Supplementary Material

Density Functional investigation of the thermo-physical and thermo-chemical properties of $2M_1$ Muscovite

by Gianfranco Ulian and Giovanni Valdrè (American Mineralogist, 2015).

This document presents 3 supplementary figures and captions related to the above paper.
In separate documents we reported the CIF file of the $2M_1$-muscovite obtained by geometry optimization at the DFT/B3LYP-D* level of theory at different pressures (static conditions, 0 K), and Tables S1-S4 (xlsx format) related to the vibrational and thermochemical properties of muscovite.

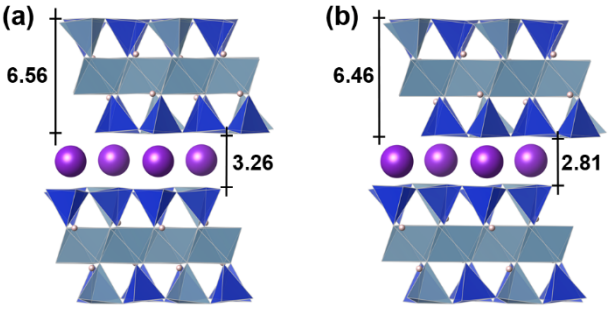

Figure S1.
[100] view of the structural deformations along [001] of Muscovite from (a) 0 GPa to (b) 10 GPa.

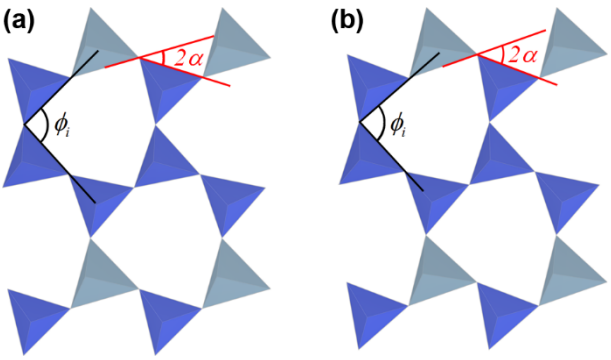

Figure S2.
Variations of tetrahedral rotation angle of Muscovite from (a) 0 GPa to (b) 10 GPa. (a) α = 13.2° and (b) α = 14.6°.

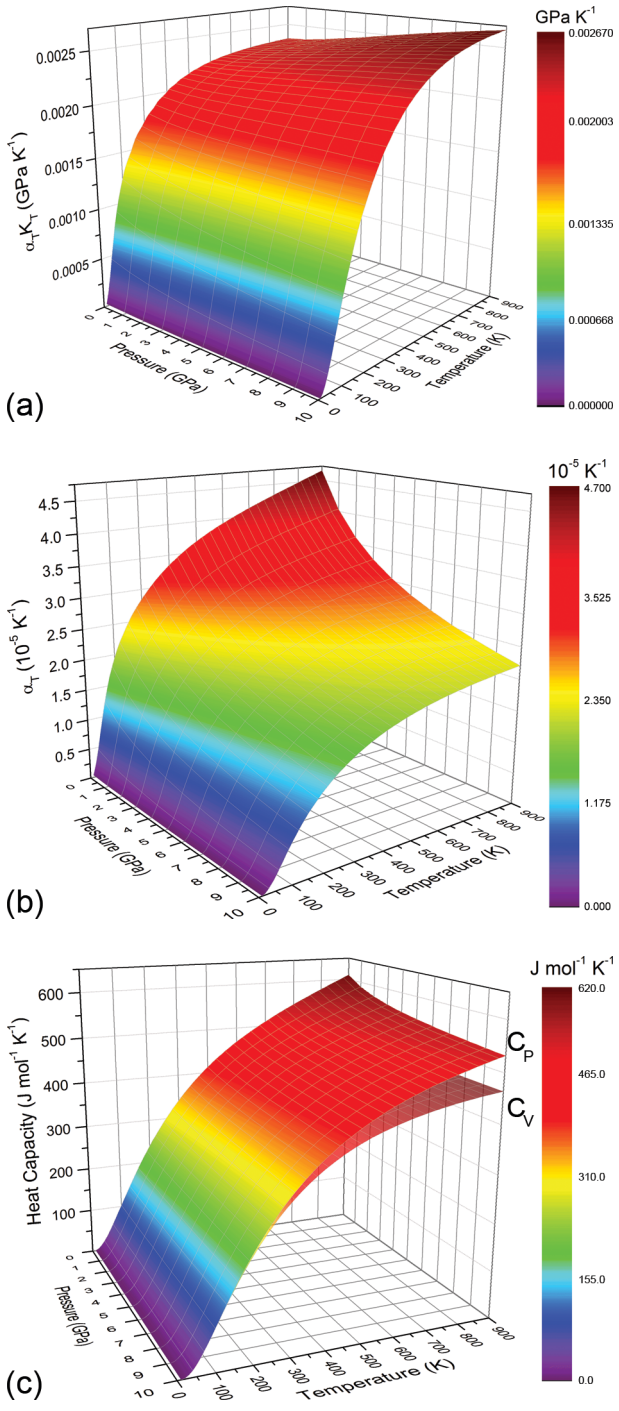

Figure S3.

Three-dimensional plots of $\alpha_T K_T$ product (a), thermal expansion coefficients (b) and (C_P, C_V) heat capacities (c), in the temperature range 10 – 900 K and pressure range 0 – 10 GPa.