

Supporting information

$\text{Pb}_2[\text{C}_2\text{O}_6]-P\bar{3}m1$: New insight into high pressure behavior of
carbonates

Maksim V. Banaev ^{*1,2}, Dinara N. Sagatova ^{†1}, Nursultan E. Sagatov^{1,2}, and Pavel N.
Gavryushkin^{1,2}

¹*Sobolev Institute of Geology and Mineralogy, Siberian Branch of the Russian Academy
of Sciences, Novosibirsk, Russian Federation*

²*Novosibirsk State University, Novosibirsk, Russian Federation*

*Electronic address:banaev@igm.nsc.ru; Corresponding author

†Electronic address:d.sagatova1729@gmail.com; Corresponding author

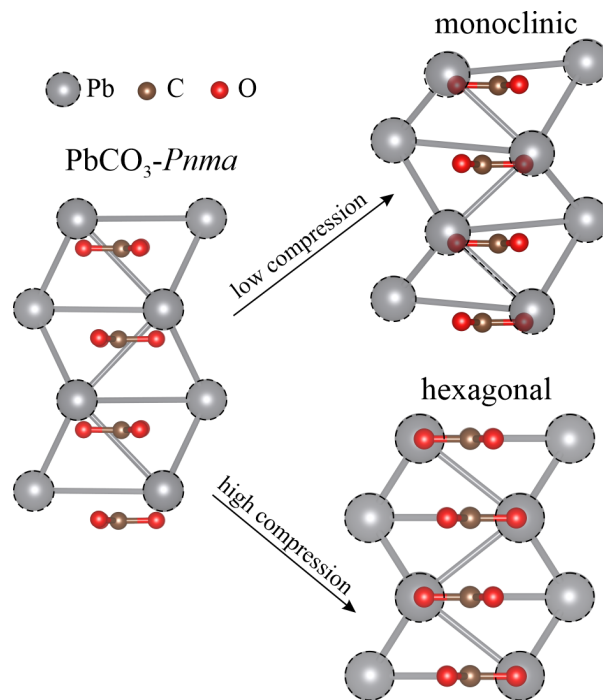


Figure S1: The results of two different compression schemes of PbCO_3 -*Pnma* to 40 GPa. The low compression is a gradual compression to 40 GPa in steps of 5 GPa, and the high compression is a sharp compression to 40 GPa.

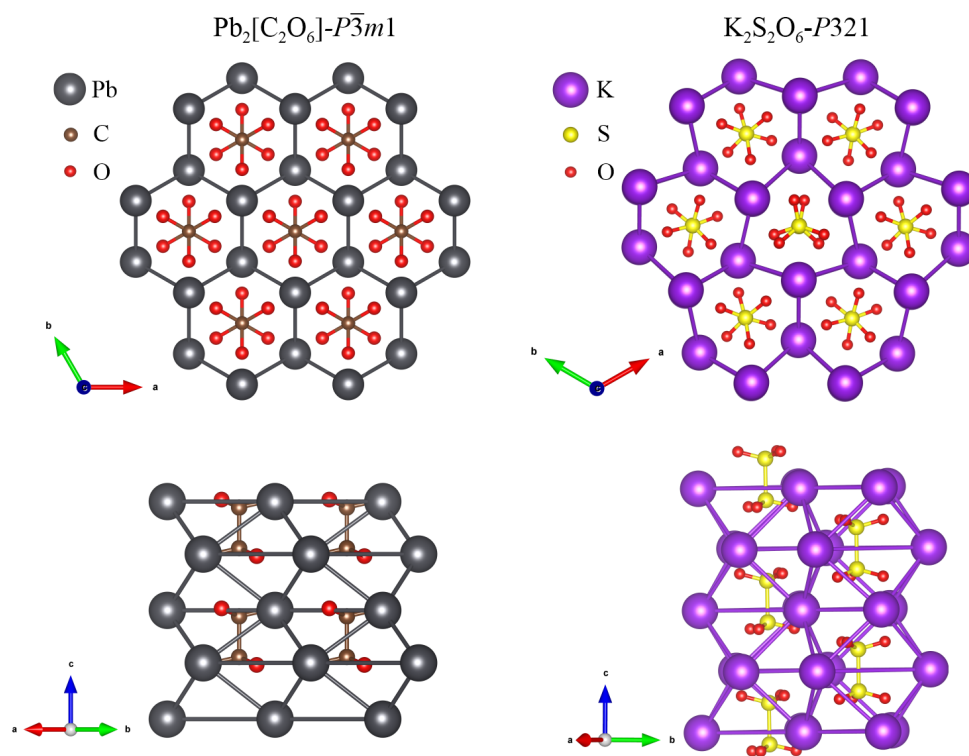


Figure S2: Comparison of the crystal structures of $\text{Pb}_2[\text{C}_2\text{O}_6]-P\bar{3}m1$ and $\text{K}_2\text{S}_2\text{O}_6-P321$.

