High-pressure and high-temperature vibrational properties and anharmonicity of carbonate minerals up to 6 GPa and 500 ˚C by Raman spectroscopy

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Supplementary material

Figure S1. Evolution of frequencies and full width half maxima (FWHM) of bands of the ν_1 internal vibrational mode in aragonite-group carbonate minerals as a function of pressure.

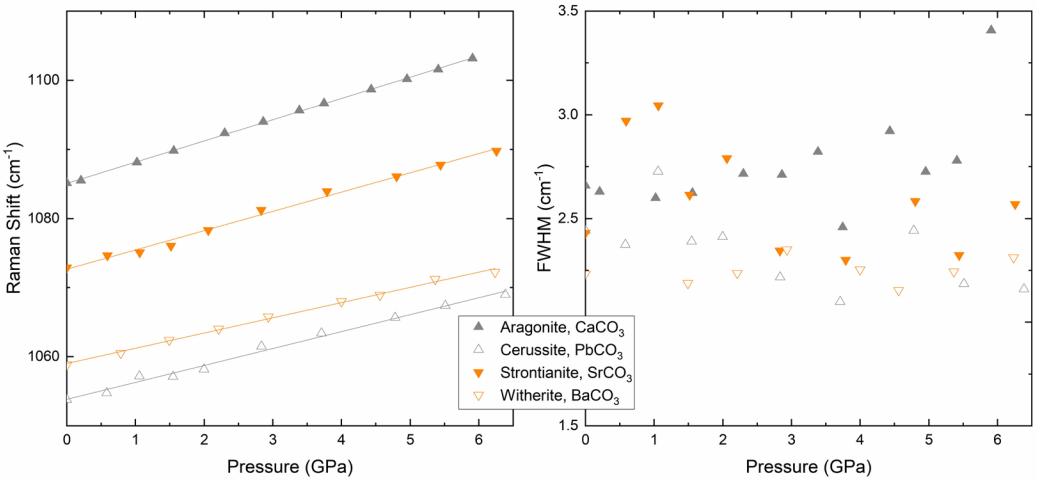

Figure S2. Evolution of frequencies and full width half maxima (FWHM) of bands of T and L external vibrational modes and ν_1 internal vibrational mode in calcite-group carbonate minerals as a function of pressure.

