

Supplementary Information

A Mechanism for Aragonite to Post-aragonite Transition in MCO_3 ($\text{M} = \text{Ca}, \text{Sr}$ and Ba) Carbonates: Evidence of a hidden metastable polymorph

Miguel A. Salvadó*, Pilar Pertierra and J. Manuel Recio

MALTA-Consolider Team and Departamento de Química Física y Analítica, Universidad de
Oviedo, E-33006 Oviedo, Spain

Email: mass@uniovi.es

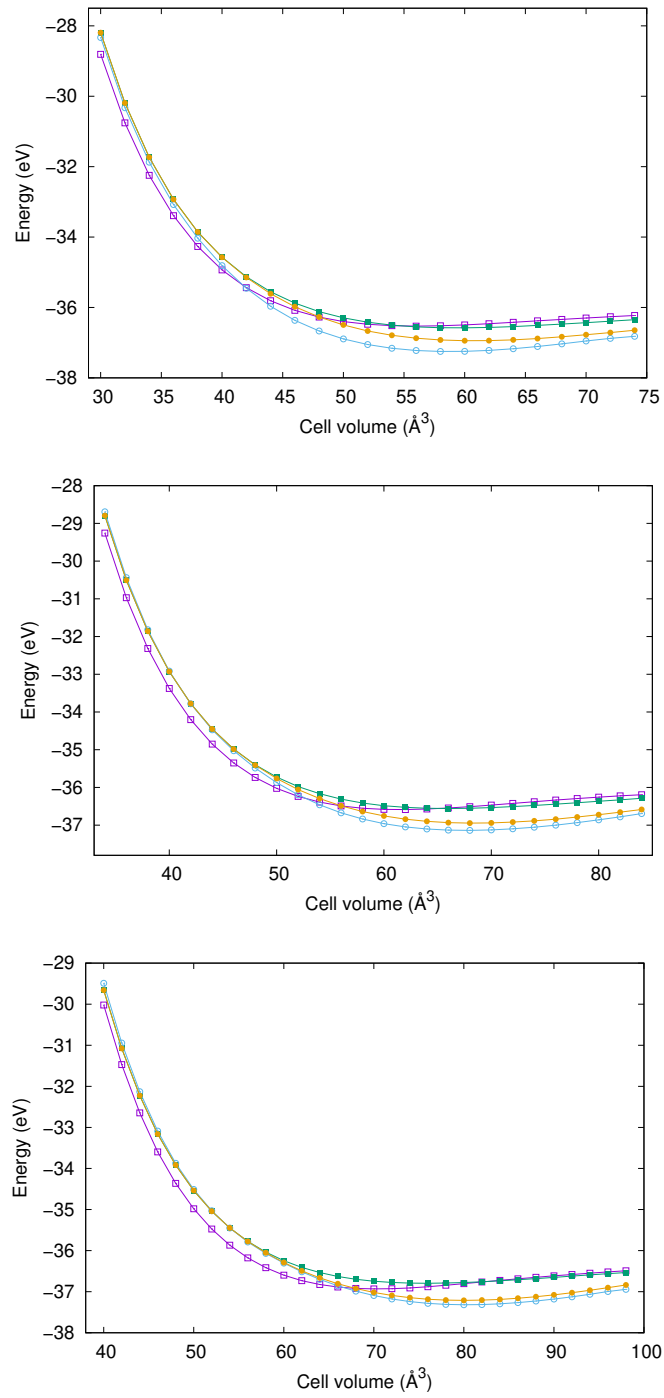


Figure S1: Energy-volume curves of aragonite (blue empty circles), post-aragonite (purple empty squares), *hexa1* (green filled squares), *hexa2* (yellow filled circles) for Ca (top), Sr (middle) and Ba (bottom) carbonates

Table S1: EOS parameters. Energy-volume data fittings using a Birch-Murnaghan third order equation. In order to obtain values easily comparable, B' was fixed in all cases to 4.0. Unit-cell volume is given per formula unit.

