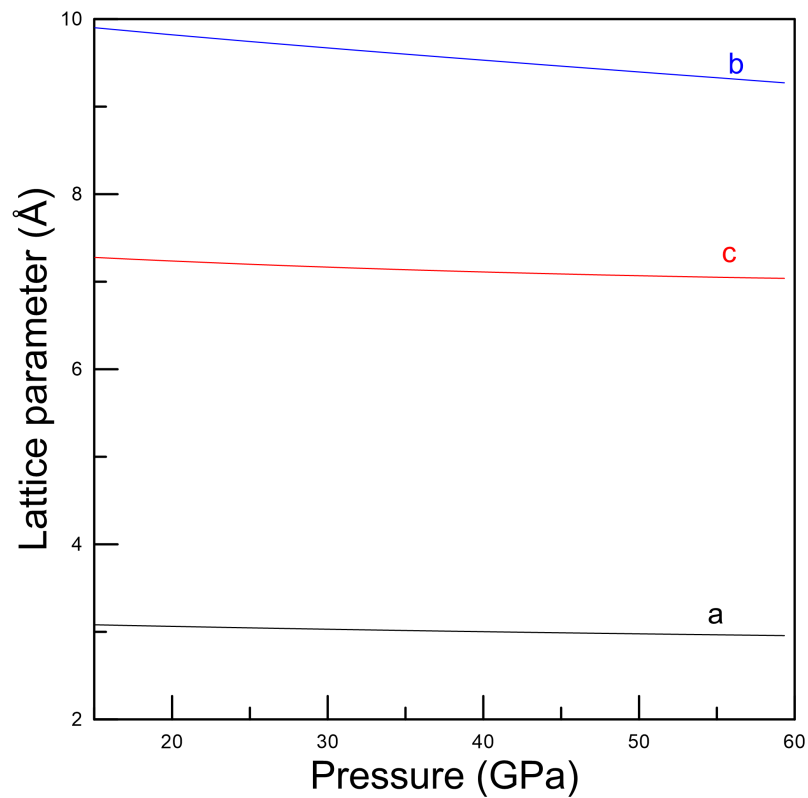


# Supplementary Materials: *Ab Initio* Theoretical Study of DyScO<sub>3</sub> at High Pressure

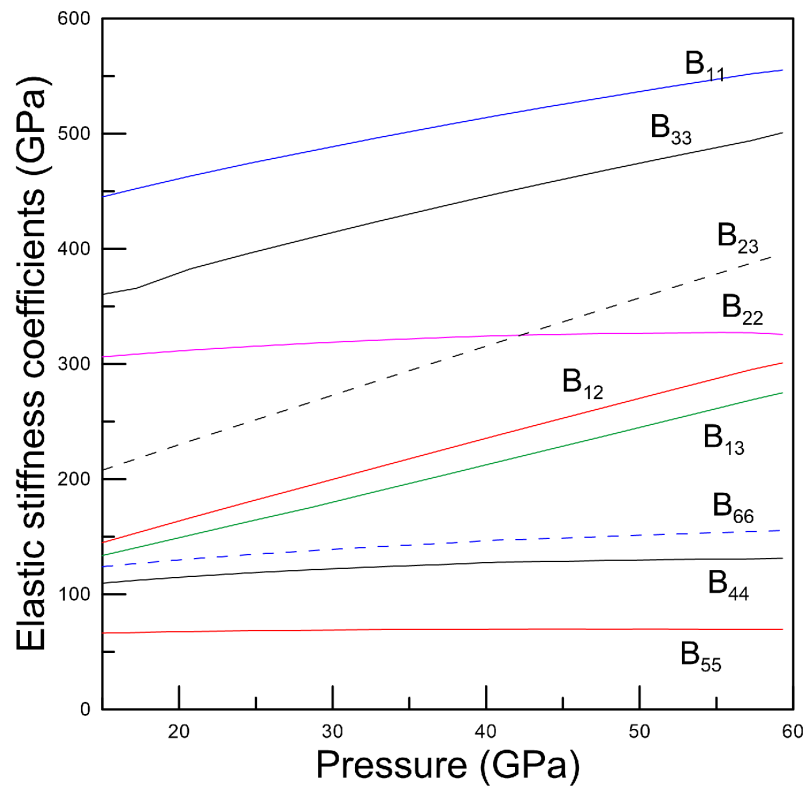
Enrique Zanardi <sup>1</sup>, Silvana Radescu <sup>1</sup>, Andrés Mujica <sup>1</sup>, Plácida Rodríguez Hernández <sup>1</sup> and Alfonso Muñoz <sup>1,\*</sup>



