

Space group (201) *Pn-3*201
cP16

| | | |
|--------------------|-------------|------------------------|
| [PH ₃] | <i>cP16</i> | (201) <i>Pn-3</i> – gb |
|--------------------|-------------|------------------------|

PH₃ [1]; AsH₃ [1]Structural features: Approximately planar PH₆ hexagonal units share atoms to form a 3D-framework.

Natta G., Casazza E. (1930) [1]

H₃P $a = 0.631 \text{ nm}$, $V = 0.2512 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|-------|---------------|---------------|------|---|
| H1 | 12g | 2.. | 0.066 | $\frac{3}{4}$ | $\frac{1}{4}$ | | 7-vertex polyhedron P ₂ H ₅ |
| P2 | 4b | .-3. | 0 | 0 | 0 | | octahedron H ₆ |

Transformation from published data (origin choice 1): origin shift $\frac{1}{4} \frac{1}{4} \frac{1}{4}$

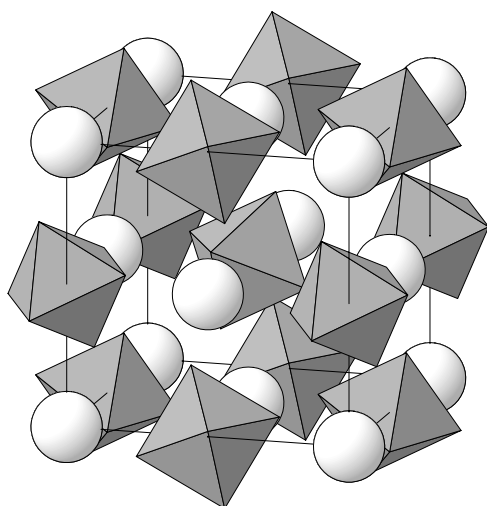
Experimental: powder, film, X-rays, T = 173 K

Remarks: H positions from crystal chemical considerations. Structure doubtful. In [1] the symmetry-equivalent positions listed under (I) are erroneously stated to correspond also to space group *P4₂32*.

References: [1] Natta G., Casazza E. (1930), Gazz. Chim. Ital. 60, 851-859.

201
cP32

| | | |
|-----------------------|-------------|-------------------------|
| CaSn[OH] ₆ | <i>cP32</i> | (201) <i>Pn-3</i> – hcb |
|-----------------------|-------------|-------------------------|

CaSn(OH)₆ [2], burtiteStructural features: Sn(OH)₆ octahedra (orientational disorder for OH) and Ca atoms in a NaCl-type arrangement. See Fig. II.61.Fig. II.61. **CaSn(OH)₆**Arrangement of Sn(OH)₆ octahedra and Ca atoms.

Basciano L.C. et al. (1998) [1]

CaD₆O₆Sn $a = 0.81221 \text{ nm}$, $V = 0.5358 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|---------------|---------------|---------------|------|---------------------------|
| O1 | 24h | 1 | 0.0787 | 0.2306 | 0.5663 | | non-colinear SnCa |
| Sn2 | 4c | .-3. | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | | octahedron O ₆ |
| Ca3 | 4b | .-3. | 0 | 0 | 0 | | octahedron O ₆ |
| D4 | 24h | 1 | 0.0638 | 0.1974 | 0.6805 | 0.5 | |
| D5 | 24h | 1 | 0.2011 | 0.2131 | 0.5346 | 0.5 | |

Experimental: powder, diffractometer, neutrons, $R_p = 0.018$, $T = 4$ K

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

References: [1] Basciano L.C., Peterson R.C., Roeder P.L., Swainson I. (1998), Can. Mineral. 36, 1203-1210. [2] Cohen Addad C. (1967), Bull. Soc. Fr. Mineral. Cristallogr. 90, 32-35.

201
cP44

| | | |
|--|------|--------------------|
| [NH ₄] ₃ Cu ₄ Ho ₂ Br ₁₃ | cP44 | (201) Pn-3 – hedba |
|--|------|--------------------|

(NH₄)₃Cu₄Ho₂Br₁₃ [1]

Structural features: Single HoBr₆ octahedra are interconnected via CuBr₄ tetrahedra to form a 3D-framework; NH₄ tetrahedra in voids.

Wickleder M.S. et al. (1996) [1]

Br₁₃Cu₄H₁₂Ho₂N₃

$a = 1.10171$ nm, $V = 1.3372$ nm³, $Z = 2$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|---------------------------------|-------|-------|---------------|---------------|---------------|------|-------------------------------------|
| Br1 | 24h | 1 | 0.0218 | 0.2509 | 0.5323 | | non-colinear CuHo |
| Cu2 | 8e | .3. | 0.3783 | 0.3783 | 0.3783 | | tetrahedron Br ₄ |
| (NH ₄) ₃ | 6d | 222.. | $\frac{1}{4}$ | $\frac{3}{4}$ | $\frac{3}{4}$ | | square prism (cube) Br ₈ |
| Ho4 | 4b | .-3. | 0 | 0 | 0 | | octahedron Br ₆ |
| Br5 | 2a | 23. | $\frac{1}{4}$ | $\frac{1}{4}$ | $\frac{1}{4}$ | | tetrahedron Cu ₄ |

Experimental: single crystal, diffractometer, X-rays, $R = 0.037$, $T = 293$ K

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

References: [1] Wickleder M.S., Bohnsack A., Meyer G. (1996), Z. Anorg. Allg. Chem. 622, 675-678.

