

Space group (206) *Ia*-3206  
*cI*16

Si	<i>cI</i> 16	(206) <i>Ia</i> -3 – c
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**Si form III** [2], BC8 (body-centered cubic, 8 atoms)

Structural features: Si forms a 3D-framework where each atom is tetrahedrally coordinated.

Kasper J.S., Richards S.M. (1964) [1]

Si

 $a = 0.6636 \text{ nm}$ ,  $V = 0.2922 \text{ nm}^3$ ,  $Z = 16$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Si1	16c	.3.	0.1003	0.1003	0.1003		tetrahedron Si <sub>4</sub>

Experimental: powder, Debye-Scherrer film, X-rays,  $R = 0.150$ 

Remarks: Metastable phase observed below 8.5 GPa on releasing pressure.

References: [1] Kasper J.S., Richards S.M. (1964), Acta Crystallogr. 17, 752-755. [2] Wentorf R.H. Jr., Kasper J.S. (1963), Science (Washington D.C.) 139, 338-339.

206  
*cI*64

KSbF <sub>6</sub>	<i>cI</i> 64	(206) <i>Ia</i> -3 – eba
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**KSbF<sub>6</sub>** [1]Structural features: Single SbF<sub>6</sub> octahedra and K atoms in a CsCl-type arrangement.

Bode H., Voss E. (1951) [1]

F<sub>6</sub>KSb $a = 1.015 \text{ nm}$ ,  $V = 1.0457 \text{ nm}^3$ ,  $Z = 8$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
F1	48e	1	0.118	0.159	0.316		single atom Sb
Sb2	8b	.-3.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		octahedron F <sub>6</sub>
K3	8a	.-3.	0	0	0		octahedron F <sub>6</sub>

Transformation from published data:  $\frac{1}{4}-y, \frac{1}{4}-x, \frac{1}{4}-z$ 

Experimental: single crystal, rotation photographs, X-rays

References: [1] Bode H., Voss E. (1951), Z. Anorg. Allg. Chem. 264, 144-150.

206  
*cI*72

[O <sub>2</sub> ]PtF <sub>6</sub>	<i>cI</i> 72	(206) <i>Ia</i> -3 – eca
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**O<sub>2</sub>PtF<sub>6</sub> cubic** [2]; N<sub>2</sub>H<sub>6</sub>TiF<sub>6</sub> [3]Structural features: Single PtF<sub>6</sub> octahedra and O<sub>2</sub> cations in a CsCl-type arrangement.

Graudejus O., Müller B.G. (1996) [1]

F<sub>6</sub>O<sub>2</sub>Pt $a = 1.0036 \text{ nm}$ ,  $V = 1.0108 \text{ nm}^3$ ,  $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
F1	48e	1	0.0583	0.3928	0.1416		single atom Pt
O2	16c	.3.	0.2223	0.2223	0.2223		single atom O
Pt3	8a	.-3.	0	0	0		octahedron F <sub>6</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.053

Remarks: The rhombohedral modification reported in [2] could not be obtained in [1]. Splitting of the O site was proposed in [4].

References: [1] Graudejus O., Müller B.G. (1996), Z. Anorg. Allg. Chem. 622, 1076-1082. [2] Bartlett N., Lohmann D.H. (1962), J. Chem. Soc. 1962, 5253-5261. [3] Kojic Prodic B., Matkovic B., Scavnicar S. (1971), Acta Crystallogr. B 27, 635-637. [4] Ibers J.A., Hamilton W.C. (1966), J. Chem. Phys. 44, 1748-1752.

206  
c/80

(Mn <sub>0.5</sub> Fe <sub>0.5</sub> ) <sub>2</sub> O <sub>3</sub>	c/80	(206) Ia-3 – eda
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**(Mn,Fe)<sub>2</sub>O<sub>3</sub>** [2], bixbyite, sesquioxide C, Strukturbericht notation D5<sub>3</sub>; Mn<sub>2</sub>O<sub>3</sub> α [2]; Yb<sub>2</sub>S<sub>3</sub> θ [3], sesquisulfide T; Mg<sub>3</sub>P<sub>2</sub> [4]

Structural features: (Mn,Fe)O<sub>6</sub> octahedra share edges and vertices to form a 3D-framework with helical chains of edge-linked octahedra along <100>. See Fig. II.36.

