

Lazurite,  $\text{Na}_3\text{Ca}(\text{Si}_3\text{Al}_3)\text{O}_{12}\text{S}$

Lazurite

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The structure of lazurite, ideally  $\text{Na}_6\text{Ca}_2(\text{Al}_6\text{Si}_6\text{O}_{24})\text{S}_2$ , a member of the sodalite group

9.105 9.105 9.105 90 90 90 P-43n

atom	x	y	z	Wyckoff
Na	0.178	0.178	0.178	8e
Al	0.25	0	0.5	6d
Si	0.25	0.5	0	6c
O1	0.133	0.147	0.545	24i
O2	0.598	0.598	0.598	8e
S	0	0	0	2a

$$(1 \times 24i) + (2 \times 8e) + (1 \times 6d) + (1 \times 6c) + (1 \times 2a)$$

**Raman Active Modes**

WP	A <sub>1</sub>	A <sub>2</sub>	E	T <sub>1</sub>	T <sub>2</sub>
24i	3	-	6	-	9
8e	1	-	2	-	3
6d	-	-	1	-	3
6c	-	-	1	-	3
2a	-	-	-	-	1

Total number of modes:

$$5A_1 + 12E + 22T_2 = 39$$