201
cP60

| | | |
|-------------------|------|--------------------|
| KSbO ₃ | cP60 | (201) Pn-3 – hgfeb |
|-------------------|------|--------------------|

KSbO₃ cubic [1]

Structural features: Pairs of edge-linked SbO₆ octahedra share vertices to form a 3D-framework.

Spiegelberg P. (1940) [1]

KO₃Sb

$a = 0.956$ nm, $V = 0.8737$ nm³, $Z = 12$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|---------------|---------------|------|------------------------------|
| O1 | 24h | 1 | 0.0389 | 0.0972 | 0.75 | | non-colinear Sb ₂ |
| Sb2 | 12g | 2.. | 0.0972 | $\frac{3}{4}$ | $\frac{1}{4}$ | | octahedron O ₆ |

| | | | | | | |
|----|-----|------|--------|---------------|---------------|------------------------------|
| O3 | 12f | 2.. | 0.6111 | $\frac{1}{4}$ | $\frac{1}{4}$ | non-colinear Sb ₂ |
| K4 | 8e | .3. | 0.3889 | 0.3889 | 0.3889 | octahedron O ₆ |
| K5 | 4b | -.3. | 0 | 0 | 0 | octahedron O ₆ |

Transformation from published data (origin choice 1): -y,-x,-z; origin shift $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: powder, film, X-rays

Remarks: On page 7 of [1] the Wyckoff position of the first K site is misprinted as 4b instead of 4c (checked on interatomic distances).

References: [1] Spiegelberg P. (1940), Ark. Kemi Mineral. Geol. 14A(5), 1-12.

201
cP64

| | | |
|---|------|--|
| K ₂ NaSb ₃ O ₉ | cP64 | (201) <i>Pn</i> -3 – hgfe ² |
|---|------|--|

K₈Na₄Sb₁₂O₃₆ [1]

Structural features: Pairs of edge-linked SbO₆ octahedra share vertices to form a 3D-framework. Ordering variant of KSbO₃ with splitting of one of the cation sites.

Watelet H. et al. (1981) [1]

K₂NaO₉Sb₃

$a = 0.9515$ nm, $V = 0.8614$ nm³, $Z = 4$

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------|------|----------|---------------|---------------|------|------------------------------|
| O1 | 24h | 1 | 0.042 | 0.092 | 0.75 | | non-colinear Sb ₂ |
| Sb2 | 12g | 2.. | 0.09 | $\frac{3}{4}$ | $\frac{1}{4}$ | | octahedron O ₆ |
| O3 | 12f | 2.. | 0.613 | $\frac{1}{4}$ | $\frac{1}{4}$ | | non-colinear Sb ₂ |
| Na4 | 8e | .3. | 0.018 | 0.018 | 0.018 | 0.5 | |
| K5 | 8e | .3. | 0.399 | 0.399 | 0.399 | | octahedron O ₆ |

Transformation from published data: -y,-x,-z

Experimental: single crystal, diffractometer, X-rays, R = 0.059

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

References: [1] Watelet H., Picard J.P., Baud G., Besse J.P., Chevalier R. (1981), Mater. Res. Bull. 16, 877-882.

201
cP66

| | | |
|---|------|--|
| Re ₆ Pb ₆ O ₁₉ | cP66 | (201) <i>Pn</i> -3 – hgfe ² a |
|---|------|--|

Pb₆Re₆O₁₉ [1]

Structural features: Pairs of edge-linked ReO₆ octahedra share vertices to form a 3D-framework; OPb₄ tetrahedra and additional Pb in voids.

Abakumov A.M. et al. (1998) [1]

O₁₉Pb₆Re₆

$a = 0.9318$ nm, $V = 0.8090$ nm³, $Z = 2$

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------|------|----------|---------------|---------------|------|------------------------------|
| O1 | 24h | 1 | 0.0495 | 0.104 | 0.7479 | | non-colinear Re ₂ |
| Re2 | 12g | 2.. | 0.11855 | $\frac{3}{4}$ | $\frac{1}{4}$ | | octahedron O ₆ |
| O3 | 12f | 2.. | 0.58 | $\frac{1}{4}$ | $\frac{1}{4}$ | | non-colinear Re ₂ |
| Pb4 | 8e | .3. | 0.0134 | 0.0134 | 0.0134 | 0.5 | |

| | | | | | | |
|-----|----|-----|---------------|---------------|---------------|------------------------------------|
| Pb5 | 8e | .3. | 0.39626 | 0.39626 | 0.39626 | 7-vertex polyhedron O ₇ |
| O6 | 2a | 23. | $\frac{1}{4}$ | $\frac{1}{4}$ | $\frac{1}{4}$ | tetrahedron Pb ₄ |

Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: powder, diffractometer, X-rays, $R_B = 0.021$

Remarks: Short interatomic distances for partly occupied site(s). In the abstract of [1] the cell parameter is misprinted as 0.93162 nm instead of 0.931795 nm (given in table 1).

