

MS14-P08 | COMPARATIVE CRYSTAL CHEMISTRY OF THE SOLID SOLUTION SYSTEMS BETWEEN KIESERITE (MgSO₄·H₂O) AND TRANSITION METAL KIESERITE-TYPE COMPOUNDS (M²⁺SO₄·H₂O; M²⁺ = (Mn, Fe, Co, Ni, Zn))

Wildner, Manfred (Institut für Mineralogie und Kristallographie, Wien, AUT); Talla, Dominik (University of Vienna, Vienna, AUT)

The extensive presence of low-hydrated sulfates, e.g. kieserite (MgSO₄·H₂O), on the surface of Mars and probably also on icy moons of Jupiter and Saturn has gained much attention during the past 40 years. Given the local abundance of cosmochemically relevant transition metals (TM), the actual composition of extraterrestrial kieserite likely differs from its ideal formula. Hence, the confirmation and characterisation of continuous solid solutions between kieserite and the isotypic 3dTM-compounds is crucial for interpretation of data from orbiter and rover space missions.

We have synthesized and structurally characterized the solid solution series between kieserite and the 3dTM-sulfate monohydrates of Mn, Fe, Ni, Zn and previously Co [1]. All these systems form continuous solid solutions with linear Vegard-type behaviour of lattice and structural parameters. Nonetheless, it appeared that kieserite itself shows crystal chemical peculiarities compared to the 3dTM-compounds, which do not follow simple expectations deduced from the different M²⁺ ionic radii: Mg-dominant phases show clearly expanded bond angles at polyhedra-linking oxygens, leading to larger cell volumes than expected.

We attribute this to the absence of 3d orbitals in Mg, in contrast to their presence in the TM-compounds, leading to anisotropy of the electron density around the TM cations and affecting the bond critical point r_c along the M–O bond path [2]. This influences the electron density at the oxygen atoms and hence the second coordination sphere.

[1] Bechtold A, Wildner M (2016) *Eur J Mineralogy* 28, 43–52

[2] Bader RFW (1998) *Encyclopedia Comput Chem* 1, 64–86