

Data Table 30 K₂PtCl₆

Cubic, space group *Fm3m*, No. 225; $a = 9.755 \text{ \AA}$; $Z = 4$, $V = 928.28 \text{ \AA}^3$

Atomic Positions

Pt in 4(a): 0,0,0; fc

Cl in 24(e): $\pm(x,0,0; 0,x,0; 0,0,x)$; $x = 0.240$; fc

K in 8(c): $\pm \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$; fc

Data Table 5 V₂O₅ (14)

Orthorhombic, space group *Pmmn*, No. 59; $a = 11.51$, $b = 3.56$, $c = 4.37 \text{ \AA}$;
 $Z = 2$, $V = 179 \text{ \AA}^3$

Atomic Positions

V in 4(f): $x, 0, z; \bar{x}, 0, z; \frac{1}{2} - x, \frac{1}{2}, \bar{z}; \frac{1}{2} + x, \frac{1}{2}, \bar{z}$; $x = 0.1487$, $z = 0.1086$

O(1) in 4(f): $x = 0.1460$, $z = 0.4713$

O(2) in 4(f): $x = 0.3191$, $z = -0.0026$

O(3) in 2(a): $0, 0, z; \frac{1}{2}, \frac{1}{2}, \bar{z}$; $z = -0.0031$

Data Table 3 Anhydrite, CaSO₄ (22)

Orthorhombic, space group *Cmcm*, No. 63; $a = 6.998$, $b = 6.245$, $c = 7.006 \text{ \AA}$,
 $b/a = 0.8924$, $b/c = 0.8914$; $Z = 4$, $V = 306.2 \text{ \AA}^3$

Atomic Positions: $(0,0,0; \frac{1}{2}, \frac{1}{2}, 0) +$

Ca in 4(c): $\pm(0, y, \frac{1}{4})$; $y = 0.6524$

S in 4(c): $y = 0.1556$

O(1) in 8(g): $\pm(x, y, \frac{1}{4}; \bar{x}, y, \frac{1}{4})$; $x = 0.1695$, $y = 0.0155$

O(2) in 8(f): $\pm(0, y, z; 0, y, \frac{1}{2} - z)$; $y = 0.2976$, $z = 0.0817$

Data Table 15 B-Type Eu₂O₃ (35)

Monoclinic, space group *C2/m*, No. 12; $a = 14.1105$, $b = 3.6021$, $c = 8.8080 \text{ \AA}$,
 $\beta = 100.037^\circ$; $Z = 6$, $V = 440.84 \text{ \AA}^3$

Atomic Positions: $(0,0,0; \frac{1}{2}, \frac{1}{2}, 0) +$

Eu(1) in 4(i): $\pm(x, 0, z)$; $x = 0.63740$, $z = 0.4897$

Eu(2) in 4(i): $x = 0.68972$, $z = 0.13760$

Eu(3) in 4(i): $x = 0.96635$, $z = 0.18763$

O(1) in 4(i): $x = 0.1291$, $z = 0.2855$

O(2) in 4(i): $x = 0.8248$, $z = 0.0267$

O(3) in 4(i): $x = 0.7961$, $z = 0.3732$

O(4) in 4(i): $x = 0.4734$, $z = 0.3431$

O(5) in 2(b): $0, \frac{1}{2}, 0$