References: [1] Abakumov A.M., Shpanchenko R.V., Antipov E.V. (1998), Z. Anorg. Allg. Chem. 624, 750-753.

201
cP68

Ru₃Bi₃O₁₁

cP68

(201) $Pn-3 - hgfe^2b$

Bi₃Ru₃O₁₁ [2]; Bi₃GaSb₂O₁₁ (see remark)

Structural features: Pairs of edge-linked RuO₆ octahedra share vertices to form a 3D-framework; units of four edge-linked OBi₄ tetrahedra (Bi₄O₄ cube with one additional O bonded to each Bi) share vertices to form a second framework. See Fig. II.62.

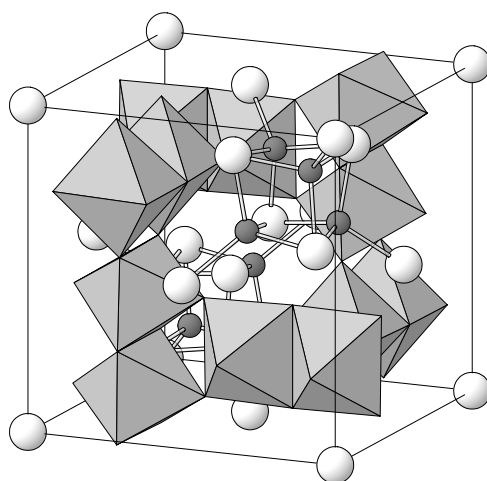


Fig. II.62. **Bi₃Ru₃O₁₁**

Arrangement of RuO₆ octahedra and Bi (large) and O (small) atoms.

Facer G.F. et al. (1993) [1]

Bi₃O₁₁Ru₃

$a = 0.9305$ nm, $V = 0.8057$ nm³, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|---------------|---------------|------|---|
| O1 | 24h | 1 | 0.0368 | 0.0974 | 0.755 | | non-colinear Ru ₂ |
| Ru2 | 12g | 2.. | 0.1103 | $\frac{3}{4}$ | $\frac{1}{4}$ | | octahedron O ₆ |
| O3 | 12f | 2.. | 0.5919 | $\frac{1}{4}$ | $\frac{1}{4}$ | | non-colinear Ru ₂ |
| O4 | 8e | .3. | 0.147 | 0.147 | 0.147 | | tetrahedron Bi ₄ |
| Bi5 | 8e | .3. | 0.3838 | 0.3838 | 0.3838 | | tricapped trigonal prism O ₉ |
| Bi6 | 4b | .-3. | 0 | 0 | 0 | | square prism (cube) O ₈ |

Transformation from published data: $-y, -x, -z$

Experimental: powder, diffractometer, neutrons, $R_B = 0.013$

Remarks: A similar structure proposal for Bi₃GaSb₂O₁₁ [3] is superseded by a model with a split Bi site (see [4]).

References: [1] Facer G.F., Elcombe M.M., Kennedy B.J. (1993), Aust. J. Chem. 46, 1897-1907. [2] Abraham F., Thomas D., Nowogrocki G. (1975), Bull. Soc. Fr. Mineral. Cristallogr. 98, 25-29. [3] Sleight A.W., Bouchard R.J. (1973), Inorg. Chem. 12, 2314-2316. [4] Kennedy I.J., Kennedy B.J., Hunter B.A. (1998), Solid State Commun. 108, 649-654.

201
cP80

| | | |
|-----------|--------------|---------------------------------------|
| W_3Br_7 | <i>cP</i> 80 | (201) <i>Pn</i> -3 – h ³ e |
|-----------|--------------|---------------------------------------|

W₆Br₁₄ [1]

Structural features: Single W₆Br₁₄ clusters (a W₆ octahedron surrounded by a Br₈ cube and a Br₆ octahedron).

Sassmannshausen J., Von Schnering H.G. (1994) [1]

Br₇W₃

$a = 1.3458$ nm, $V = 2.4375$ nm³, $Z = 8$

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------------|------|----------|----------|----------|------|---|
| W1 | 24 <i>h</i> | 1 | 0.0351 | 0.3680 | 0.5277 | | tricapped trigonal prism Br ₅ W ₄ |
| Br2 | 24 <i>h</i> | 1 | 0.0668 | 0.6226 | 0.3084 | | non-coplanar triangle W ₃ |
| Br3 | 24 <i>h</i> | 1 | 0.0861 | 0.1889 | 0.5695 | | single atom W |
| Br4 | 8 <i>e</i> | .3. | 0.1383 | 0.1383 | 0.1383 | | non-coplanar triangle W ₃ |

Experimental: single crystal, diffractometer, X-rays, $wR = 0.055$, $T = 298$ K

Remarks: Space group (195) *P*23 was tested and rejected ($R = 0.11$).

References: [1] Sassmannshausen J., Von Schnering H.G. (1994), Z. Anorg. Allg. Chem. 620, 1312-1320.