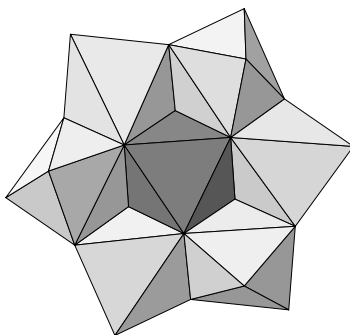


Fig. II.36. **(Mn,Fe)<sub>2</sub>O<sub>3</sub>**

Arrangement of (Mn,Fe)O<sub>6</sub> octahedra (light) around a central (Mn,Fe)O<sub>6</sub> octahedron (dark) at the origin.

Geller S. (1971) [1]

Fe<sub>0.03</sub>Mn<sub>1.97</sub>O<sub>3</sub>

*a* = 0.94146 nm, *V* = 0.8345 nm<sup>3</sup>, *Z* = 16

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	48e	1	0.08347	0.37087	0.14708		tetrahedron Mn <sub>4</sub>
M2	24d	2..	0.28508	0	1/4		octahedron O <sub>6</sub>
M3	8a	.-3.	0	0	0		octahedron O <sub>6</sub>

M2 = 0.983Mn + 0.017Fe; M3 = 0.983Mn + 0.017Fe

Experimental: single crystal, diffractometer, X-rays, R = 0.027

Remarks: Pure α-Mn<sub>2</sub>O<sub>3</sub> crystallizes with an orthorhombic structure up to 302 K; beyond a substitution of 0.75 at.% Fe for Mn the phase remains cubic down to rt. The atom coordinates were not refined in [3] but isotypism with Tl<sub>2</sub>O<sub>3</sub> is stated. A report on Be<sub>3</sub>P<sub>2</sub> with this structure type [4] is superseded (see [5]).

References: [1] Geller S. (1971), Acta Crystallogr. B 27, 821-828. [2] (1937), Strukturberichte 2, 38. [3] Patrie M. (1969), Bull. Soc. Chim. Fr. 1969, 1600-1601. [4] Stackelberg M.V., Paulus R. (1933), Z. Phys. Chem., Abt. B 22, 305-322. [5] El Maslout A., Motte J.P., Courtois A., Protas J., Gleitzer C. (1975), J. Solid State Chem. 15, 223-228.

206  
c/80

$\text{Cu}_3[\text{TeO}_6]$	<i>c/80</i>	(206) <i>Ia-3</i> – eda
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### $\text{Cu}_3\text{TeO}_6$ [1]

Structural features: Distorted close-packed O layers in c stacking; Cu and Te in octahedral voids. Cu atoms and  $\text{TeO}_6$  octahedra in an approximate  $\text{Cu}_3\text{Au}$ -type arrangement.

Falck L. et al. (1978) [1]

$\text{Cu}_3\text{O}_6\text{Te}$

$a = 0.9537 \text{ nm}$ ,  $V = 0.8674 \text{ nm}^3$ ,  $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	48e	1	0.0758	0.3825	0.145		non-coplanar triangle $\text{TeCu}_2$
Cu2	24d	2..	0.28093	0	$1/4$		octahedron $\text{O}_6$
Te3	8a	.-3.	0	0	0		octahedron $\text{O}_6$

Transformation from published data:  $1/4-y, 1/4-x, 1/4-z$

Experimental: single crystal, diffractometer, X-rays,  $R = 0.022$

References: [1] Falck L., Lindqvist O., Moret J. (1978), Acta Crystallogr. B 34, 896-897.

