**Supplementary Information**

Study of the Structural, Vibrational and Thermodynamic Properties of Natroxalate Mineral Using

 Density Functional Theory

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**Appendix A.** Raman active normal modes of natroxalate.

**Figure A.1** The atomic motions associated to some Raman active vibrational normal mode of natroxalate.

Mode ν=1656 cm-1 –$ ν^{a}(CO)$ – Antisymmetric CO bond stretching.



Mode ν=1442 cm-1 – $ν^{a}\left(CC\right)+ ν^{s}\left(CO\right) $– Antisymmetric CC bond stretching plus symmetric CO bond stretching.



Mode ν=884 cm-1 – $ν^{s}\left(CC\right)+δ\left(OCO\right) $– Symmetric CC bond stretching plus OCO bending (scissoring).



Mode ν=876 cm-1 – $ϱ(C\_{2}O\_{4})$ – Oxalate fragment deformation. The motion involves a CC bond rotation (C atoms move perpendicularly to oxalate plane but in opposite directions).



Mode ν=578 cm-1 – $ϱ(C\_{2}O\_{4})$ – Oxalate fragment deformation. The motion involves a CC bond rotation (C atoms move within oxalate plane but in opposite directions).



Mode ν=471 cm-1– $T^{ip}\left(CO\_{2}\right)$ – CO2 translation within the oxalate plane. The two CO2 groups of C2O4 fragment nearly translate in opposite directions within the oxalate plane.



Mode ν=235 cm-1– $T^{op}\left(CO\_{2}\right)$ – CO2 translation out of the oxalate plane. The two CO2 groups of C2O4 fragment nearly translate in opposite directions perpendicular to the oxalate plane.



Mode ν=152 cm-1– $t(OCO)$ – OCO twisting.



Mode ν=126 cm-1– $t(OCO)$ – OCO twisting.