201
cP84

| | | |
|------------------------------------|--------------|--|
| $(Ga_{0.33}Sb_{0.67})_3Bi_3O_{11}$ | <i>cP</i> 84 | (201) <i>Pn</i> -3 – h ² gfeb |
|------------------------------------|--------------|--|

Bi₃GaSb₂O₁₁ [1]

Structural features: Pairs of edge-linked (Sb,Ga)O₆ octahedra share vertices to form a 3D-framework; units of four edge-linked OBi₄ tetrahedra (small orientational disorder around <111>) share vertices to form a second framework. Distorted variant of Ru₃Bi₃O₁₁.

Kennedy I.J. et al. (1998) [1]

Bi₃GaO₁₁Sb₂

$a = 0.949$ nm, $V = 0.8547$ nm³, $Z = 4$

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------------|------|----------|-----------------------------|-----------------------------|-------|------------------------------------|
| O1 | 24 <i>h</i> | 1 | 0.0393 | 0.0895 | 0.7539 | | non-colinear Sb ₂ |
| Bi2 | 24 <i>h</i> | 1 | 0.0958 | 0.1328 | 0.3672 | 0.333 | |
| M3 | 12 <i>g</i> | 2.. | 0.0919 | ³ / ₄ | ¹ / ₄ | | octahedron O ₆ |
| O4 | 12 <i>f</i> | 2.. | 0.6112 | ¹ / ₄ | ¹ / ₄ | | non-colinear Sb ₂ |
| O5 | 8 <i>e</i> | .3. | 0.1474 | 0.1474 | 0.1474 | | |
| Bi6 | 4 <i>b</i> | .-3. | 0 | 0 | 0 | | square prism (cube) O ₈ |

$M3 = 0.667Sb + 0.333Ga$

Transformation from published data: -*y*, -*x*, -*z*

Experimental: powder, diffractometer, neutrons, $R_B = 0.020$, $T = 295$ K

Remarks: Short interatomic distances for partly occupied site(s). Refinement of a similar model with Bi in Wyckoff position 8*e* gave a slightly less good agreement ($R_B = 0.032$).

References: [1] Kennedy I.J., Kennedy B.J., Hunter B.A. (1998), Solid State Commun. 108, 649-654.

201
cP84

| | | |
|------------------------------------|------|--|
| HgMo ₆ Cl ₁₄ | cP84 | (201) <i>Pn</i> -3 – h ³ eb |
|------------------------------------|------|--|

Hg[Mo₆Cl₈]Cl₆ [1]

Structural features: Mo₆Cl₁₄ clusters (a Mo₆ octahedron surrounded by a Cl₈ cube and a Cl₆ octahedron) and Hg atoms in a NaCl-type arrangement. See Fig. II.63.

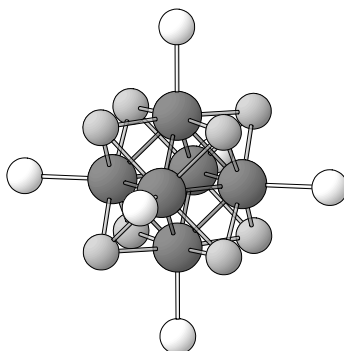


Fig. II.63. Hg[Mo₆Cl₈]Cl₆

20-atom cluster: Mo₆ octahedron + Cl₈ cube + Cl₆ octahedron.

Von Schnering H.G. (1971) [1]

Cl₁₄HgMo₆

$a = 1.2706 \text{ nm}$, $V = 2.0513 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------------|------|----------|----------|----------|------|--|
| Mo1 | 24 <i>h</i> | 1 | 0.0342 | 0.139 | 0.5274 | | tricapped trigonal prism Cl ₅ Mo ₄ |
| Cl2 | 24 <i>h</i> | 1 | 0.0731 | 0.6249 | 0.1896 | | non-coplanar triangle Mo ₃ |
| Cl3 | 24 <i>h</i> | 1 | 0.0804 | 0.3265 | 0.5645 | | non-colinear MoHg |
| Cl4 | 8 <i>e</i> | .3. | 0.3623 | 0.3623 | 0.3623 | | non-coplanar triangle Mo ₃ |
| Hg5 | 4 <i>b</i> | -.3. | 0 | 0 | 0 | | octahedron Cl ₆ |

Transformation from published data (origin choice 1): origin shift $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: powder, Guinier film, X-rays, $R = 0.060$

References: [1] Von Schnering H.G. (1971), Z. Anorg. Allg. Chem. 385, 75-84.

201
cP84

| | | |
|--|------|--|
| KRe ₆ (Se _{0.6} Cl _{0.4}) ₈ Cl ₆ | cP84 | (201) <i>Pn</i> -3 – h ³ eb |
|--|------|--|

KRe₆Se₅Cl₉ [1]

Structural features: Re₆Se_{4.8}Cl_{9.2} clusters (a Re₆ octahedron surrounded by a (Se,Cl)₈ cube and a Cl₆ octahedron) and K atoms in a NaCl-type arrangement. Ordering variant of HgMo₆Cl₁₄.