206  
c/96

$\text{UN}_{1.6}$	<i>c/96</i>	(206) <i>Ia-3</i> – eda
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### $\text{U}_2\text{N}_{3+x}$ α [2]

Structural features: Close-packed U layers in c stacking, N in tetrahedral voids (partial disorder).

Masaki N., Tagawa H. (1975) [1]

$\text{N}_{1.60}\text{U}$

$a = 1.0676 \text{ nm}$ ,  $V = 1.2168 \text{ nm}^3$ ,  $Z = 32$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
N1	48e	1	0.11	0.37	0.13		trigonal bipyramid $\text{U}_4\text{N}$
U2	24d	2..	0.265	0	$1/4$		square prism (cube) $\text{N}_8$
N3	16c	.3.	0.10	0.10	0.10	0.20	single atom U
U4	8a	.-3.	0	0	0		square prism (cube) $\text{N}_8$

Transformation from published data:  $1/4-y, 1/4-x, 1/4-z$

Experimental: powder, diffractometer, neutrons,  $R = 0.210$

Remarks: Homogeneity range  $\text{N}_{100-x}\text{U}_x$ ,  $36.5 < x < 38.5$ . Preliminary data in [3].

References: [1] Masaki N., Tagawa H. (1975), J. Nucl. Mater. 57, 187-192. [2] Tobisch J., Hase W. (1967), Phys. Status Solidi 21, K11-K12. [3] Rundle R.E., Baenziger N.C., Wilson A.S., McDonald R.A. (1948), J. Am. Chem. Soc. 70, 99-105.

206  
cI96

$(\text{Pr}_{0.6}\text{Gd}_{0.4})_2\text{O}_{3.32}$	<i>cI96</i>	(206) <i>Ia-3</i> – edca
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**Pr<sub>0.6</sub>Gd<sub>0.4</sub>O<sub>1.5+δ</sub>** [1]

Structural features: Distorted (Pr,Gd)O<sub>6</sub> octahedra share edges and vertices to form a 3D-framework; additional O in tetrahedral voids. Structure intermediate between (Mn,Fe)<sub>2</sub>O<sub>3</sub> (bixbyite) and CaF<sub>2</sub> (fluorite).

Endo K. et al. (1976) [1]

Gd<sub>0.80</sub>O<sub>3.32</sub>Pr<sub>1.20</sub> $a = 1.0897 \text{ nm}$ ,  $V = 1.2940 \text{ nm}^3$ ,  $Z = 16$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	48 <i>e</i>	1	0.103	0.363	0.123	0.927	square pyramid OPr <sub>4</sub>
M2	24 <i>d</i>	2..	0.2666	0	$\frac{1}{4}$		8-vertex polyhedron O <sub>8</sub>
O3	16 <i>c</i>	.3.	0.196	0.196	0.196	0.54	7-vertex polyhedron O <sub>4</sub> Pr <sub>3</sub>
M4	8 <i>a</i>	-.3.	0	0	0		octahedron O <sub>6</sub>

M2 = 0.6Pr + 0.4Gd; M4 = 0.6Pr + 0.4Gd

Transformation from published data:  $\frac{1}{4}-y, \frac{1}{4}-x, \frac{1}{4}-z$ Experimental: powder, diffractometer, X-rays,  $R_B = 0.037$ 

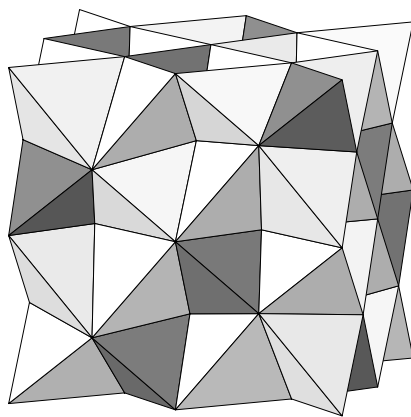
References: [1] Endo K., Yamauchi S., Fueki K., Mukaibo T. (1976), Bull. Chem. Soc. Jpn. 49, 1191-1193.