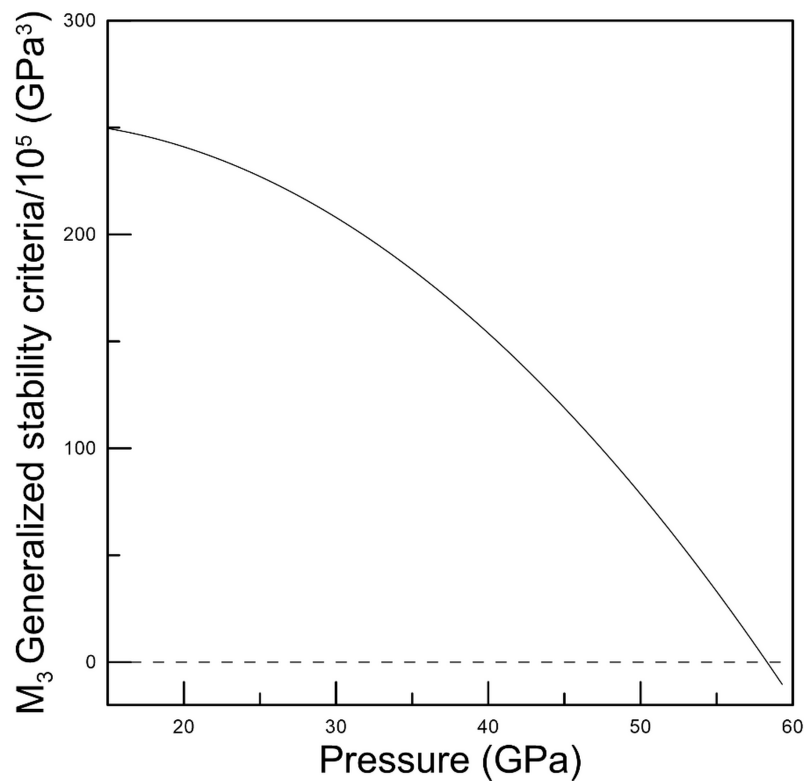
**Figure S1.** Variation of the lattice parameters *a*, *b*, *c* with pressure for the proposed *Cmcm* phase.

**Table S1.** Elastic moduli *B*, *E* and *G*; *B*/*G* ratio; and Poisson’s ratio *ν* for the proposed *Cmcm* phase., calculated using the Voigt, Reuss, and Hill approximations from the calculated elastic coefficients at 15 GPa.

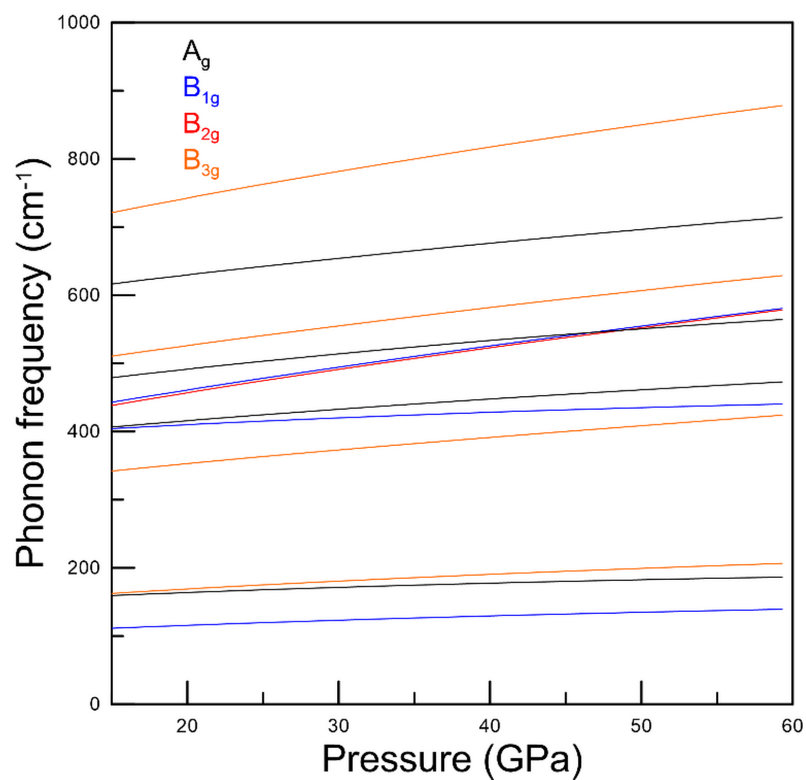
	Voigt	Reuss	Hill
Bulk modulus $B_0$ (GPa)	231.6	230.1	230.9
Shear modulus $G_0$ (GPa)	101.7	90.1	95.9
Young modulus $E_0$ (GPa)	266.1	239.2	252.6
Poisson’s ratio $\nu_0$	0.309	0.327	0.318
Bulk/Shear ratio $B_0/G_0$	2.278	2.553	2.407 (ductile)



