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**Raman scattering of omphacite at high pressure: towards its possible application to elastic
geothermobarometry**

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Cámara¹**

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Supplemental Material

Table S1. Selected interatomic distances (Å) and polyhedral volumes. Mean quadratic elongation (λ) and the angle variance (σ^2) were computed according to Robinson et al. (1971).

		Natural-8	Natural-11			Annealed-3	Annealed-7
<i>T1</i>	–O11	1.6176(7)	1.6163(7)	<i>T</i>	–O1	1.6186(8)	1.6166(5)
	–O31	1.6545(8)	1.6548(8)		–O2	1.5934(10)	1.5919(5)
	–O32	1.6656(7)	1.6636(7)		–O3	1.6528(10)	1.6519(5)
	–O21	1.5974(7)	1.5972(8)		–O3	1.6683(9)	1.6671(5)
	< <i>T1</i> –O>	1.6338(8)	1.6330(8)		< <i>T</i> –O>	1.6333(10)	1.6319(5)
	$V(\text{\AA}^3)$	2.2194	2.2162		$V(\text{\AA}^3)$	2.2179	2.2126
	σ^2	25.4620	25.5402		σ^2	24.7182	24.2834
	λ	1.0059	1.0059		λ	1.0057	1.0056
<i>T2</i>	–O12	1.6194(8)	1.6181(7)	<i>M1</i>	–O1 ($\times 2$)	2.0671(11)	2.0666(5)
	–O22	1.5880(7)	1.5878(8)		–O1 ($\times 2$)	2.0035(8)	2.0025(5)
	–O31	1.6706(7)	1.6699(7)		–O2 ($\times 2$)	1.9638(11)	1.9633(6)
	–O32	1.6511(8)	1.6515(8)		< <i>M1</i> –O>	2.0115(10)	2.0108(6)
	< <i>T2</i> –O>	1.6323(8)	1.6318(8)		$V(\text{\AA}^3)$	10.7093	10.6999
	$V(\text{\AA}^3)$	2.2155	2.2138		σ^2	29.9119	29.7099
	σ^2	22.2385	22.0892		λ	1.0093	1.0092
	λ	1.0053	1.0053	<i>M2</i>	–O1 ($\times 2$)	2.3761(11)	2.3736(5)
<i>M1</i>	–O11 ($\times 2$)	2.1326(8)	2.1358(8)		–O2 ($\times 2$)	2.3762(8)	2.3751(4)
	–O12 ($\times 2$)	2.0611(7)	2.0636(6)		–O3 ($\times 2$)	2.7242(10)	2.7215(5)
	–O22 ($\times 2$)	2.0345(8)	2.0372(8)		–O3 ($\times 2$)	2.4804(10)	2.4783(5)
	< <i>M1</i> –O>	2.0761(8)	2.0789(8)		< <i>M2</i> –O>	2.4892(10)	2.4871(5)
	$V(\text{\AA}^3)$	11.7101	11.7509		$V(\text{\AA}^3)$	25.4019	25.3416
	σ^2	41.9800	43.3542				
	λ	1.0129	1.0133				
<i>M11</i>	–O11 ($\times 2$)	1.9479(7)	1.9408(6)				
	–O12 ($\times 2$)	2.0033(8)	1.9989(8)				
	–O21 ($\times 2$)	1.9071(8)	1.8990(8)				
	< <i>M11</i> –O>	1.9528	1.9462(8)				
	$V(\text{\AA}^3)$	9.8418	9.7434				
	σ^2	20.2378	20.2028				
	λ	1.0063	1.0063				
<i>M2</i>	–O31 ($\times 2$)	2.6936(8)	2.6923(8)				
	–O32 ($\times 2$)	2.4779(7)	2.4731(8)				
	–O21 ($\times 2$)	2.3609(7)	2.3618(6)				
	–O11 ($\times 2$)	2.3577(8)	2.3581(8)				
	< <i>M2</i> –O>	2.4725(8)	2.4714(8)				

	$V(\text{\AA}^3)$	24.8083	24.7544
<i>M21</i>	–O12 (×2)	2.3926(7)	2.3938(8)
	–O22 (×2)	2.3824(7)	2.3815(6)
	–O31 (×2)	2.4933(7)	2.4890(7)
	–O32 (×2)	2.7700(8)	2.7737(8)
	< <i>M21</i> –O>	2.5096(8)	2.5095(8)
	$V(\text{\AA}^3)$	26.0091	25.9948

Table S2. Raman wavenumbers (ω , in cm^{-1}) of the A_g and B_g modes and relative intensities (I , in arbitrary units) of omphacite ($\text{Jd}_{50}\text{Aug}_{50}$) calculated with HF/DFT simulations. Note that the calculated intensities correspond to the components of the Raman polarizability tensor for a single crystal.