206  
cI96

$\text{Li}_3\text{AlN}_2$	<i>cI96</i>	(206) <i>Ia-3</i> – edca
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**Li<sub>3</sub>AlN<sub>2</sub>** [2], Strukturbericht notation E9<sub>d</sub>; Li<sub>5</sub>GeN<sub>3</sub> [3]; Li<sub>5</sub>SiN<sub>3</sub> [3]; Li<sub>5</sub>TiN<sub>3</sub> [3]

Structural features: Close-packed N layers in c stacking; Li and Al in tetrahedral voids. AlN<sub>4</sub> tetrahedra share vertices to form a 3D-framework. See Fig. II.37.

Fig. II.37. **Li<sub>3</sub>AlN<sub>2</sub>**

Arrangement of LiN<sub>4</sub> (light) and AlN<sub>4</sub> (dark) tetrahedra.

Juza R., Hund F. (1948) [1]

AlLi<sub>3</sub>N<sub>2</sub> $a = 0.9461 \text{ nm}$ ,  $V = 0.8469 \text{ nm}^3$ ,  $Z = 16$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Li1	48 <i>e</i>	1	0.11	0.16	0.382		pseudo Frank-Kasper N <sub>4</sub> Li <sub>5</sub> Al <sub>2</sub>
N2	24 <i>d</i>	2..	0.205	0	<sup>1</sup> / <sub>4</sub>		square prism (cube) Al <sub>2</sub> Li <sub>6</sub>
Al3	16 <i>c</i>	.3.	0.115	0.115	0.115		tetrahedron N <sub>4</sub>
N4	8 <i>a</i>	.-3.	0	0	0		square prism (cube) Al <sub>2</sub> Li <sub>6</sub>

Experimental: powder, film, X-rays

Remarks: The same data are reported in [2]. Mixed occupation corresponding to Li<sub>3</sub>(Li,M)N<sub>2</sub> is reported for the compounds Li<sub>5</sub>MN<sub>3</sub> (M = Ge, Si, Ti) in [3].

References: [1] Juza R., Hund F. (1948), Z. Anorg. Chem. 257, 13-25. [2] Juza R., Hund F. (1946), Naturwissenschaften 33, 121-122. [3] Juza R., Weber H.H., Meyer Simon E. (1953), Z. Anorg. Allg. Chem. 273, 48-64.

206  
c/96

TiTe <sub>3</sub> O <sub>8</sub>	c/96	(206) Ia-3 – edca
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### TiTe<sub>3</sub>O<sub>8</sub> [1]

Structural features: TiO<sub>6</sub> octahedra and :TeO<sub>4</sub> trigonal ψ-bipyramids share vertices to form a 3D-framework. Distorted substitution derivative of fluorite.

Meunier G., Galy J. (1971) [1]

O<sub>8</sub>Te<sub>3</sub>Ti

*a* = 1.0956 nm, *V* = 1.3151 nm<sup>3</sup>, *Z* = 8

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	48 <i>e</i>	1	0.06	0.367	0.104		non-colinear TeTi
Te2	24 <i>d</i>	2..	0.2101	0	<sup>1</sup> / <sub>4</sub>		4-vertex polyhedron O <sub>4</sub>
O3	16 <i>c</i>	.3.	0.175	0.175	0.175		non-coplanar triangle Te <sub>3</sub>
Ti4	8 <i>a</i>	.-3.	0	0	0		octahedron O <sub>6</sub>

Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.054

References: [1] Meunier G., Galy J. (1971), Acta Crystallogr. B 27, 602-608.

206  
c/104

[O <sub>2</sub> ]PtF <sub>6</sub>	c/104	(206) Ia-3 – e <sup>2</sup> a
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### O<sub>2</sub>PtF<sub>6</sub> [1]

Structural features: Single PtF<sub>6</sub> octahedra and O<sub>2</sub> cations (orientational disorder) in a CsCl-type arrangement.

