**Supplementary Information**

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

Density Functional Theory

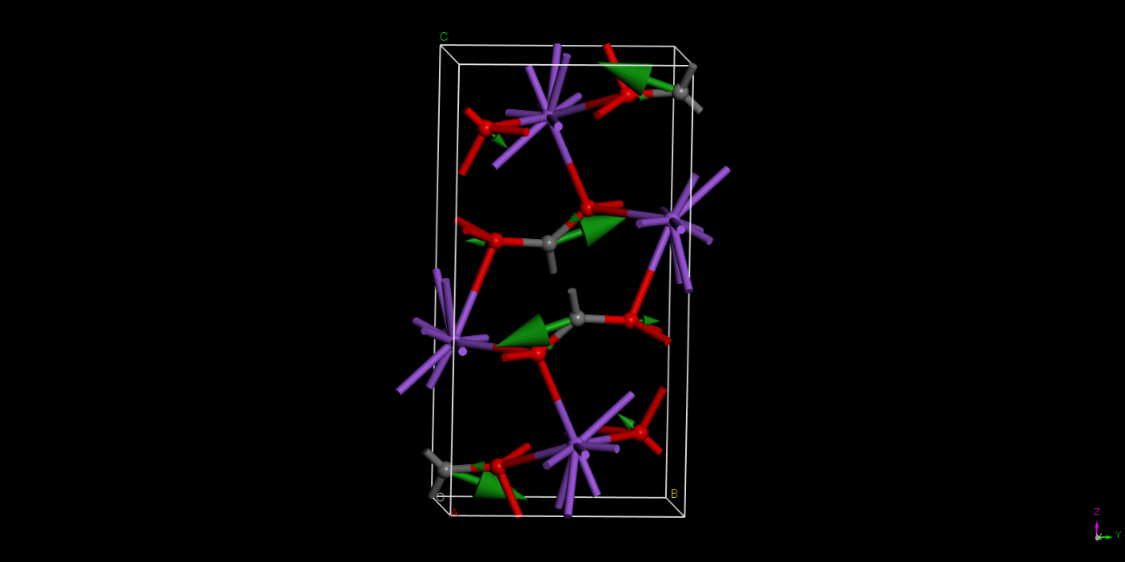
Francisco Colmenero and Vicente Timón

*Instituto de Estructura de la Materia, CSIC. C/ Serrano, 113. 28006 Madrid, Spain*

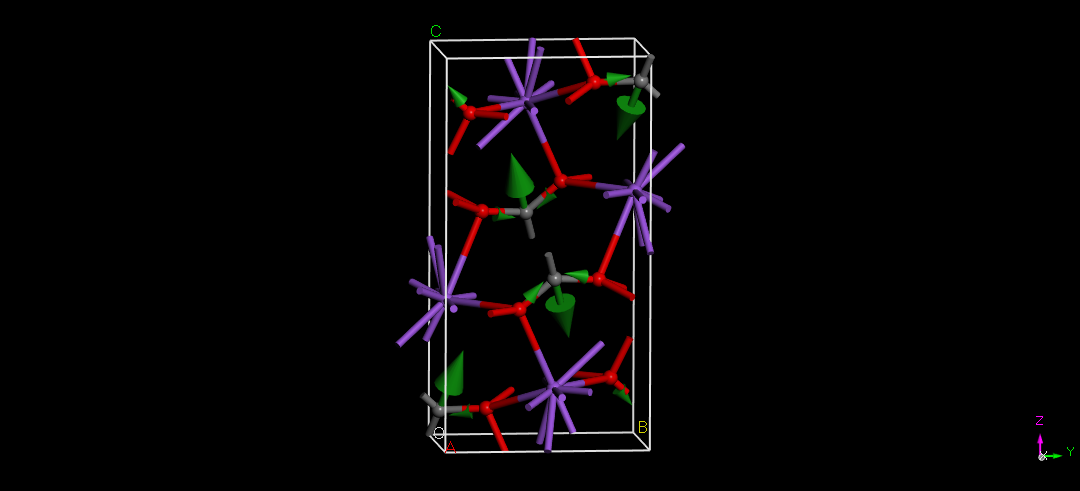
**Appendix A.** Raman active normal modes of natroxalate.