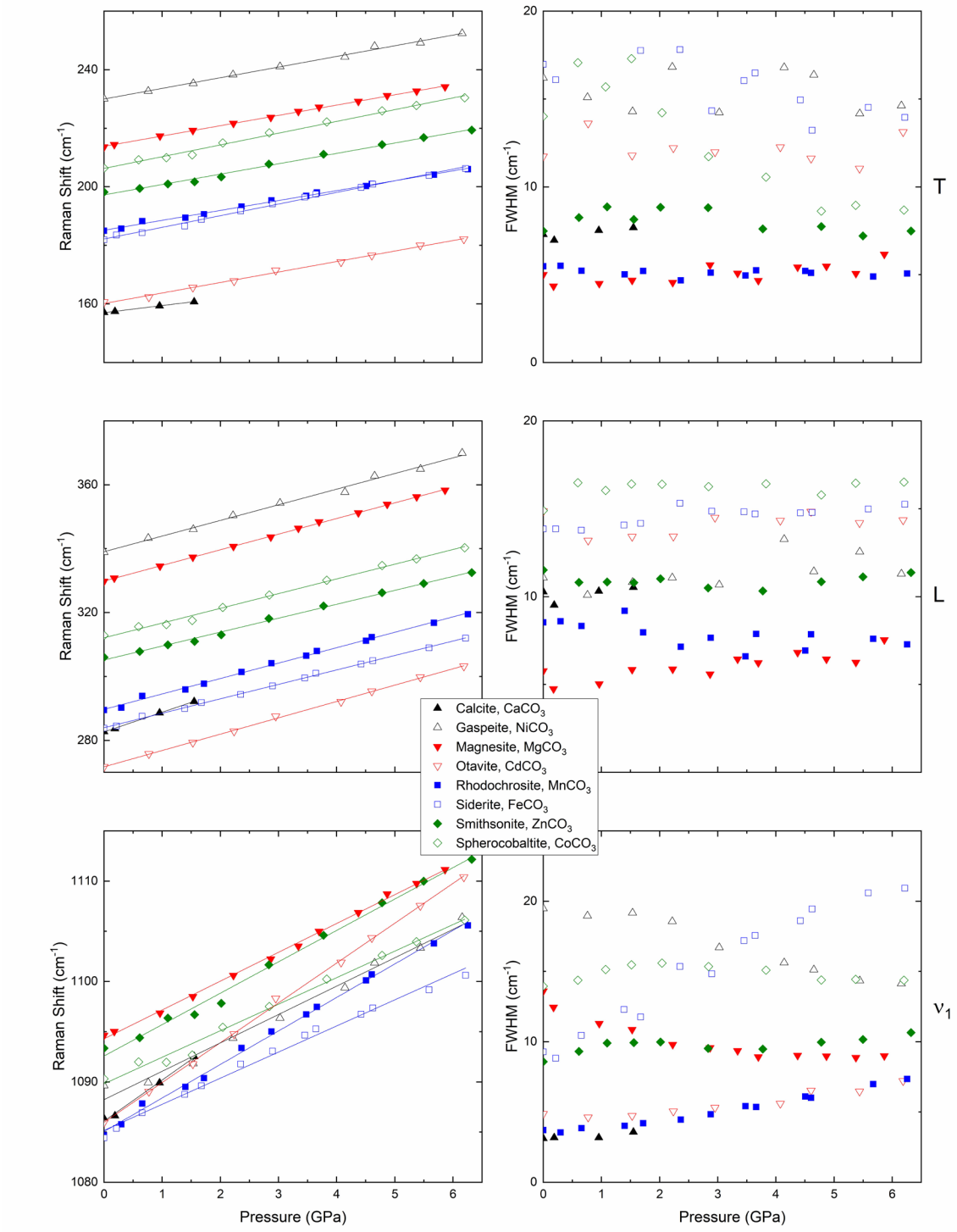

Figure S3. Evolution of frequencies and full width half maxima (FWHM) of bands of the ν_1 internal vibrational mode in aragonite-group carbonate minerals as a function of temperature.

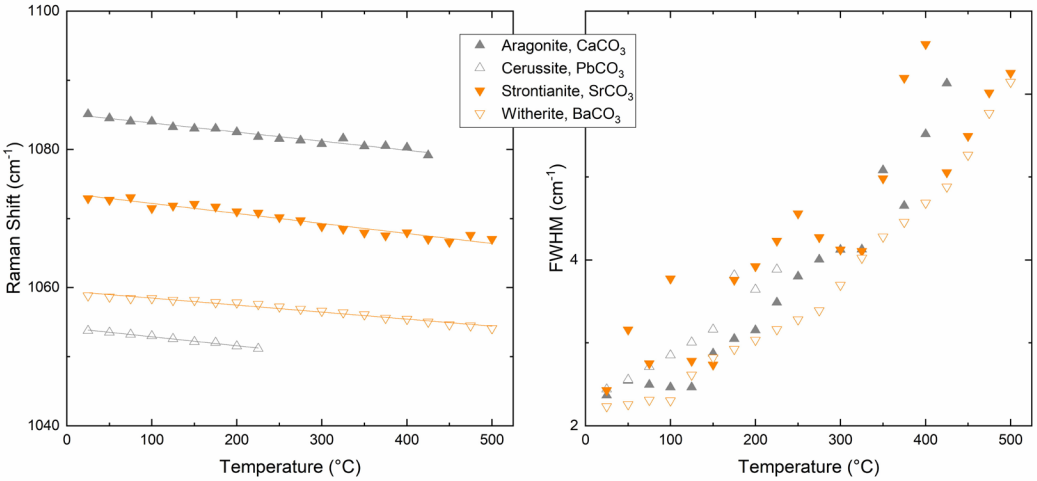

Figure S4. Phase transition of aragonite to calcite recorded by Raman spectra taken at 425 ˚C and 450 ˚C.