Perrin A. et al. (1990) [1]

Cl_{9.20}KRe₆Se_{4.80}

$a = 1.3034 \text{ nm}$, $V = 2.2143 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|---------|---------|------|--|
| Re1 | 24h | 1 | 0.0422 | 0.13121 | 0.53193 | | tricapped trigonal prism ClSe ₄ Re ₄ |
| M2 | 24h | 1 | 0.0543 | 0.6171 | 0.1956 | | non-coplanar triangle Re ₃ |
| Cl3 | 24h | 1 | 0.0984 | 0.2988 | 0.5755 | | single atom Re |
| M4 | 8e | .3. | 0.3636 | 0.3636 | 0.3636 | | non-coplanar triangle Re ₃ |
| K5 | 4b | -.3. | 0 | 0 | 0 | | octahedron Cl ₆ |

M2 = 0.62Se + 0.38Cl; M4 = 0.54Se + 0.46Cl

Transformation from published data: -y, -x, -z; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.040

References: [1] Perrin A., Leduc L., Pote M., Sergent M. (1990), Mater. Res. Bull. 25, 1227-1234.

201
cP88

| | | |
|---|------|--|
| K ₅ CeFe ₂ [NO ₂] ₁₂ | cP88 | (201) <i>Pn</i> -3 – h ³ dcba |
|---|------|--|

K₅Ce[Fe(NO₂)₆]₂ [1]

Structural features: Fe(NO₂)₆ octahedral units (FeN₆ octahedron, non-linear NO₂ units), K and Ce atoms in a BiF₃-type arrangement (K and Ce ordered).

Ferrari A. et al. (1951) [1]

CeFe₂K₅N₁₂O₂₄

a = 1.038 nm, *V* = 1.1184 nm³, *Z* = 2

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|-------|---------------|---------------|---------------|------|------------------------------|
| N1 | 24h | 1 | 0.0 | 0.0 | 0.204 | | non-collinear O ₂ |
| O2 | 24h | 1 | 0.0 | 0.245 | 0.602 | | single atom N |
| O3 | 24h | 1 | 0.0 | 0.255 | 0.102 | | single atom N |
| K4 | 6d | 222.. | $\frac{1}{4}$ | $\frac{3}{4}$ | $\frac{3}{4}$ | | icosahedron O ₁₂ |
| K5 | 4c | -.3. | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | | icosahedron O ₁₂ |
| Fe6 | 4b | -.3. | 0 | 0 | 0 | | octahedron N ₆ |
| Ce7 | 2a | 23. | $\frac{1}{4}$ | $\frac{1}{4}$ | $\frac{1}{4}$ | | icosahedron O ₁₂ |

Transformation from published data (origin choice 1): origin shift $\frac{1}{4} \frac{1}{4} \frac{1}{4}$

Experimental: powder, X-rays

References: [1] Ferrari A., Cavalca L., Nardelli M. (1951), Gazz. Chim. Ital. 81, 964-981.

201
cP88

| | | |
|-----------------------------------|------|--|
| CuMo ₃ Cl ₇ | cP88 | (201) <i>Pn</i> -3 – h ³ e ² |
|-----------------------------------|------|--|

Cu₂Mo₆Cl₁₄ [1]

Structural features: Mo₆Cl₁₄ clusters (a Mo₆ octahedron surrounded by a Cl₈ cube and a Cl₆ octahedron) and CuCl₃ trigonal units share vertices to form a 3D-framework.

Peppenhurst A., Keller H.L. (1996) [1]

Cl₇CuMo₃

a = 1.2772 nm, *V* = 2.0834 nm³, *Z* = 8

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|--------|------|--|
| Mo1 | 24h | 1 | 0.0339 | 0.1376 | 0.5269 | | tricapped trigonal prism Cl ₅ Mo ₄ |
| Cl2 | 24h | 1 | 0.0718 | 0.6249 | 0.1861 | | non-coplanar triangle Mo ₃ |

| | | | | | | |
|-----|-----|-----|--------|--------|--------|---------------------------------------|
| Cl3 | 24h | 1 | 0.0831 | 0.3187 | 0.5672 | non-colinear CuMo |
| Cu4 | 8e | .3. | 0.0647 | 0.0647 | 0.0647 | tetrahedron Cl ₃ Cu |
| Cl5 | 8e | .3. | 0.3623 | 0.3623 | 0.3623 | non-coplanar triangle Mo ₃ |

Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.072

References: [1] Peppenhorst A., Keller H.L. (1996), Z. Anorg. Allg. Chem. 622, 663-669.

201
cP90

| | | |
|---------------------------------|------|---------------------------------|
| KW ₃ Br ₇ | cP90 | (201) Pn-3 – h ³ edb |
|---------------------------------|------|---------------------------------|

K₂W₆Br₁₄ [1]

Structural features: W₆Br₁₄ clusters (a W₆ octahedron surrounded by a Br₈ cube and a Br₆ octahedron) in a Cu-type (c.c.p.) arrangement; K in "octahedral" and "tetrahedral" voids (partial disorder for the latter).