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

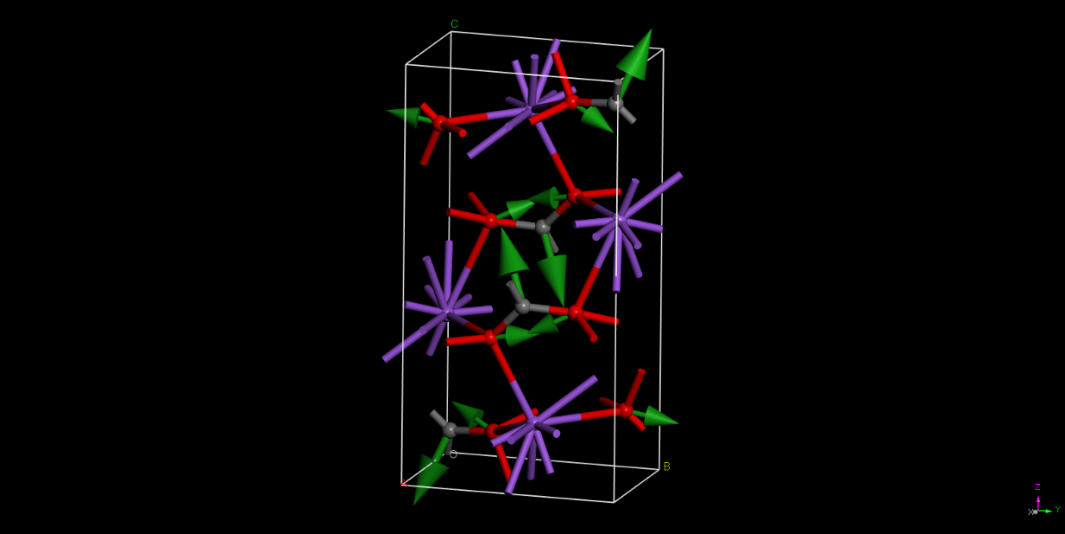
Mode ν=1656 cm-1 – – Antisymmetric CO bond stretching.



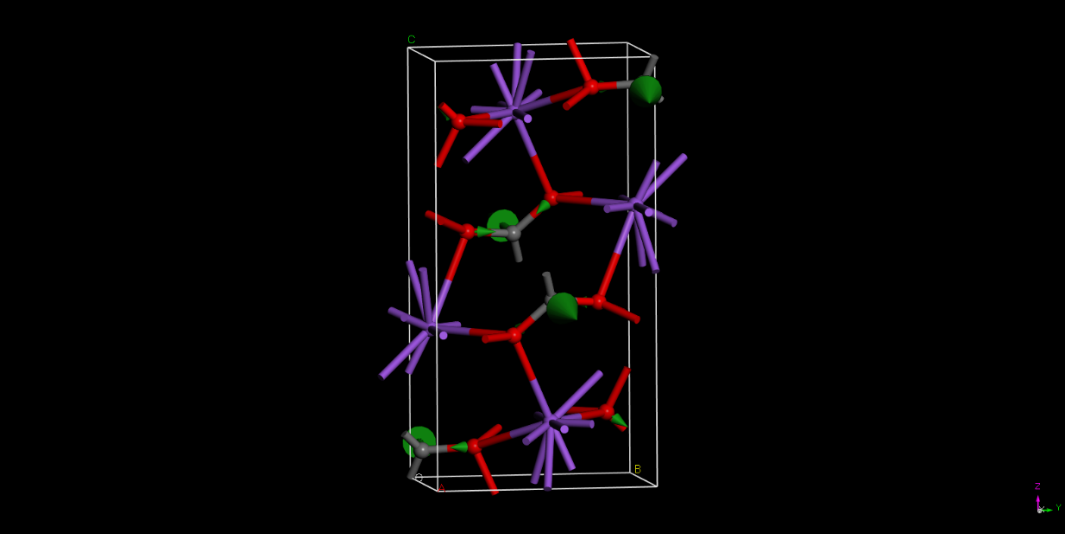
Mode ν=1442 cm-1 – – Antisymmetric CC bond stretching plus symmetric CO bond stretching.