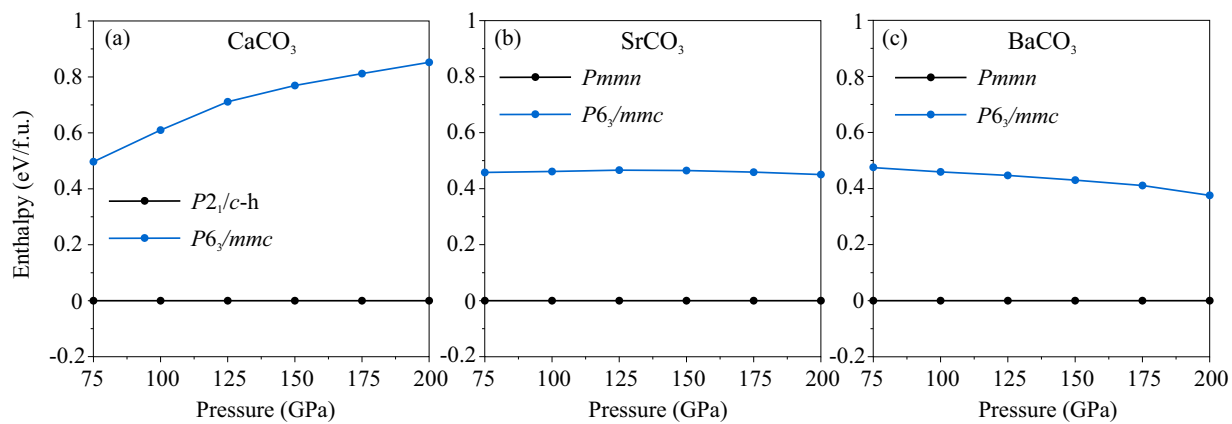


Figure S3: Relative enthalpy–pressure dependencies of CaCO_3 (a), SrCO_3 (b), and BaCO_3 (c).

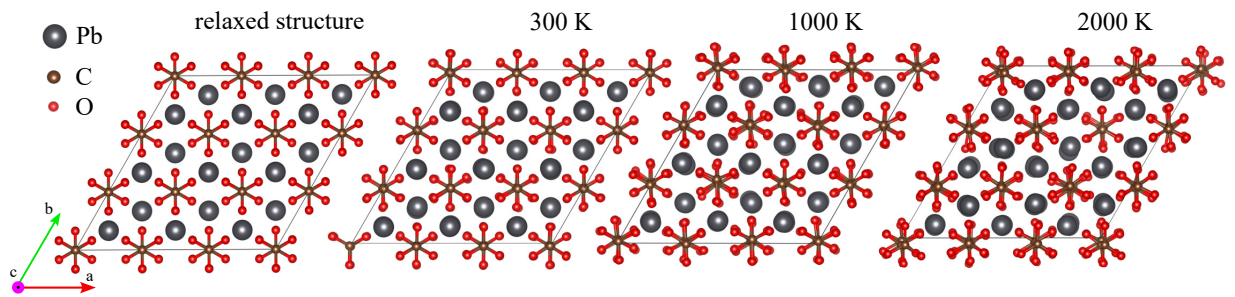


Figure S4: Optimized structure of $\text{Pb}_2[\text{C}_2\text{O}_6]-P\bar{3}m1$ and snapshots of the last step of MD calculations at 100 GPa and 300, 1000 and 2000 K.

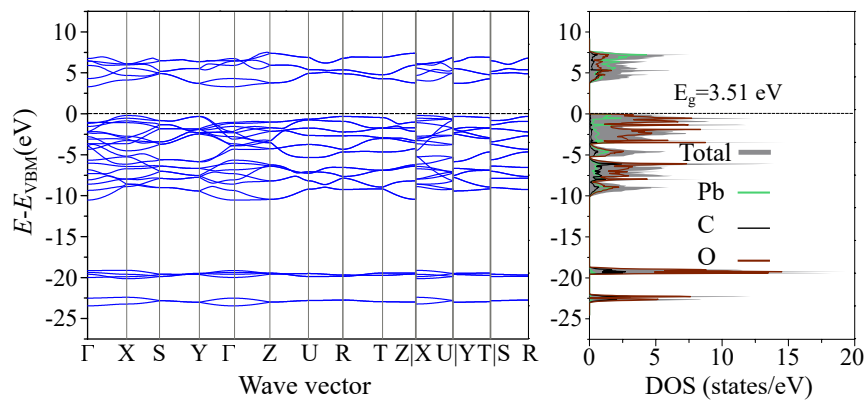


Figure S5: Band structure of PbCO_3-Pmmn at 30 GPa.

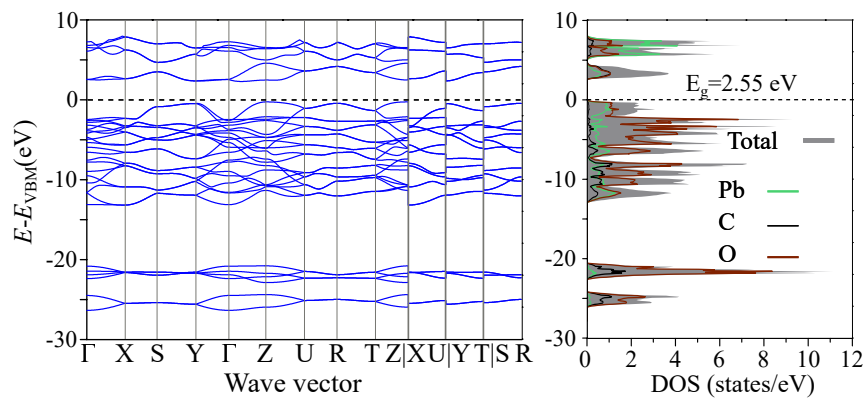


Figure S6: Band structure of PbCO_3-Pmmn at 100 GPa.