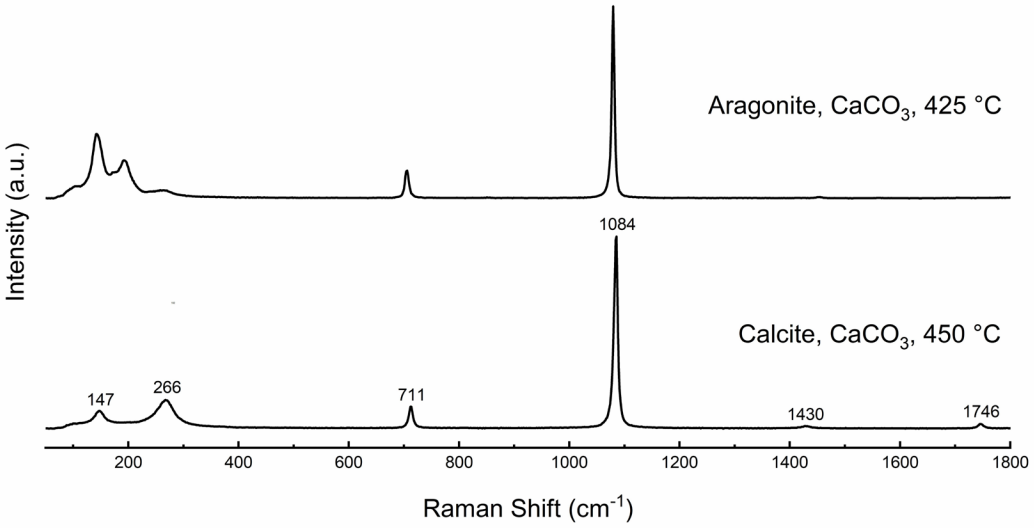

Figure S5. Thermal decomposition of cerussite recorded by Raman spectra taken at 225 ˚C and 250 ˚C.

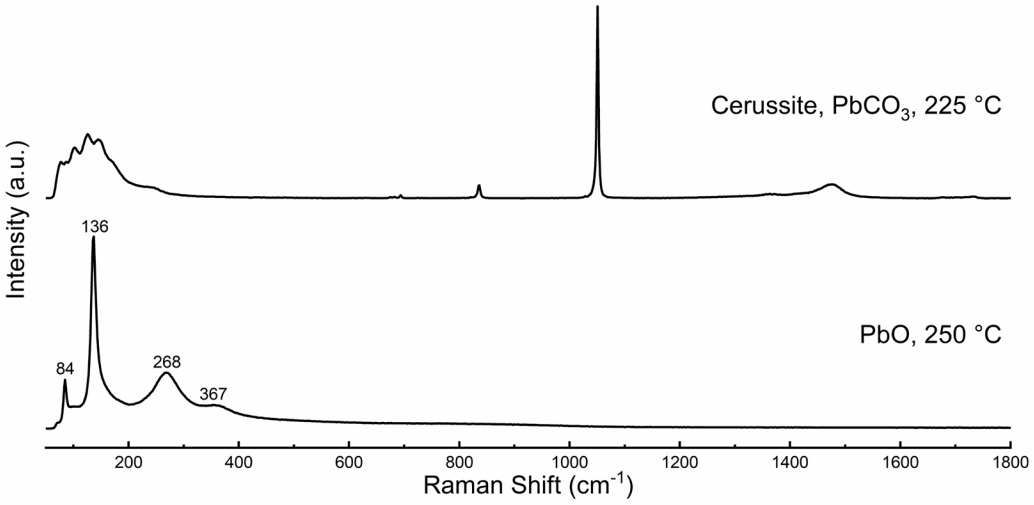

Figure S6. Evolution of frequencies and full width half maxima (FWHM) of bands of T and L external vibrational modes and ν_1 internal vibrational mode in calcite-group carbonate minerals as a function of temperature.