Ibers J.A., Hamilton W.C. (1966) [1]

F<sub>6</sub>O<sub>2</sub>Pt

*a* = 1.0032 nm, *V* = 1.0096 nm<sup>3</sup>, *Z* = 8

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	48 <i>e</i>	1	0.0579	0.3951	0.1364		single atom Pt
O2	48 <i>e</i>	1	0.1942	0.2294	0.2424	0.333	
Pt3	8 <i>a</i>	.-3.	0	0	0		octahedron F <sub>6</sub>

Experimental: powder, diffractometer, neutrons,  $wR = 0.008$

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Ibers J.A., Hamilton W.C. (1966), J. Chem. Phys. 44, 1748-1752.

206  
cI160

$K(Al_{0.33}Si_{0.67})_3O_6$	<i>cI160</i>	(206) <i>Ia-3</i> – $e^3c$
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**KAISi<sub>2</sub>O<sub>6</sub> ht** [1], leucite high, zeolite ANA-K

Structural features: (Si,Al)O<sub>4</sub> tetrahedra share vertices to form an ANA-type zeolite framework with 4-, 6- and 8-rings; K in non-intersecting channels along  $\langle 111 \rangle$ .

Ito Y. et al. (1995) [1]

AlKO<sub>6</sub>Si<sub>2</sub>

$a = 1.3547$  nm,  $V = 2.4862$  nm<sup>3</sup>,  $Z = 16$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	48 <i>e</i>	1	0.03059	0.11828	0.35244		non-colinear Si <sub>2</sub>
O2	48 <i>e</i>	1	0.10476	0.36641	0.21995		non-colinear Si <sub>2</sub>
M3	48 <i>e</i>	1	0.12514	0.16217	0.41215		tetrahedron O <sub>4</sub>
K4	16 <i>c</i>	.3.	0.12492	0.12492	0.12492		icosahedron O <sub>12</sub>

M3 = 0.667Si + 0.333Al

Transformation from published data:  $\frac{1}{4}-y, \frac{1}{4}-x, \frac{1}{4}-z$

Experimental: single crystal, diffractometer, X-rays,  $R = 0.054$ ,  $T = 973$  K

Remarks: Phase stable at  $T > 948$  K. Supersedes refinements of high leucite in space group (230) *Ia-3d* ([2], [3]). The structure was, however, later again refined in this space group [4].

References: [1] Ito Y., Kuehner S., Ghose S. (1995), Solid State Ionics 79, 120-123. [2] Wyart M.J. (1940), Bull. Soc. Fr. Mineral. 63, 5-17. [3] Peacor D.R. (1968), Z. Kristallogr. 127, 213-224. [4] Palmer D.C., Dove M.T., Ibberson R.M., Powell B.M. (1997), Am. Mineral. 82, 16-29.

206  
cI168

$[CN_3H_6]_3Be_2F_7$	<i>cI168</i>	(206) <i>Ia-3</i> – $e^2d^2ca$
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**[C(NH<sub>2</sub>)<sub>3</sub>]<sub>3</sub>Be<sub>2</sub>F<sub>7</sub>** [1]

Structural features: Be<sub>2</sub>F<sub>7</sub> units (two vertex-linked BeF<sub>4</sub> tetrahedra) and planar C(NH<sub>2</sub>)<sub>3</sub> (guanidinium) trigonal units.

Aléonard S., Gorius M.F. (1989) [1]

Be<sub>2</sub>C<sub>3</sub>F<sub>7</sub>H<sub>18</sub>N<sub>9</sub>

$a = 1.4596$  nm,  $V = 3.1096$  nm<sup>3</sup>,  $Z = 8$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
N1	48 <i>e</i>	1	0.0157	0.173	0.3362		single atom C
F2	48 <i>e</i>	1	0.0264	0.0502	0.1585		single atom Be
N3	24 <i>d</i>	2..	0.203	0	$\frac{1}{4}$		single atom C
C4	24 <i>d</i>	2..	0.2918	0	$\frac{1}{4}$		coplanar triangle N <sub>3</sub>
Be5	16 <i>c</i>	.3.	0.0606	0.0606	0.0606		tetrahedron F <sub>4</sub>
F6	8 <i>a</i>	-.3.	0	0	0		colinear Be <sub>2</sub>
H7	48 <i>e</i>	1	0.007	0.176	0.391		
H8	48 <i>e</i>	1	0.01	0.205	0.177		

