

Ferro-axinite, $\text{Ca}_2\text{Fe}^{2+}\text{Al}_2\text{BSi}_4\text{O}_{15}(\text{OH})$

Ferro-axinite

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The crystal structure of near-end-member ferroaxinite from an iron-contaminated pegmatite at Malesov, Czech Republic

7.152 9.206 8.962 91.84 98.17 77.33 P-1

atom	x	y	z	Wyckoff
CaX1	0.74654	0.34815	0.39531	2i
CaX2	0.18294	0.10007	0.08383	2i
FeY	0.76793	0.590928	0.111915	2i
AlZ1	0.05241	0.80071	0.25398	2i
AlZ2	0.35207	0.93593	0.42115	2i
BT5	0.46146	0.63436	0.28684	2i
SiT1	0.21024	0.44997	0.23430	2i
SiT2	0.21917	0.27475	0.52333	2i
SiT3	0.69820	0.25644	0.01151	2i
SiT4	0.64140	0.01946	0.23044	2i
O1	0.05360	0.60321	0.18957	2i
O2	0.23119	0.33833	0.09578	2i
O3	0.41844	0.48704	0.31215	2i
O4	0.13537	0.37210	0.36980	2i
O5	0.02163	0.24270	0.56436	2i
O6	0.32702	0.38060	0.64393	2i
O7	0.38056	0.12747	0.49578	2i
O8	0.53476	0.34395	0.87689	2i
O9	0.87563	0.15555	0.93367	2i
O10	0.76780	0.36672	0.13914	2i
O11	0.60268	0.13512	0.08713	2i
O12	0.43624	0.98117	0.24413	2i
O13	0.72081	0.10006	0.38469	2i
O14	0.79432	0.87507	0.17743	2i
O15	0.32502	0.74622	0.35434	2i
Oh16	0.09682	0.99539	0.32260	2i
H	0.993	0.963	0.631	2i

(27 × 2i)

Raman Active Modes

WP	A _g	A _u
2i	3	.

Total number of modes:

$$81A_g = 81$$