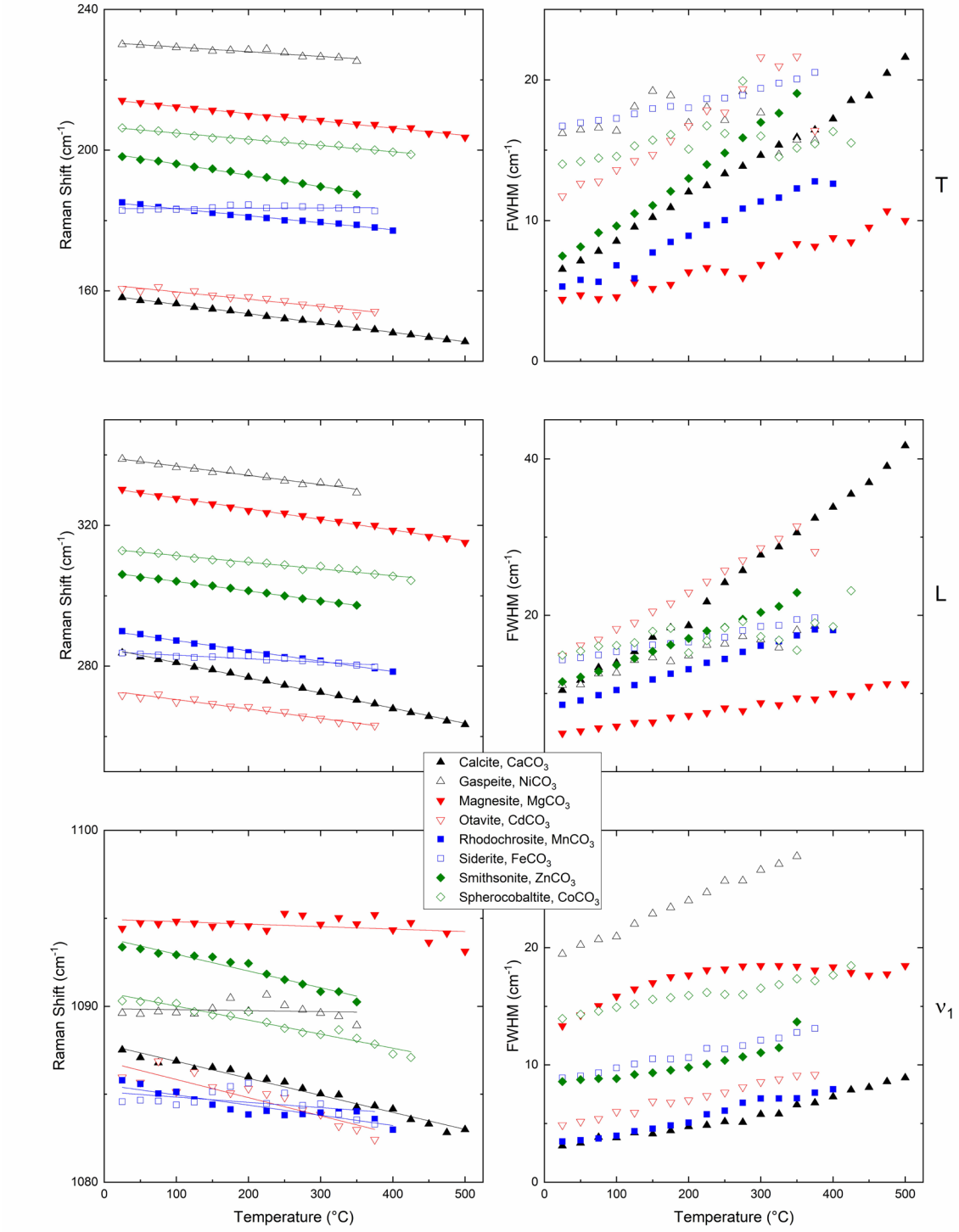

Figure S7. Thermal decomposition of gaspeite recorded by Raman spectra taken at 375 ˚C and 400 ˚C.