Zheng Y.Q. et al. (1998) [1]

Br₇KW₃

$a = 1.3808 \text{ nm}$, $V = 2.6326 \text{ nm}^3$, $Z = 8$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|-------|---------------|---------------|---------------|-------|---|
| W1 | 24h | 1 | 0.04199 | 0.12425 | 0.53126 | | tricapped trigonal prism Br ₅ W ₄ |
| Br2 | 24h | 1 | 0.0502 | 0.6139 | 0.1968 | | non-coplanar triangle W ₃ |
| Br3 | 24h | 1 | 0.0981 | 0.2977 | 0.5761 | | single atom W |
| Br4 | 8e | .3. | 0.3652 | 0.3652 | 0.3652 | | non-coplanar triangle W ₃ |
| K5 | 6d | 222.. | $\frac{1}{4}$ | $\frac{3}{4}$ | $\frac{3}{4}$ | 0.667 | square antiprism Br ₈ |
| K6 | 4b | -.3. | 0 | 0 | 0 | | octahedron Br ₆ |

Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.061

References: [1] Zheng Y.Q., Peters K., Grin Y., Von Schnering H.G. (1998), Z. Anorg. Allg. Chem. 624, 506-512.

201
cP90

| | | |
|---|------|---------------------------------|
| KRe ₃ (S _{0.75} Br _{0.25}) ₄ Br ₃ | cP90 | (201) Pn-3 – h ³ edb |
|---|------|---------------------------------|

K₂Re₆S₆Br₈ [1]

Structural features: Re₆(Br,S)₁₄ clusters (a Re₆ octahedron surrounded by a (S,Br)₈ cube and a Br₆ octahedron) in a Cu-type (c.c.p.) arrangement; K in "octahedral" and "tetrahedral" voids (partial disorder). Ordering variant of KW₃Br₇.

Slougui A. et al. (1997) [1]

Br_{4.14}K_{0.85}Re₃S_{2.86}

$a = 1.3433 \text{ nm}$, $V = 2.4239 \text{ nm}^3$, $Z = 8$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|-------|---------------|---------------|---------------|------|---|
| Re1 | 24h | 1 | 0.0417 | 0.126 | 0.5322 | | tricapped trigonal prism S ₃ Br ₂ Re ₄ |
| M2 | 24h | 1 | 0.048 | 0.6106 | 0.1869 | | non-coplanar triangle Re ₃ |
| Br3 | 24h | 1 | 0.1003 | 0.2993 | 0.5785 | | single atom Re |
| M4 | 8e | .3. | 0.3653 | 0.3653 | 0.3653 | | non-coplanar triangle Re ₃ |
| K5 | 6d | 222.. | $\frac{1}{4}$ | $\frac{3}{4}$ | $\frac{3}{4}$ | 0.53 | square antiprism Br ₄ S ₄ |

K6 4b -3. 0 0 0 0.9 octahedron Br₆

M2 = 0.87S + 0.13Br; M4 = 0.755Br + 0.245S

Transformation from published data: -y, -x, -z; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.046

References: [1] Slougui A., Ferron S., Perrin A., Sergent M. (1997), J. Cluster Sci. 8, 349-359.

201
cP134

Lu₂Nb₄Pb_{0.67}Cl₁₀O₄

cP134

(201) *Pn*-3 – h⁴g²eba

PbLu₃Nb₆Cl₁₅O₆ [1]

Structural features: Nb₆Cl₁₂O₆ clusters (a Nb₆ octahedron surrounded by a (Cl₆O₆) cuboctahedron and a Cl₆ octahedron) in a Cu-type (c.c.p.) arrangement; Lu₂Cl₂ rhombs and Pb atoms between the units (partial disorder for the latter).

Gulo F. et al. (2001) [1]

Cl₁₀Lu₂Nb₄O₄Pb_{0.64}

a = 1.38327 nm, *V* = 2.6468 nm³, *Z* = 6

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------|------|---------------|---------------|---------------|-------|---|
| Cl1 | 24h | 1 | 0.0039 | 0.3004 | 0.1441 | | non-colinear Nb ₂ |
| Nb2 | 24h | 1 | 0.0185 | 0.1449 | 0.527 | | non-colinear O ₂ |
| O3 | 24h | 1 | 0.0437 | 0.1227 | 0.6671 | | non-coplanar triangle Nb ₂ Lu |
| Cl4 | 24h | 1 | 0.0508 | 0.3217 | 0.5789 | | non-coplanar triangle NbLuPb |
| Cl5 | 12g | 2.. | 0.1345 | $\frac{3}{4}$ | $\frac{1}{4}$ | | non-colinear Lu ₂ |
| Lu6 | 12g | 2.. | 0.591 | $\frac{3}{4}$ | $\frac{1}{4}$ | | trigonal prism O ₂ Cl ₄ |
| Pb7 | 8e | .3. | 0.1353 | 0.1353 | 0.1353 | 0.414 | square prism (cube) Pb ₂ Cl ₆ |
| Pb8 | 4b | -.3. | 0 | 0 | 0 | 0.05 | square prism (cube) Cl ₆ Pb ₂ |
| Pb9 | 2a | 23. | $\frac{1}{4}$ | $\frac{1}{4}$ | $\frac{1}{4}$ | 0.156 | tetrahedron Pb ₄ |

Experimental: single crystal, diffractometer, X-rays, R = 0.032, T = 295 K

References: [1] Gulo F., Roisnel T., Perrin C. (2001), J. Mater. Chem. 11, 1237-1241.