H9      48e    1            0.03      0.121      0.301

Experimental: single crystal, diffractometer, X-rays, R = 0.051

Remarks: Guanidinium pyrofluoroberyllate. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Aléonard S., Gorius M.F. (1989), C. R. Acad. Sci., Ser. II 309, 683-687.

206  
cI192

UN <sub>1.82</sub>	cI192	(206) Ia-3 – e <sup>4</sup>
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### U<sub>2</sub>N<sub>3+x</sub> **a** [1]

Structural features: Distorted close-packed U layers in c stacking; N in tetrahedral voids (high degree of disorder).

Serizawa H. et al. (1994) [1]

N<sub>1.77</sub>U

*a* = 1.0596 nm, *V* = 1.1897 nm<sup>3</sup>, *Z* = 32

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
U1	48e	1	0.005	0.245	0.265	0.5	
N2	48e	1	0.107	0.126	0.139	0.27	
N3	48e	1	0.123	0.125	0.366	0.91	
U4	48e	1	0.24	0.24	0.26	0.167	

Experimental: powder, diffractometer, neutrons, R = 0.054

Remarks: Homogeneity range N<sub>100-x</sub>U<sub>x</sub>, 35.2 < *x* < 37.3. Short interatomic distances for partly occupied site(s).

References: [1] Serizawa H., Fukuda K., Ishii Y., Morii Y., Katsura M. (1994), J. Nucl. Mater. 208, 128-134.

206  
cI208

P <sub>4</sub> S <sub>9</sub>	cI208	(206) Ia-3 – e <sup>4</sup> c
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### P<sub>4</sub>S<sub>9</sub> form II [1]

Structural features: P<sub>4</sub>S<sub>9</sub> molecules consisting of three PS<sub>4</sub> tetrahedra and a :PS<sub>3</sub> ψ-tetrahedron sharing vertices (a P<sub>4</sub>S<sub>6</sub> cage with an additional S bonded to three P atoms).

Hilmer V.W. (1969) [1]

P<sub>4</sub>S<sub>9</sub>

*a* = 1.760 nm, *V* = 5.4518 nm<sup>3</sup>, *Z* = 16

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
S1	48e	1	0.0337	0.0816	0.1889		non-colinear P <sub>2</sub>
S2	48e	1	0.0628	0.1505	0.3613		single atom P
P3	48e	1	0.1040	0.1495	0.2595		tetrahedron S <sub>4</sub>
S4	48e	1	0.1062	0.2626	0.2153		non-colinear P <sub>2</sub>
P5	16c	.3.	0.0771	0.0771	0.0771		non-coplanar triangle S <sub>3</sub>

Transformation from published data:  $\frac{1}{4}-y, \frac{1}{4}-x, \frac{1}{4}-z$

Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.123

References: [1] Hilmer V.W. (1969), Acta Crystallogr. B 25, 1229-1232.

206  
cI240

$\text{Cs}_3\text{KRe}_6\text{S}_8[\text{CN}]_6$	<i>cI240</i>	(206) <i>Ia-3</i> – $e^4dca$
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**Cs<sub>3</sub>KRe<sub>6</sub>S<sub>8</sub>(CN)<sub>6</sub>** [1]

Structural features: Single  $\text{Re}_6\text{S}_8(\text{CN})_6$  clusters (a  $\text{Re}_6$  octahedron surrounded by a  $\text{S}_8$  cube and a large  $(\text{CN})_6$  octahedron, linear Re-C-N segments).

