

## Danburite, CaB<sub>2</sub>Si<sub>2</sub>O<sub>8</sub>

Danburite

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The crystal structure of danburite: A comparison with anorthite, albite, and reedmergnerite

8.038 8.752 7.730 90 90 90 Pnam

atom	x	y	z	Wyckoff
Ca	0.3854	0.0765	0.25	4c
B1	0.2590	0.4192	0.4201	8d
Si2	0.0533	0.1924	0.9442	8d
O1	0.1930	0.0680	0.9968	8d
O2	0.1263	0.3650	0.9567	8d
O3	0.3998	0.3135	0.0781	8d
O4	0.5136	0.6636	0.25	4c
O5	0.1838	0.4282	0.25	4c

$(5 \times 8d) + (3 \times 4c)$

### Raman Active Modes

WP	A <sub>g</sub>	A <sub>u</sub>	B <sub>1g</sub>	B <sub>1u</sub>	B <sub>2g</sub>	B <sub>2u</sub>	B <sub>3g</sub>	B <sub>3u</sub>
8d	3	.	3	.	3	.	3	.
4c	2	.	1	.	2	.	1	.

Total number of modes:

$$21A_g + 18B_{1g} + 21B_{2g} + 18B_{3g} = 78$$