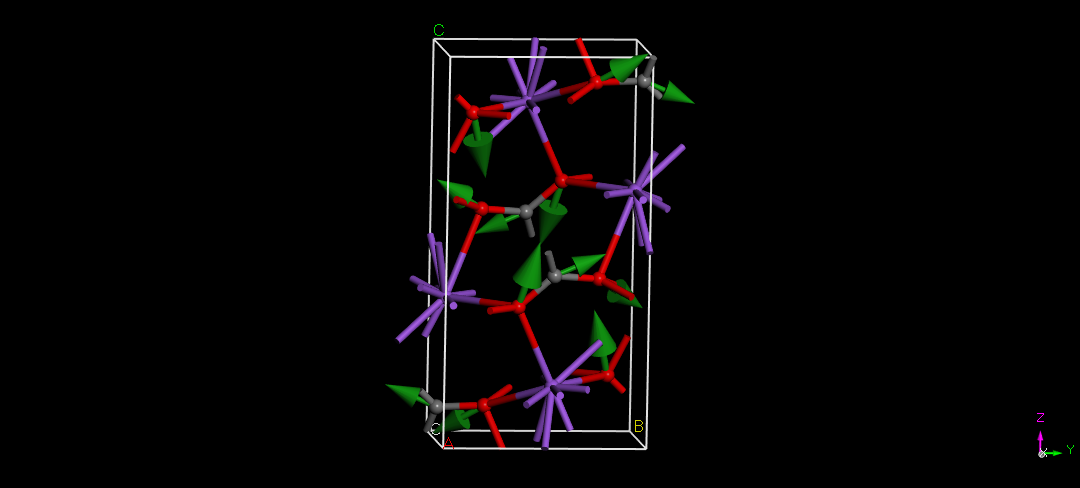
Mode ν=884 cm-1 – – Symmetric CC bond stretching plus OCO bending (scissoring).



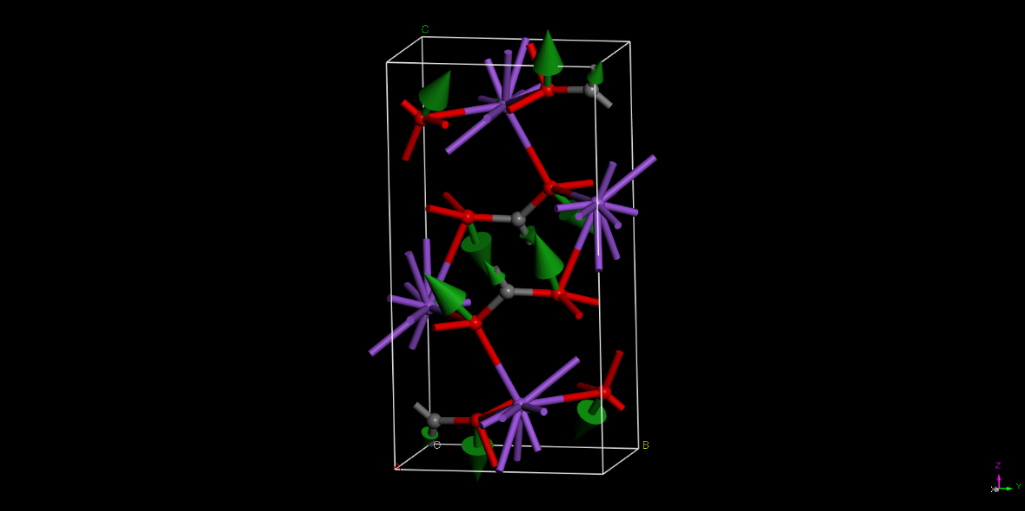
Mode ν=876 cm-1 – – Oxalate fragment deformation. The motion involves a CC bond rotation (C atoms move perpendicularly to oxalate plane but in opposite directions).