Slogui A. et al. (1995) [1]

$\text{C}_6\text{Cs}_{3.22}\text{K}_{0.78}\text{N}_6\text{Re}_6\text{S}_{7.40}\text{Te}_{0.60}$

$a = 1.778 \text{ nm}$ ,  $V = 5.6208 \text{ nm}^3$ ,  $Z = 8$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
N1	48 <i>e</i>	1	0.061	0.0694	0.3643		single atom C
S2	48 <i>e</i>	1	0.0907	0.2892	0.2736		non-coplanar triangle $\text{Re}_3$
C3	48 <i>e</i>	1	0.098	0.109	0.3321		single atom N
Re4	48 <i>e</i>	1	0.17721	0.18503	0.28462		tricapped trigonal prism $\text{CS}_4\text{Re}_4$
Cs5	24 <i>d</i>	2..	0.4473	0	$\frac{1}{4}$		non-collinear $\text{N}_2$
M6	16 <i>c</i>	.3.	0.1472	0.1472	0.1472		non-coplanar triangle $\text{Re}_3$
M7	8 <i>a</i>	-.3.	0	0	0		octahedron $\text{N}_6$

$\text{M6} = 0.70\text{S} + 0.30\text{Te}$ ;  $\text{M7} = 0.78\text{K} + 0.22\text{Cs}$

Transformation from published data:  $\frac{1}{4}-y, \frac{1}{4}-x, \frac{1}{4}-z$

Experimental: single crystal, diffractometer, X-rays,  $R = 0.033$

Remarks: Small amounts of Te are ignored in the chemical formula above.

References: [1] Slogui A., Mironov Y.V., Perrin A., Fedorov V.E. (1995), Croat. Chem. Acta 68, 885-890.

206  
cI320

$\text{Na}_4\text{BaCu}_3\text{F}_{12}$	<i>cI320</i>	(206) <i>Ia-3</i> – $e^5d^2cba$
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**Na<sub>4</sub>BaCu<sub>3</sub>F<sub>12</sub>** [1], perovskite family

Structural features:  $\text{NaF}_6$  and  $\text{CuF}_6$  octahedra (the latter distorted towards square coordination) share vertices to form a 3D-framework, additional Na and Ba in "cuboctahedral" voids. Derivative of  $\text{CaTiO}_3$  of composition  $[\text{A}_3\text{A}'][\text{AB}_3]\text{X}_{12}$ .

Frit B. et al. (1990) [1]

$\text{BaCu}_3\text{F}_{12}\text{Na}_4$

$a = 1.6135 \text{ nm}$ ,  $V = 4.2006 \text{ nm}^3$ ,  $Z = 16$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	48 <i>e</i>	1	0.0132	0.4099	0.142		single atom Cu
F2	48 <i>e</i>	1	0.0919	0.146	0.4831		single atom Cu
F3	48 <i>e</i>	1	0.0983	0.2406	0.3491		non-coplanar triangle $\text{Cu}_2\text{Na}$
F4	48 <i>e</i>	1	0.1075	0.2557	0.1508		non-collinear $\text{CuNa}$
Cu5	48 <i>e</i>	1	0.1204	0.3787	0.1276		octahedron $\text{F}_6$
Na6	24 <i>d</i>	2..	0.0332	0	$\frac{1}{4}$		trigonal prism $\text{F}_6$
Na7	24 <i>d</i>	2..	0.2614	0	$\frac{1}{4}$		tetrahedron $\text{F}_4$
Na8	16 <i>c</i>	.3.	0.1315	0.1315	0.1315		octahedron $\text{F}_6$
Ba9	8 <i>b</i>	-.3.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		icosahedron $\text{F}_{12}$



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Ba10	8a	.-3.	0	0	0	icosahedron F <sub>12</sub>
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Experimental: single crystal, diffractometer, X-rays, wR = 0.038

Remarks: Space group (230) *Ia-3d* was tested and rejected (wR = 0.157).

References: [1] Frit B., Mercurio J.P., Renaudin J., Ferey G. (1990), Eur. J. Solid State Inorg. Chem. 27, 771-782.