

## MS17-P01 | SYMMETRY LOWERING IN NATROCHALCITE $\text{NaCu}_2(\text{H}_3\text{O}_2)(\text{SO}_4)_2$ UNDER PRESSURE.

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Natrochalcite compounds, currently discussed as an anode material for Li-/Na-ion batteries [1], exhibit hydrogen-bond lengths that are among hydrogen-bearing solids some of the shortest ones reported so far [2]. Furthermore, at high-pressure the formation of an extremely short single-well no-barrier hydrogen bond is possible.

At ambient pressure the space group of natrochalcite is  $C2/m$  [3]. The XRD measurements performed between 0.4 and 10 GPa showed the Bravais lattice centering to remain and the continuous decrease of the hydrogen bonds, respectively their O...O distances. However, the Raman spectra show clear changes in the  $\text{SO}_4$  bending region. Furthermore, all the oxygen atoms of the  $\text{SO}_4$ -tetrahedron clearly show higher isotropic displacement parameters compared to the only oxygen not involved in this polyhedron. The acceptor oxygen for the longer hydrogen bond, shrinks about  $0.18(2)$  Å until 10 GPa and shows the strongest displacement starting at ambient pressure up to 10 GPa, when refined in  $C2/m$ .

Since all the oxygens of the  $\text{SO}_4$ -tetrahedron are shared with Na-polyhedra it is very likely that at least for these polyhedra the symmetry is lowered above 2 GPa. Due to the preserved C-centering only two space groups are reasonable then,  $Cm$  and  $C2$ .

[1] Liu Z., Zhou H., Ang S. S., Zhang J.-J., (2016) *Electrochim. Acta*, **211**, 619-626.

[2] Krickl R., Wildner M., (2007) *Eur. J. Mineral.*, **19**, 805-816.

[3] Giester G., Zemann J. (1987) *Z. Kristallogr.*, **179**, 431-442