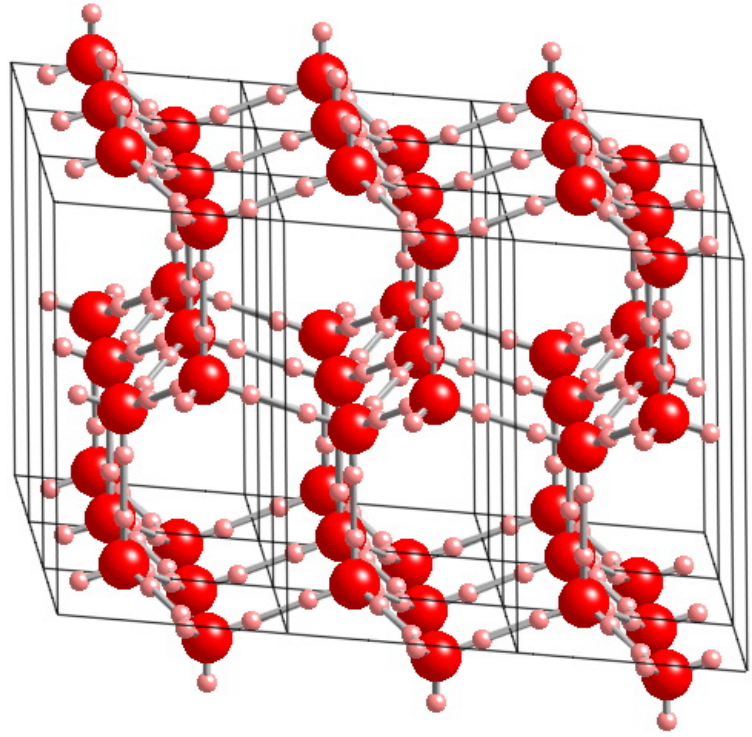
Structure 93 *Prototype:* Lepidocrocite γ-FeO(OH)
SBS/PS: —/oC24 *SG # 63:* **Bbmm** $(D_{2h}{}^{17})$
Lattice parameters: $a = 1.24, b = 0.387, c = 0.307$
Lattice complex: Fe@ $0.822, 0.25, 0.0$); O@ $0.21, 0.25, 0.0$); OH@ $0.425, 0.25, 0.0$.



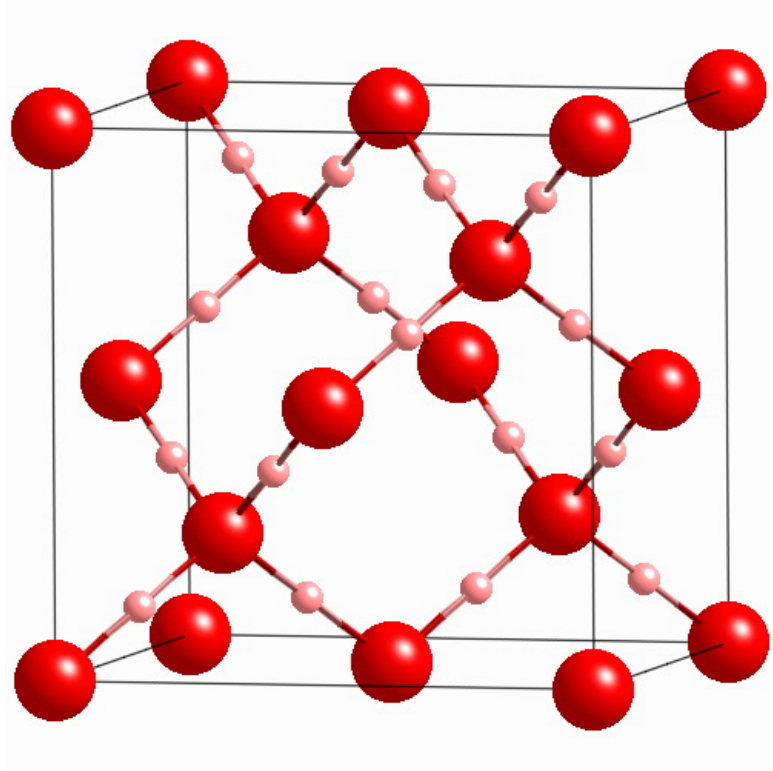
Structure 94 *Prototype:* Jarosite $KFe_3(SO_4)_2(OH)_6$
SBS/PS: —/R60 *SG # 166:* **R − 3m** $(D_{3d}{}^5)$
Lattice parameters: $a = 0.7304, c = 1.7268$ (hexagonal axes)
Lattice complex: Fe@ $9d(x,-x,z)$ with $x = 0.166667, z = 0.166667$; S@ $6c(0,0,z)$ with $z = 0.3084$; O@ $6c(0,0,z)$ with $z = 0.3934$; O@ $18h(x,-x,z)$ with $x = 0.218, z = 0.9457$; K@ $3a(0,0,0)$; OH@ $18h(x,-x,z)$ with $x = 0.1247, z = 0.1351$.



