Crystal structure of manganese chlorine boracite, $Mn_3B_7O_{13}Cl$

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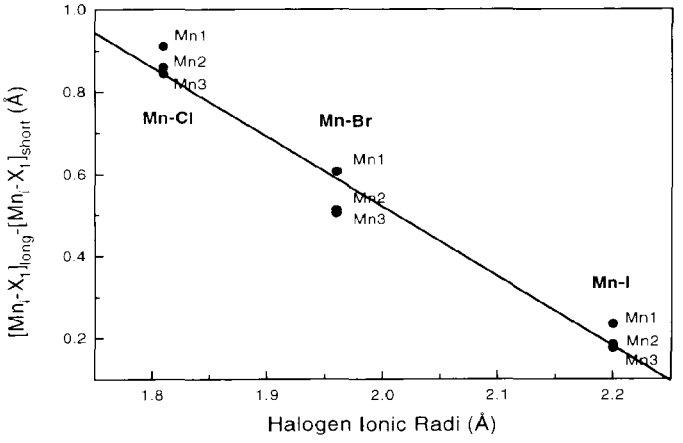

Source of material: The compound is synthesized from a mixture of MnO, $MnCl_2$, B_2O_3 and H_2O traces in a sealed quartz ampoule at 1200 K. The three crucible method described in ref. 1 was used. Data collection on an optically controlled ferroelectric single domain crystal. The figure shows the difference between the two metal-halogen distances as a function of the halogen ionic radii for the three orthorombic manganese boracites. A linear behavior is found as for others boracites (see ref. 2).

$B_7ClMn_3O_{13}$, orthorhombic, $Pca2_1$ (No. 29), a =8.678(1) Å, b =8.688(1) Å, c =12.290(1) Å, V =926.6 Å^3, Z =4, $R(F)$ =0.028, $R_w(F)$ =0.023.

References

1. Schmid, H: Die Synthese von Boraziten mit Hilfe chemischer Transportreaktionen. J. Phys. Chem. Solids **26** (1965) 973-988.
2. Kubel, F.; Janner, A.-M.: Structure of the Fully Ferroelectric/Fully Ferro-elastic Orthorhombic Room-Temperature Phase of Iron Iodine Boracite, $Fe_3B_7O_{13}I$. Acta Crystallogr. C**49** (1993) 657-659.

Table 1. Parameters used for the X-ray data collection

Crystal:	platelet, size 0.23 x 0.15 x 0.03 mm
Wavelength:	Mo K_α radiation (0.71070 Å)
μ:	44.00 cm^{-1}
Diffractometer:	Stoe
Scan mode:	ω/2θ
$T_{measurement}$:	293 K
$2\theta_{max}$:	49°
$N(hkl)_{unique}$:	1734
Criterion for F_o:	$F_o > 3\,\sigma(F_o)$
$N(param)_{refined}$:	118
Program:	Xtal3.2

Table 2. Final atomic coordinates and displacement parameters (in Å^2)

Atom	Site	x	y	z	U_{iso}
B(1)	4a	0.503(1)	0.496(2)	0.249(1)	0.01(1)
B(2)	4a	0.2561(7)	0.249(2)	0.4958(7)	0.009(9)
B(3)	4a	0.002(1)	−0.005(2)	0.2495(9)	0.009(9)
B(4)	4a	0.4561(8)	0.249(1)	0.3506(7)	0.01(1)
B(5)	4a	0.2474(9)	0.401(2)	0.169(1)	0.008(8)
B(6)	4a	0.9045(7)	0.751(1)	0.8209(6)	0.01(1)
B(7)	4a	0.7528(9)	0.902(2)	0.669(1)	0.007(7)
O(1)	4a	0.2283(5)	0.250(1)	0.236(5)	0.009(9)
O(2)	4a	0.5401(5)	0.3317(6)	0.2758(5)	0.009(9)
O(3)	4a	0.3827(5)	0.3241(5)	0.4343(4)	0.009(9)
O(4)	4a	0.9717(5)	0.1599(6)	0.2744(5)	0.009(9)
O(5)	4a	0.3171(6)	0.3629(6)	0.0653(5)	0.008(8)
O(6)	4a	0.1657(6)	0.9750(6)	0.2254(5)	0.009(9)
O(7)	4a	0.1432(5)	0.1810(6)	0.4222(4)	0.01(1)
O(8)	4a	0.3390(6)	0.5136(6)	0.2275(5)	0.009(9)
O(9)	4a	0.1765(6)	0.1243(5)	0.0639(5)	0.01(1)
O(10)	4a	0.9515(6)	0.5933(6)	0.8395(4)	0.009(9)
O(11)	4a	0.5347(5)	0.9088(5)	0.8513(5)	0.007(7)
O(12)	4a	0.9081(6)	0.5365(5)	0.6528(4)	0.008(8)
O(13)	4a	0.5897(6)	0.9429(5)	0.6588(5)	0.008(8)

Table 3. Final atomic coordinates and displacement parameters (in Å^2)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cl(1)	4a	0.7691(2)	0.2504(4)	0.50870[a]	0.0164(7)	0.0151(7)	0.016(1)	0.000(1)	0.0014(9)	0.002(2)
Mn(1)	4a	0.7617(1)	0.2520(3)	0.2211(2)	0.0077(4)	0.0081(4)	0.0159(7)	0.0004(5)	0.0015(5)	0.000(1)
Mn(2)	4a	0.4823(2)	0.5333(2)	0.4994(2)	0.0137(6)	0.0129(5)	0.0083(8)	−0.0045(6)	−0.0001(7)	−0.0003(6)
Mn(3)	4a	−0.0162(2)	0.0334(2)	0.5028(2)	0.0153(6)	0.0126(5)	0.0074(8)	0.0042(6)	−0.0002(7)	−0.0001(6)

a: arbitrarily fixed for definition of the origin.