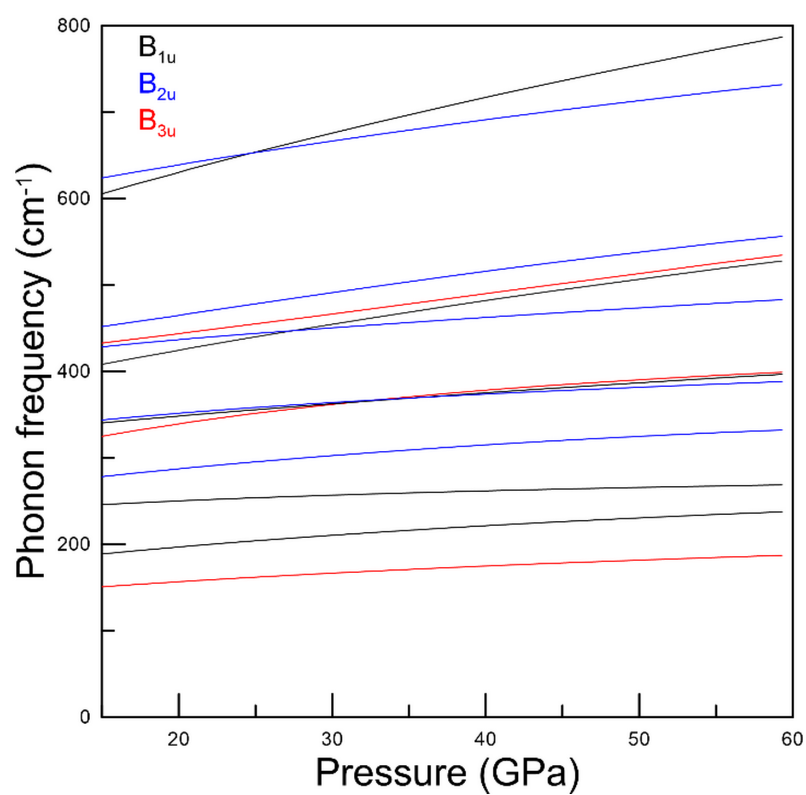
**Figure S2.** Calculated pressure evolution of the elastic stiffness coefficients for the proposed *Cmcm* phase.



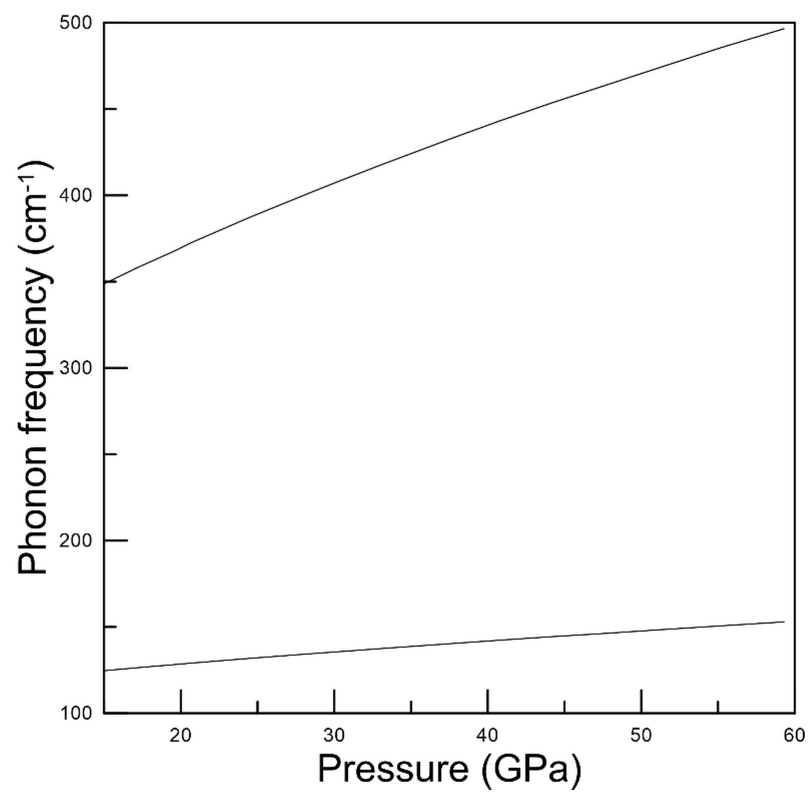
**Figure S3.**  $M_3$  generalized stability criteria as a function of pressure for the proposed *Cmcm* phase..