	<i>aragonite</i>			<i>post-aragonite</i>			<i>hexa1</i>			<i>hexa2</i>		
	Ca	Sr	Ba	Ca	Sr	Ba	Ca	Sr	Ba	Ca	Sr	Ba
V_0 (\AA^3)	59.28	67.52	79.07	56.82	63.14	72.88	58.80	65.59	75.83	60.35	67.58	78.56
B_0 (GPa)	64.7	52.2	41.4	67.8	62.2	54.5	62.7	55.0	46.4	57.8	49.9	41.2

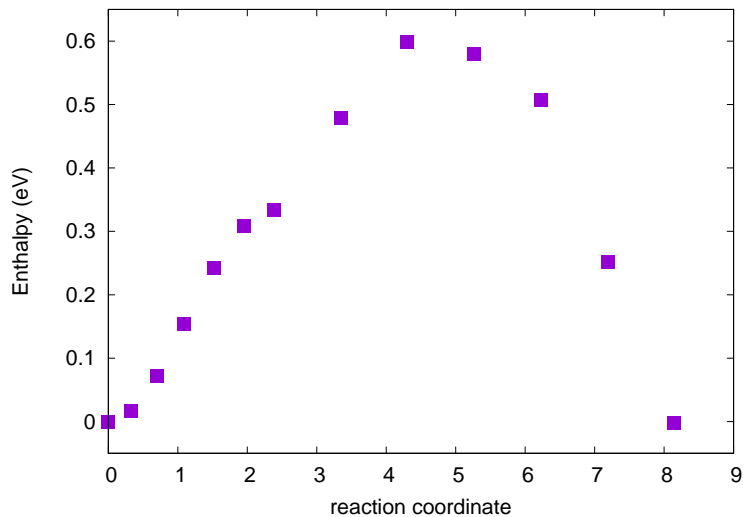


Figure S2: Enthalpy profile of CaCO_3 aragonite to post-aragonite transition obtained using NEB method

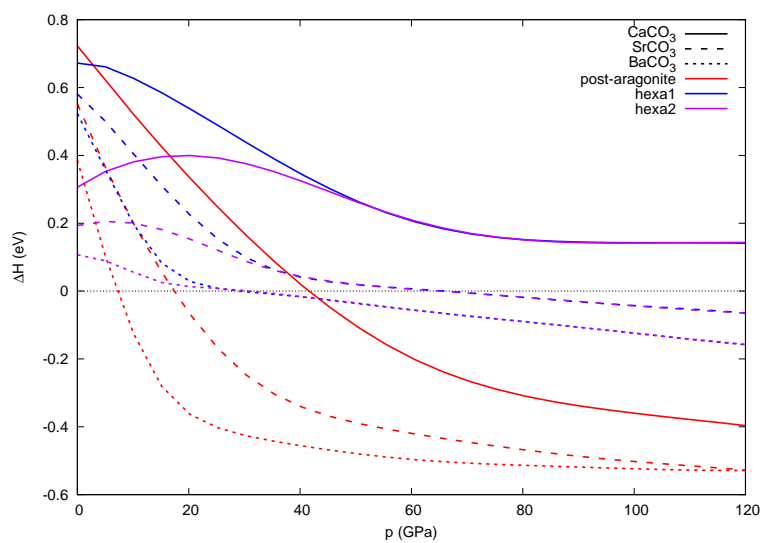


Figure S3: Enthalpy differences relative to the aragonite phase. Line segments joining calculated data points are plotted for greater clarity

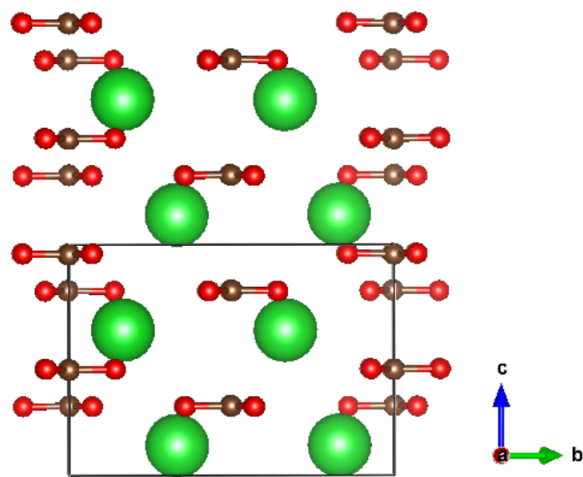


Figure S4: An example of structure for BaCO₃ with carbonate groups alternating *aragonite* and *hexa2* positions. Green, brown, and red balls stand for barium, carbon, and oxygen, respectively.