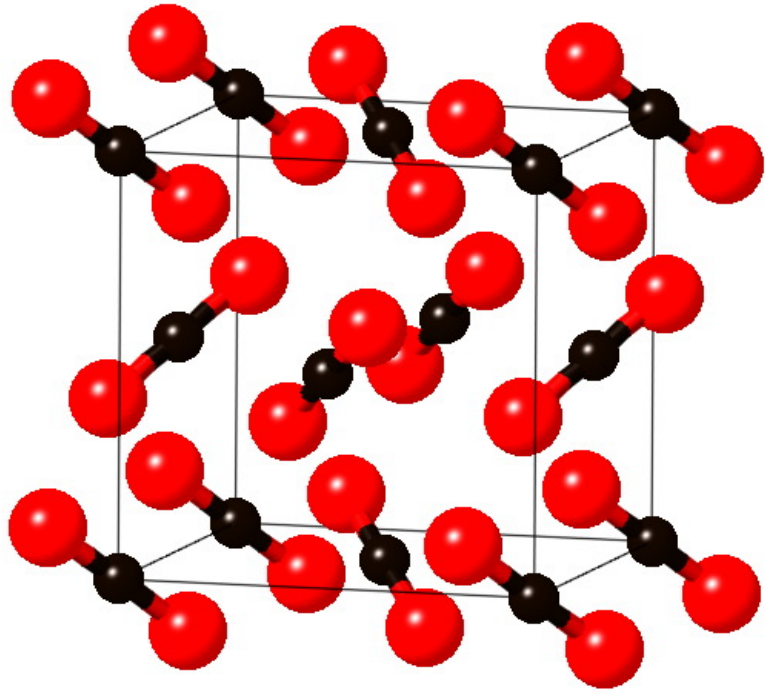
Structure 95 *Prototype:* Ice- I_h H_2O
SBS/PS: —/hP12 *SG # 194:* **$P6_3/mmc$** $(D_{6h}{}^4)$
Lattice parameters: $a = 0.45227, c = 0.73671$
Lattice complex: H@ $4f(\frac{1}{3},\frac{2}{3},z)$ with $z = 0.173$; $12k(x,2x,z)$ with $x = 0.437$ and $z = 0.024$; O@ @ $4f(\frac{1}{3},\frac{2}{3},z)$ with $z = 0.0618$.



Structure 96 *Prototype:* Ice- I_c H_2O
SBS/PS: —/cF24 *SG # 227:* **Fd$\bar{3}$m** $(O_h{}^7)$
Lattice parameters: $a = 0.635$
Lattice complex: H@ $16c(\frac{1}{8},\frac{1}{8},\frac{1}{8})$; O@ $8a(0,0,0)$.



Structure 97 *Prototype:* CO_2-Cubic
SBS/PS: —/cP12 *SG # 205:* **Pa$\bar{3}$** $(T_h{}^6)$
Lattice parameters: $a = 0.5056$
Lattice complex: O@ $8c(x,x,x)$ with $x = 0.1324$ and $x = -0.1324$; C@ $4a(0,0,0)$.

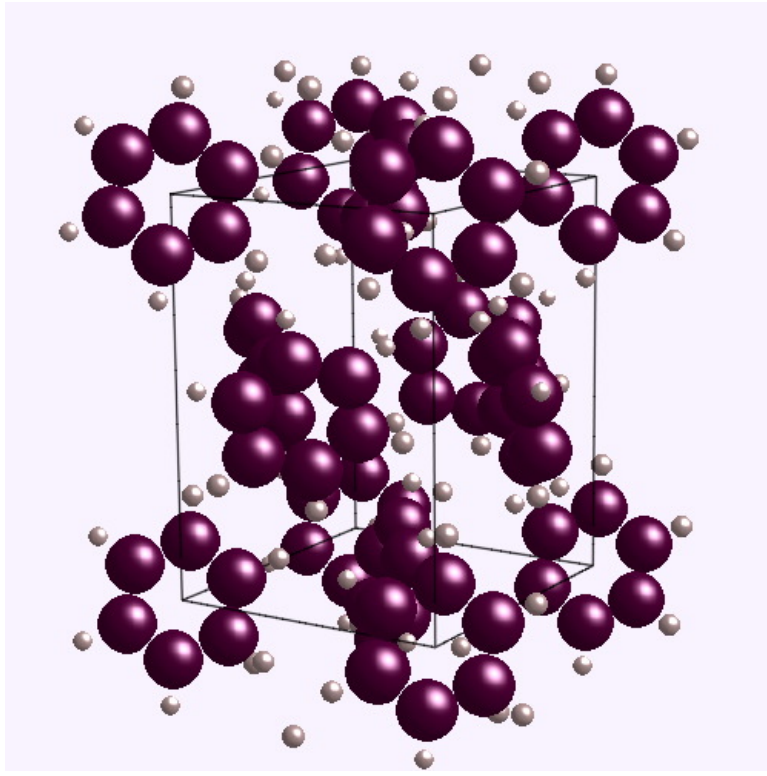


Structure 98 *Prototype:* C_6H_6

SBS/PS: —/oP48 *SG # 61:* **Pbca** $(D_{2h}{}^{15})$

Lattice parameters: $a = 0.744, b = 0.955, c = 0.692$

Lattice complex: All positions $8c(x,y,z)$: C@ $(-0.0569, 0.1387, -0.0054)$, $(-0.1335, 0.046, 0.1264)$ and $(-0.0774, -0.0925, 0.1295)$; H@ $(-0.0976, 0.2477, -0.0177)$, $(-0.2409, 0.0794, 0.2218)$ and $(-0.1371, -0.1631, 0.2312)$.



Structure 99 *Prototype:* $Sr_8Ga_{16}Ge_{30}$

SBS/PS: —/cP48 *SG # 223:* **Pm$\bar{3}$n** $(O_h{}^3)$

Lattice complex: $a = 1.0734$ Sr@ $2a(0,0,0)$; $24k(0,y,z)$ with $y = 0.2387$ and $z = 0.4623$; Ge,Ga@ $6c(\frac{1}{4},0,\frac{1}{2})$; $16i(x,x,x)$ with $x = 0.18459$; $24k(0,y,z)$ with $y = 0.30939$ and $z = 0.11770$.