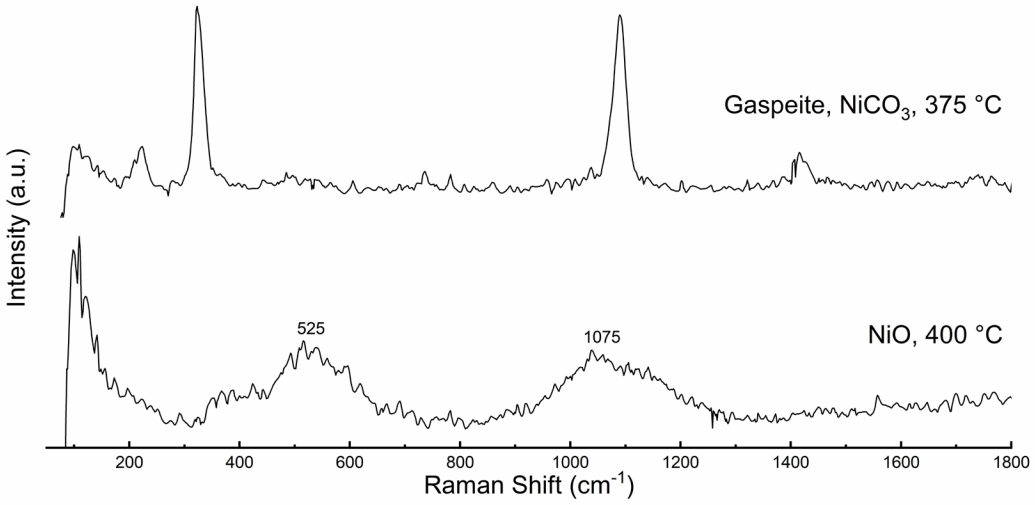

Figure S8. Thermal decomposition of smithsonite recorded by Raman spectra taken at 325 ˚C, 350 ˚C, 375 ˚C, and 400 ˚C.

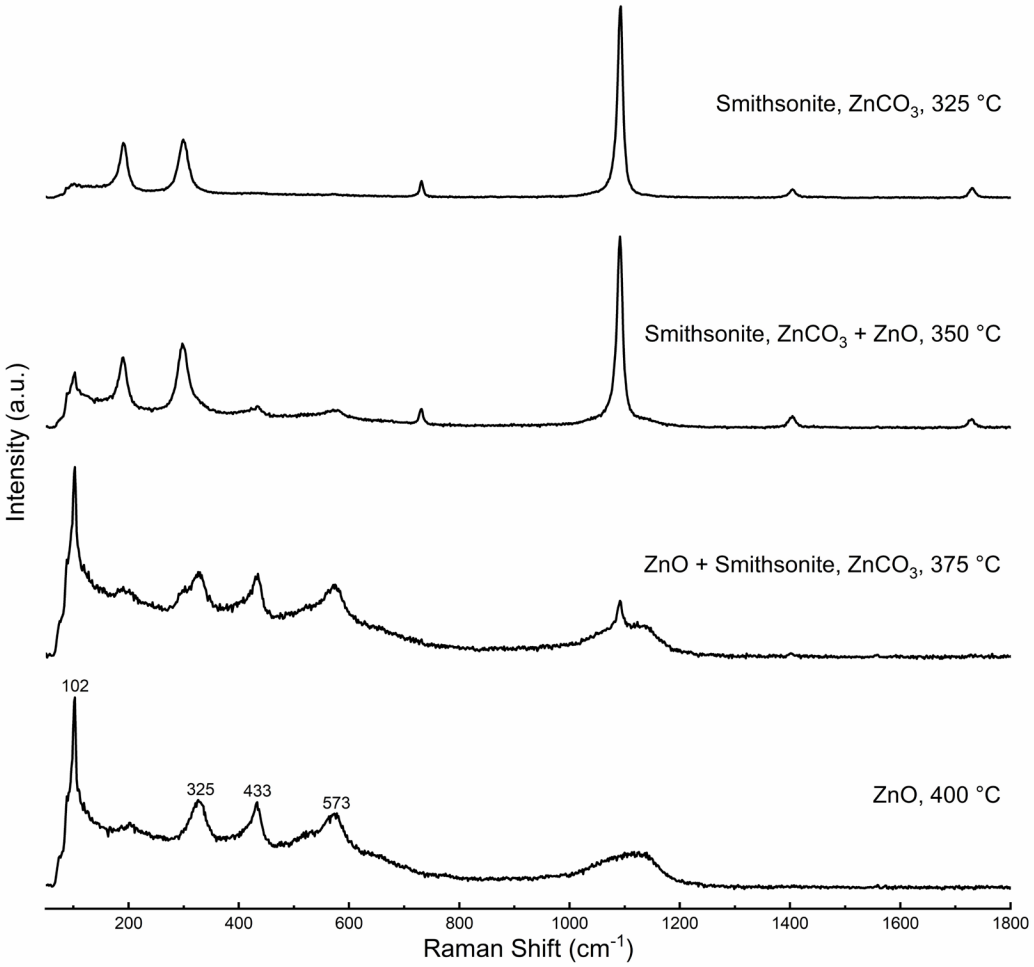

Figure S9. a) isobaric Grüneisen parameters (γ_{iP}), b) isothermal Grüneisen parameters (γ_{iT}), and c) intrinsic anharmonic parameters (a_i) of the Raman-active vibrational modes of aragonite-group carbonate minerals as a function of band frequencies.

