

Spinel, MgAl₂O₄

Spinel

Martignago F, Dal Negro A, Carbonin S

Physics and Chemistry of Minerals 30 (2003) 401-408

How Cr³⁺ and Fe³⁺ affect Mg-Al order-disorder transformation
at high temperature in natural spinels

8.1080 8.1080 8.1080 90 90 90 *Fd3m

.125 .125 .125

atom	x	y	z	Wyckoff
MgT	0.125	0.125	0.125	8a
AlM	0.5	0.5	0.5	16d
O	0.26338	0.26338	0.26338	32e

Raman Active Modes

WP	A _{1g}	A _{1u}	A _{2g}	A _{2u}	E _u	E _g	T _{2u}	T _{2g}	T _{1u}	T _{1g}
32e	1	-	-	-	-	1	-	2	-	-
16d	-	-	-	-	-	-	-	-	-	-
8a	-	-	-	-	-	-	-	1	-	-

Total number of modes:

$$1A_{1g} + 1E_g + 3T_{2g} = 5$$