

Chrysoberyl, BeAl₂O₄

Chrysoberyl

Weber S U, Grodzicki M, Lottermoser W, Redhammer G J, Tippelt G, Ponahlo J, Amthauer G
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⁵⁷Fe Mossbauer spectroscopy, X-ray single-crystal diffractometry, and
 electronic structure calculations on natural alexandrite

9.4082 5.4790 4.4288 90 90 90 Pnma

atom	x	y	z	Wyckoff
Al1	0	0	0	4a
Al2	0.27282	0.25	-0.00503	4c
Be	0.09289	0.25	0.43360	4c
O1	0.09022	0.25	0.78822	4c
O2	0.43316	0.25	0.24167	4c
O3	0.16324	0.01554	0.25728	8d

$$(1 \times 8d) + (4 \times 4c) + (1 \times 4a)$$

Raman Active Modes

WP	A _g	A _u	B _{1g}	B _{1u}	B _{2g}	B _{2u}	B _{3g}	B _{3u}
8d	3	-	3	-	3	-	3	-
4c	2	-	1	-	2	-	1	-
4a	-	-	-	-	-	-	-	-

Total number of modes:

$$11A_g + 7B_{1g} + 11B_{2g} + 7B_{3g} = 36$$