

Corundum, Al₂O₃

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Electric field gradients and charge density in corundum alpha-Al₂O₃

4.7602 4.7602 12.9933 90 90 120 R-3c

atom	x	y	z	Wyckoff
Al	0	0	.35216	12c
O	.30624	0	0.25	18e

Raman Active Modes

WP	A _{1g}	A _{1u}	A _{2g}	A _{2u}	E _u	E _g
18e	1	3
12c	1	2

Total number of modes:

$$2A_{1g} + 5 E_g = 7$$