Mode	ω	$I(xx)$	$I(xy)$	$I(xz)$	$I(yy)$	$I(yz)$	$I(zz)$
Bg	90.1882	0	0.06	0	0	1.3	0
Bg	121.7017	0	0.31	0	0	0.27	0
Ag	142.3413	5.47	0	9.42	0.01	0	3.81
Bg	147.8224	0	0.02	0	0	0.09	0
Ag	157.8623	0.48	0	0	0	0	1.89
Bg	160.961	0	2.67	0	0	2.09	0
Bg	180.8623	0	0.41	0	0	1.12	0
Ag	190.9421	0.11	0	0.97	7.66	0	3.07
Bg	192.9386	0	4.34	0	0	4.63	0
Ag	215.4766	7.92	0	0.31	1.38	0	6.18
Bg	219.6555	0	5.59	0	0	1.62	0
Ag	229.6004	0.02	0	0.27	3.75	0	0
Bg	232.9456	0	7.33	0	0	0	0
Bg	240.0151	0	14.43	0	0	1.96	0
Bg	269.662	0	2.15	0	0	0.7	0
Ag	271.3843	13.7	0	2.36	14.01	0	10.43
Ag	281.1903	4.03	0	1.44	0.09	0	0.54
Bg	293.2131	0	5.34	0	0	12.81	0
Ag	300.3654	12.43	0	0.9	0	0	0.09
Bg	315.8276	0	8.84	0	0	9.26	0
Bg	325.7705	0	7.15	0	0	6.93	0
Ag	329.337	3.46	0	1.94	104.67	0	1.8
Ag	337.4799	47.56	0	1.94	103.54	0	95.78
Bg	342.3721	0	0.08	0	0	6.66	0
Ag	348.9098	0.95	0	4.04	37.83	0	19.52
Bg	354.9189	0	20.93	0	0	3.59	0
Ag	375.2446	0.51	0	3.88	78.45	0	13.92
Bg	381.4427	0	10.28	0	0	22.8	0
Ag	381.968	56.11	0	15.92	158.12	0	32.87
Bg	398.6208	0	22.89	0	0	31.11	0
Ag	401.9073	1.05	0	0.34	10.5	0	4.9
Ag	410.6266	97.37	0	24.16	133.01	0	18.34
Bg	427.7318	0	16.95	0	0	0.44	0
Bg	450.0975	0	2.05	0	0	0.17	0

Ag	452.3757	0.67	0	0.12	1.14	0	0.18
Bg	494.2334	0	2.24	0	0	21.21	0
Bg	517.2296	0	3.59	0	0	0.44	0
Ag	519.3322	11.91	0	0.02	0.46	0	32.68
Bg	541.7877	0	3.26	0	0	0.35	0
Ag	544.9493	1.97	0	3.21	40.15	0	10.14
Bg	552.8327	0	1.67	0	0	28.7	0
Ag	562.5376	78.95	0	0.33	4.5	0	26.96
Bg	575.7787	0	56.77	0	0	3.62	0
Ag	609.1143	48.95	0	0.01	25.05	0	26.67
Ag	688.0756	995.28	0	9.51	329.19	0	694.58
Bg	701.7361	0	6.98	0	0	0.39	0
Ag	734.6369	7.81	0	1.75	6.66	0	17.97
Bg	749.5436	0	2.59	0	0	22.09	0
Bg	891.2765	0	5.43	0	0	16.06	0
Ag	899.2192	34.79	0	9.87	22.02	0	3.72
Bg	912.8104	0	0.17	0	0	1.53	0
Ag	916.3339	97.55	0	23.95	27.56	0	6.53
Bg	936.2462	0	17.94	0	0	3.3	0
Ag	1007.438	436.84	0	42.75	433.68	0	279.99
Bg	1009.107	0	0.16	0	0	5.94	0
Ag	1020.806	356.98	0	16.32	180.59	0	46.03
Bg	1028.623	0	5.98	0	0	0	0
Ag	1028.96	547.01	0	70.67	1000	0	107.55
Bg	1040.292	0	25.48	0	0	10.48	0
Ag	1067.446	4.47	0	5.88	6.73	0	50.41