201
cP188

Cd₃₇Ce₆

cP188

(201) *Pn*-3 – h⁶gfe²b

Ce₆Cd₃₇ [1]

Structural features: CeCd₁₈ polyhedra (bicapped double pentagonal antiprism, additional Cd above an edge of the central pentagon) are interconnected to form a 3D-framework; the centering atoms form large Ce₁₂ icosahedra.

Armbrüster M., Lidin S. (2000) [1]

Cd₃₇Ce₆

a = 1.5808 nm, *V* = 3.9503 nm³, *Z* = 4

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------|------|----------|----------|----------|------|--|
| Cd1 | 24h | 1 | 0.00683 | 0.25549 | 0.15888 | | |
| Cd2 | 24h | 1 | 0.04995 | 0.59326 | 0.13164 | | pseudo Frank-Kasper Cd ₁₀ Ce ₃ |
| Cd3 | 24h | 1 | 0.05476 | 0.59643 | 0.35627 | | pseudo Frank-Kasper Cd ₁₀ Ce ₃ |
| Ce4 | 24h | 1 | 0.05875 | 0.25519 | 0.54745 | | |
| Cd5 | 24h | 1 | 0.1007 | 0.15581 | 0.74718 | | icosahedron Cd ₉ Ce ₃ |

| | | | | | | | |
|------|-----|------|---------|---------------|---------------|-------|---|
| Cd6 | 24h | 1 | 0.1648 | 0.1877 | 0.2942 | 0.333 | |
| Cd7 | 12g | 2.. | 0.05464 | $\frac{3}{4}$ | $\frac{1}{4}$ | | icosahedron Cd ₁₀ Ce ₂ |
| Cd8 | 12f | 2.. | 0.65639 | $\frac{1}{4}$ | $\frac{1}{4}$ | | 15-vertex Frank-Kasper Cd ₁₃ Ce ₂ |
| Cd9 | 8e | .3. | 0.11147 | 0.11147 | 0.11147 | | |
| Cd10 | 8e | .3. | 0.41892 | 0.41892 | 0.41892 | | |
| Cd11 | 4b | -.3. | 0 | 0 | 0 | | square prism (cube) Cd ₈ |

Transformation from published data (origin choice 1): origin shift $\frac{1}{4} \frac{1}{4} \frac{1}{4}$

Experimental: single crystal, diffractometer, X-rays, wR = 0.014, T = 298 K

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

References: [1] Armbrüster M., Lidin S. (2000), J. Alloys Compd. 307, 141-148.

201
cP290

| | | |
|--|-------|--|
| Ca _{5.92} Ti ₃ Mn _{1.7} Fe ₃ [AsO ₃] ₁₂ [H ₂ O] _{4.5} | cP290 | (201) <i>Pn</i> -3 - h ¹⁰ gfe ² db |
|--|-------|--|

Ca_{5.9}Mn_{1.7}Fe_{3.0}Ti_{3.0}(AsO₃)₁₂·4·5H₂O [1], cafarsite

Structural features: Single :AsO₃ ψ-tetrahedra, distorted FeO₄ squares, TiO₆, MnO₆ and (Fe,Mn)O₆ octahedra share atoms to form a 3D-framework.

Edenharter A. et al. (1977) [1]

As_{11.18}Ca_{5.92}Fe_{2.97}Mn_{1.70}O_{40.68}Ti₃
a = 1.5984 nm, V = 4.0837 nm³, Z = 4

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|-------|---------------|---------------|---------------|------|--------------------------------------|
| O1 | 24h | 1 | 0.0032 | 0.1941 | 0.1369 | 0.94 | non-collinear AsFe |
| O2 | 24h | 1 | 0.0329 | 0.2239 | 0.6621 | | non-collinear AsTi |
| As3 | 24h | 1 | 0.0376 | 0.5237 | 0.27 | 0.9 | non-coplanar triangle O ₃ |
| O4 | 24h | 1 | 0.0465 | 0.6332 | 0.2915 | | non-collinear AsTi |
| O5 | 24h | 1 | 0.0852 | 0.1746 | 0.2822 | | non-collinear AsFe |
| Ca6 | 24h | 1 | 0.0934 | 0.3556 | 0.6258 | 0.66 | square prism (cube) O ₈ |
| As7 | 24h | 1 | 0.1082 | 0.1492 | 0.6399 | 0.68 | non-coplanar triangle O ₃ |
| O8 | 24h | 1 | 0.1381 | 0.5166 | 0.5027 | 0.97 | single atom As |
| O9 | 24h | 1 | 0.1467 | 0.7367 | 0.1657 | 0.87 | non-coplanar triangle AsTiFe |
| O10 | 24h | 1 | 0.173 | 0.2228 | 0.5911 | | non-collinear AsFe |
| Ti11 | 12g | 2.. | 0.0489 | $\frac{3}{4}$ | $\frac{1}{4}$ | | octahedron O ₆ |
| M12 | 12f | 2.. | 0.5031 | $\frac{1}{4}$ | $\frac{1}{4}$ | 0.92 | octahedron O ₆ |
| Ca13 | 8e | .3. | 0.1561 | 0.1561 | 0.1561 | 0.98 | octahedron O ₆ |
| As14 | 8e | .3. | 0.3735 | 0.3735 | 0.3735 | 0.85 | non-coplanar triangle O ₃ |
| Fe15 | 6d | 222.. | $\frac{1}{4}$ | $\frac{3}{4}$ | $\frac{3}{4}$ | 0.74 | tetrahedron O ₄ |
| Mn16 | 4b | -.3. | 0 | 0 | 0 | 0.8 | octahedron O ₆ |