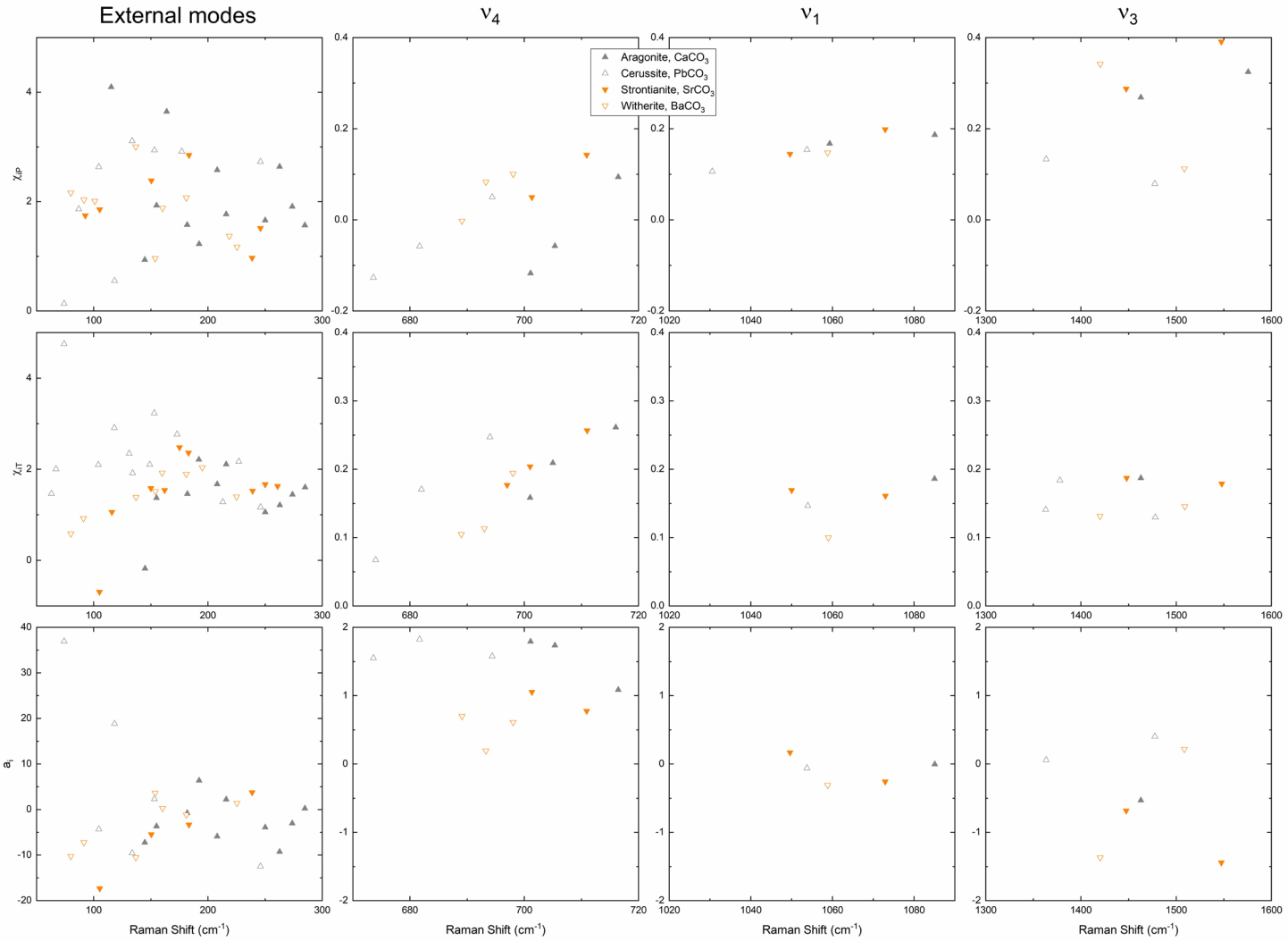

Figure S10. a) isobaric Grüneisen parameters (γ_{iP}), b) isothermal Grüneisen parameters (γ_{iT}), and c) intrinsic anharmonic parameters (a_i) of the Raman-active vibrational modes of calcite-group carbonate minerals as a function of band frequencies.