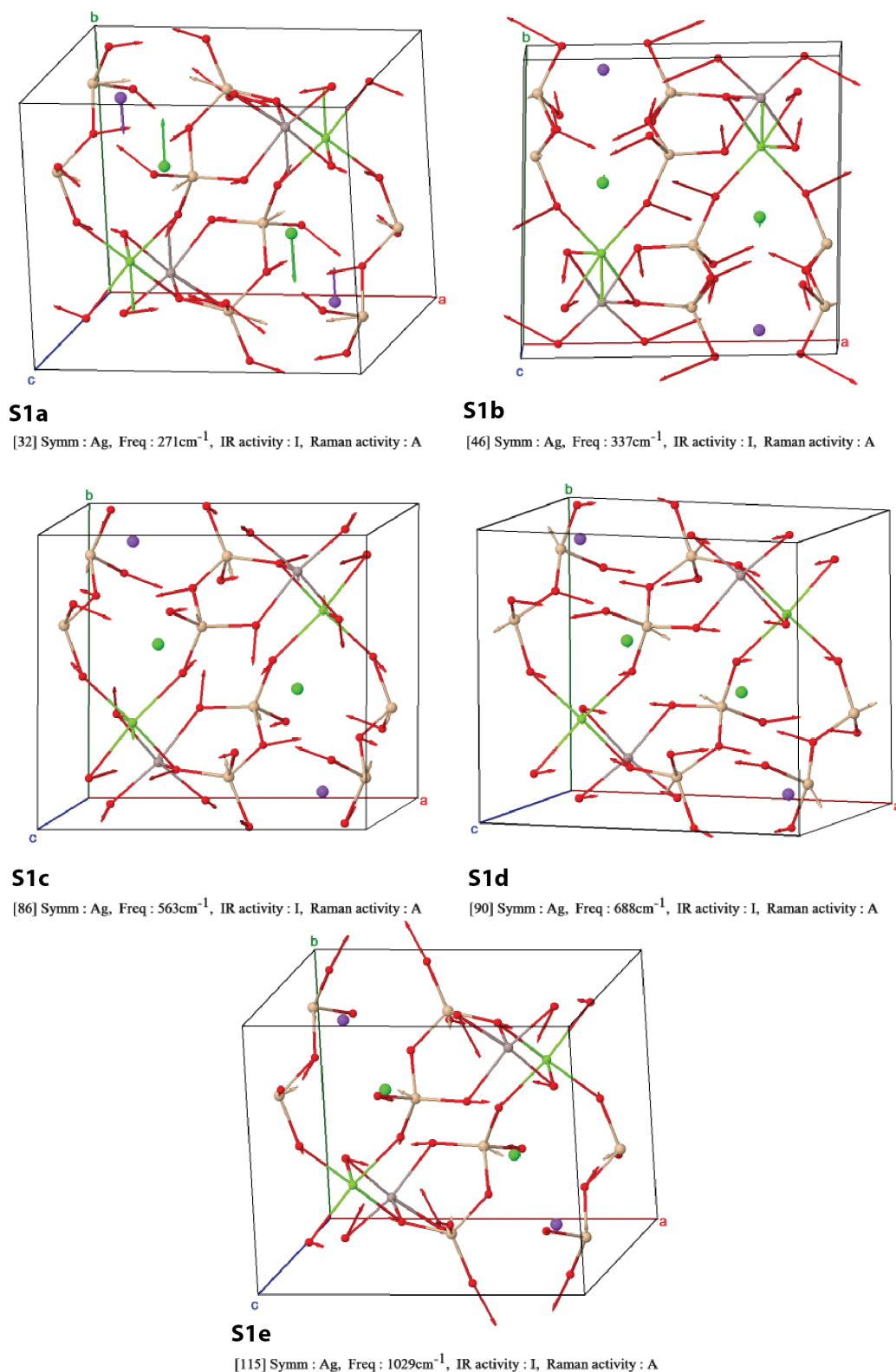


Fig. S1. Sketches of selected A_g vibrational modes obtained with HF/DFT simulations. The mode at 271 cm^{-1} is associated with vibrations of M -site cations along b and TO_4 translation along a (S1a); the mode at 337 cm^{-1} is related to $M1$ -cation vibrations parallel to b axis and TO_4 rotation around c (S1b); the Raman mode at 563 cm^{-1} is dominated by O-Si-O bond bending modes (S1c); the strong peak at 680 cm^{-1} arises from Si-O_b-Si bond bending vibrations (S1d); the mode at 1029 cm^{-1} is related to the Si-O_{nb} bond stretching (S1e). Si atoms are shown in pink, Al in grey, Mg in light green, Ca in dark green, Na in purple, and O in red. The sketches were prepared using CRYSPLOT (Beata et al. 2019).