**Figure S4.** Pressure dependence of the calculated Raman-active modes of the *Cmcm* phase.



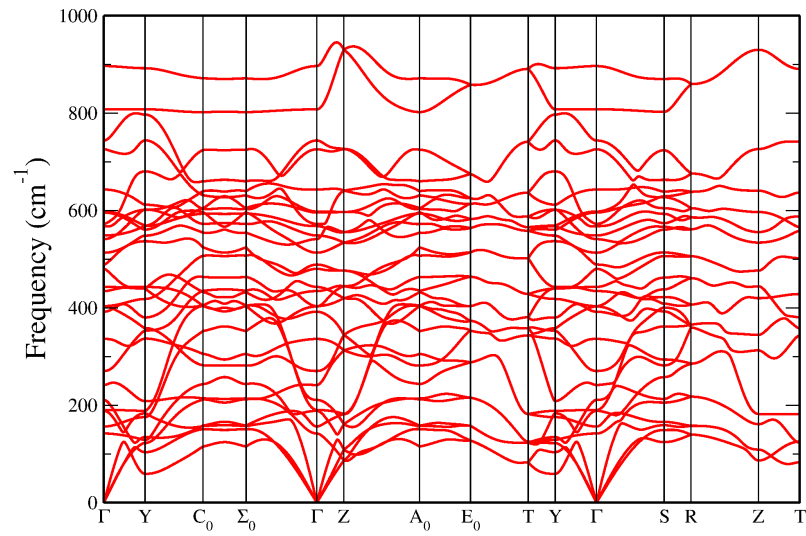
**Figure S5.** Pressure dependence of the calculated infrared modes of the *Cmcm* phase.



**Figure S6.** Pressure dependence of the calculated silent modes of the *Cmcm* phase.

**Table S2.** Calculated Raman (R), infrared (IR), and silent (S) mode frequencies for the proposed *Cmcm* phase as calculated in this work, and their respective pressure coefficients obtained by fitting in the range up to 60 GPa with a quadratic equation  $\omega(p) = \omega_o + \alpha p + \beta p^2$ .

Mode	$\omega_o$ (cm <sup>-1</sup> )	$\alpha$ (cm <sup>-1</sup> GPa <sup>-1</sup> )	$\beta$ (cm <sup>-1</sup> GPa <sup>-2</sup> )
<b>Raman</b>			
A <sub>g</sub>	145.1	1.06	-0.0061
	377.4	2.08	-0.0081
	438.5	2.92	-0.0134
	575.1	2.93	-0.0100
B <sub>1g</sub>	97.8	0.99	-0.0050
	385.4	1.38	-0.0078
	387.6	3.87	-0.0105
B <sub>2g</sub>	381.2	4.01	-0.0117
B <sub>3g</sub>	142.0	1.49	-0.0068
	309.1	2.32	-0.0066
	462.3	3.38	-0.0097
	654.3	4.72	-0.0161
<b>Infrared</b>			
B <sub>1u</sub>	163.1	1.90	-0.0110
	232.9	0.99	-0.0065
	316.0	1.74	-0.0065
	356.5	3.66	-0.0130
	527.7	5.51	-0.0194
B <sub>2u</sub>	248.7	2.19	-0.0133
	320.3	1.77	-0.0107
	404.7	1.73	-0.0070
	406.6	3.13	-0.0100
	575.9	3.42	-0.0134
B <sub>3u</sub>	132.2	1.37	-0.0076
	279.7	3.46	-0.0247
	398.7	2.23	0.0011
<b>Silent</b>			
A <sub>u</sub>	113.0	0.83	-0.0027
	283.9	4.63	-0.0178



**Figure S7.** Phonon dispersion curves at 65.7 GPa for the proposed *Cmcm* phase.