

Beryl,  $\text{Be}_3\text{Al}_2\text{Si}_6\text{O}_{18}$

Beryl

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High-pressure crystal chemistry of beryl ( $\text{Be}_3\text{Al}_2\text{Si}_6\text{O}_{18}$ ) and euclase ( $\text{BeAlSi}_4\text{O}_7\text{OH}$ )

9.208 9.208 9.188 90 90 120 P6/mcc

atom	x	y	z	Wyckoff
Be	0.5	0	0.25	6f
Al	1/3	2/3	0.25	4c
Si	0.3876	0.1159	0	12l
O1	0.3103	0.2369	0	12l
O2	0.4985	0.1456	0.1453	24m

$$(1 \times 24m) + (2 \times 12l) + (1 \times 6f) + (1 \times 4c)$$

**Raman Active Modes**

WP	$A_{1g}$	$A_{1u}$	$A_{2g}$	$A_{2u}$	$B_{1g}$	$B_{1u}$	$B_{2g}$	$B_{2u}$	$E_{2u}$	$E_{2g}$	$E_{1u}$	$E_{1g}$
24m	3	-	-	-	-	-	-	-	-	6	-	6
12l	2	-	-	-	-	-	-	-	-	4	-	2
6f	-	-	-	-	-	-	-	-	-	1	-	2
4c	-	-	-	-	-	-	-	-	-	1	-	1

Total number of modes:

$$7A_{1g} + 16E_{2g} + 13E_{1g} = 36$$