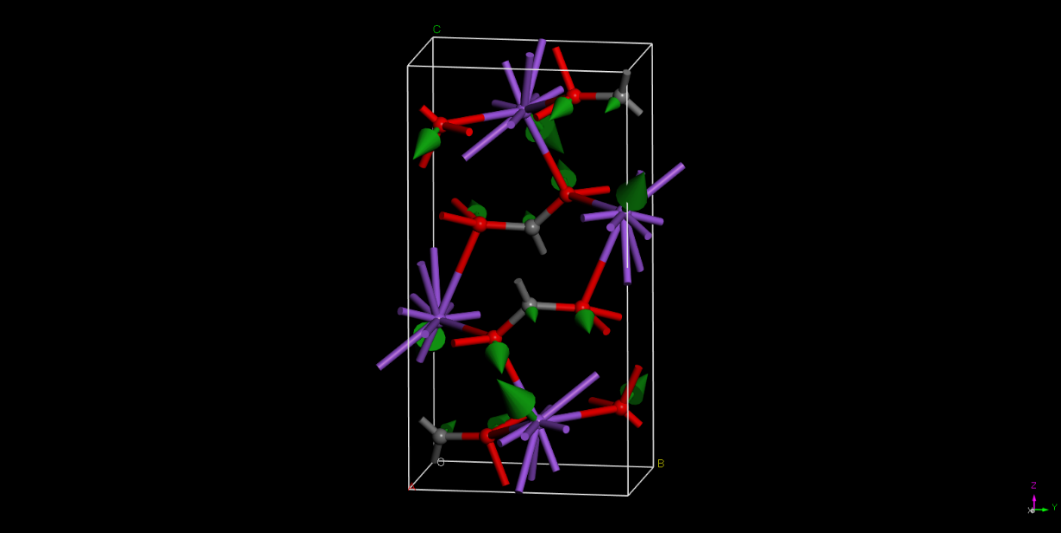
Mode ν=578 cm-1 – – Oxalate fragment deformation. The motion involves a CC bond rotation (C atoms move within oxalate plane but in opposite directions).



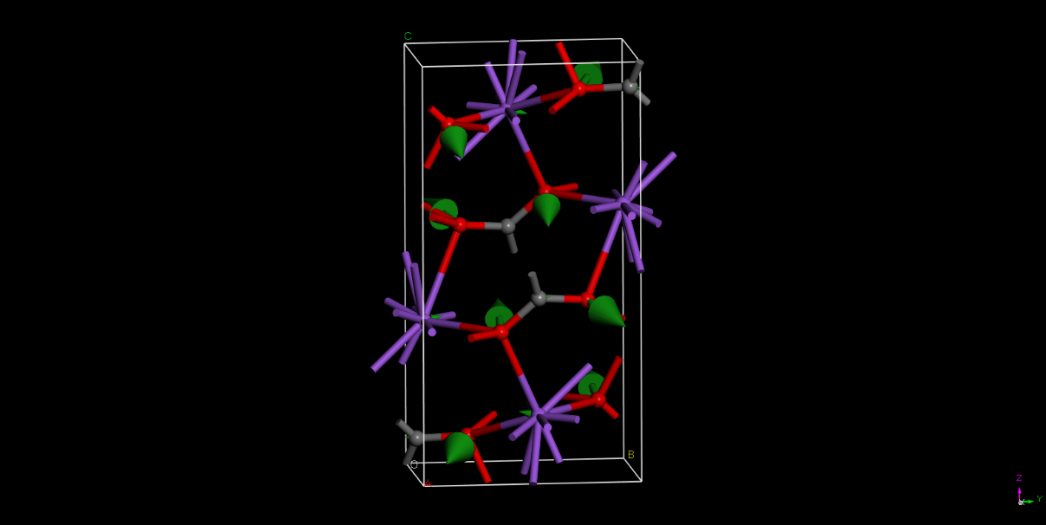
Mode ν=471 cm-1– – CO2 translation within the oxalate plane. The two CO2 groups of C2O4 fragment nearly translate in opposite directions within the oxalate plane.



Mode ν=235 cm-1– – 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– – OCO twisting.



Mode ν=126 cm-1– – OCO twisting.