M12 = 0.674Fe + 0.326Mn

Transformation from published data: -y, -x, -z

Experimental: single crystal, diffractometer, X-rays, R = 0.068

Remarks: Natural specimen from Monte Leone, Binnatal, Switzerland. Composition (Ca_{6.35}Mn_{0.79}Na_{0.77})(Ti_{3.81}Sn_{0.02}Al_{0.30}Fe²⁺_{2.34})As_{12.01}O₃₆·1.92H₂O from chemical analysis. H₂O not located. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Edenharter A., Nowacki W., Weibel M. (1977), Schweiz. Mineral. Petrogr. Mitt. 57, 1-16.

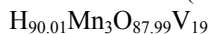


cP304

(201) $Pn-3 - h^{11}\bar{1}^2\text{eda}$ **[H₆Mn₃V₁₉O₄₆(H₂O)₁₂·30H₂O [1]**

Structural features: V₁₉O₄₀(OH)₆ units consisting of eighteen V(O,OH)₅ square pyramids sharing edges and vertices around a VO₄ tetrahedron (orientational disorder) are loosely interconnected via Mn(H₂O)₄ units to form a 3D-framework; additional H₂O in channels.

Khan M.I. et al. (1999) [1]

 $a = 1.55623 \text{ nm}$, $V = 3.7690 \text{ nm}^3$, $Z = 2$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|-------|---------|---------|---------|-------|--------------------------------------|
| O1 | 24h | 1 | 0.003 | 0.6717 | 0.2163 | 0.251 | |
| O2 | 24h | 1 | 0.0038 | 0.2158 | 0.6705 | 0.249 | |
| O3 | 24h | 1 | 0.01242 | 0.01244 | 0.25682 | | single atom V |
| O4 | 24h | 1 | 0.02739 | 0.16165 | 0.16156 | | non-coplanar triangle V ₃ |
| O5 | 24h | 1 | 0.0493 | 0.17404 | 0.32587 | | non-coplanar triangle V ₃ |
| V6 | 24h | 1 | 0.08507 | 0.08507 | 0.24528 | | square pyramid O ₅ |
| O7 | 24h | 1 | 0.08729 | 0.60933 | 0.41249 | | |
| O8 | 24h | 1 | 0.0918 | 0.598 | 0.092 | | |
| O9 | 24h | 1 | 0.1183 | 0.7468 | 0.1985 | 0.333 | |
| O10 | 24h | 1 | 0.1185 | 0.1979 | 0.7473 | 0.333 | |
| O11 | 24h | 1 | 0.1499 | 0.7472 | 0.1502 | 0.333 | |
| V12 | 12f | 2.. | 0.50737 | 1/4 | 1/4 | | square pyramid O ₅ |
| O13 | 12f | 2.. | 0.6127 | 1/4 | 1/4 | | colinear VMn |
| O14 | 8e | .3. | 0.18836 | 0.18836 | 0.18836 | | single atom V |
| Mn15 | 6d | 222.. | 1/4 | 3/4 | 3/4 | | |
| V16 | 2a | 23. | 1/4 | 1/4 | 1/4 | | tetrahedron O ₄ |
| H17 | 24h | 1 | 0.0008 | 0.1524 | 0.6601 | 0.249 | |
| H18 | 24h | 1 | 0.0009 | 0.1524 | 0.6551 | 0.251 | |
| H19 | 24h | 1 | 0.0278 | 0.0939 | 0.5959 | 0.667 | |
| H20 | 24h | 1 | 0.0278 | 0.5976 | 0.097 | 0.667 | |
| H21 | 24h | 1 | 0.0399 | 0.4519 | 0.6274 | | |
| H22 | 24h | 1 | 0.0462 | 0.7215 | 0.2104 | 0.249 | |
| H23 | 24h | 1 | 0.0513 | 0.714 | 0.2181 | 0.251 | |
| H24 | 24h | 1 | 0.0852 | 0.4117 | 0.5451 | | |
| H25 | 24h | 1 | 0.1084 | 0.1406 | 0.6992 | | |
| H26 | 24h | 1 | 0.118 | 0.1199 | 0.5464 | 0.667 | |
| H27 | 24h | 1 | 0.1275 | 0.3579 | 0.6932 | | |
| H28 | 24h | 1 | 0.1412 | 0.3493 | 0.5125 | 0.5 | |

Transformation from published data: origin shift $1/2 \ 1/2 \ 1/2$

Experimental: single crystal, diffractometer, X-rays, R = 0.041, T = 133 K

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Khan M.I., Yohannes E., Powell D. (1999), Inorg. Chem. 38, 212-213.