Scapolite Series

The end members, marialite, meionite and silvialite, exhibit I4/m symmetry. The intermediate members exhibit $P4_2/n$ symmetry. The analysis is presented for both symmetries. The I4/m phases have less Raman modes than the $P4_2/n$ phases.

Marialite, $(Na,Ca)_4(Si,Al)_{12}O_{24}(Cl,CO_3,SO_4)$

Marialite
Sokolova E V, Kabalov Y K, Sherriff B L, Teertstra D K, Jenkins D M, Kunath-Fandrei G, Goetz S, Jager C
The Canadian Mineralogist 34 (1996) 1039-1050
Marialite: Rietveld structure-refinement and Si MAS and Al satellite transition NMR spectroscopy
12.0396 12.0396 7.5427 90 90 90 I4/m

atom	x	y	z	Wyckoff
NaM	0.3741	0.2997	0.5	8h
SiT1	0.3386	0.4107	0	8h
SiT2	0.6611	0.9154	0.7936	16i
O1	0.4564	0.3522	0	8h
O2	0.6909	0.8823	0	8h
O3	0.3538	0.9488	0.7845	16i
O4	0.2691	0.3729	0.8250	16i
Cl	0.5	0.5	0.5	2a

$(1 \times 16i) + (4 \times 8h) + (1 \times 2a)$

Raman Active Modes

WP	A_g	A_u	B_g	B_u	E_g^1	E_u^1	E_g^2	E_u^2
16i	3	·	3	·	3	·	3	·
8h	2	·	2	·	1	·	1	·
2a	·	·	·	·	·	·	·	·

Total number of modes:
$11A_g + 11B_g + 7E_g^1 + 7E_g^2 = 36$

Meionite, $(Ca,Na)_4(Si,Al)_{12}O_{24}(CO_3,SO_4,Cl)$

Meionite
Lin S B, Burley B J
Tschermaks Mineralogische und Petrographische Mitteilungen 21 (1974) 196-215
The crystal structure of an intermediate scapolite - wernerite
12.1164 12.1164 7.581 90 90 90 P4_2/n

atom	x	y	z	Wyckoff
Ca	0.3603	0.2841	0.5126	8g
C	0.5	0.5	0.5	2a
Si1	0.3390	0.4092	0.9978	8g
Si2	0.6593	0.9155	0.7967	8g
Si3	0.4125	0.8363	0.7103	8g
O1	0.4576	0.3503	0.0019	8g
O2	0.6902	0.8757	0.0088	8g
O3	0.3498	0.9420	0.7947	8g
O4	0.5459	0.8472	0.7160	8g
O5	0.2677	0.3667	0.8307	8g
O6	0.3703	0.7287	0.8256	8g
O7	0.3978	0.4793	0.4598	8g
O8	0.4007	0.4819	0.5871	8g

$(12 \times 8g) + (1 \times 2a)$

Raman Active Modes

WP	A_g	A_u	B_g	B_u	E_g^1	E_u^1	E_g^2	E_u^2
8g	3	·	3	·	3	·	3	·
2a	·	·	1	·	1	·	1	·

Total number of modes:
$36A_g + 37B_g + 37E_g^1 + 37E_g^2 = 147$