MS14-P05 | SYNTHESIS AND CRYSTAL STRUCTURES OF $Zr_2(OH)_2(XO_4)_3{\cdot}4H_2O$ (X=S,Se) AND $Zr(SeO_3)_2$

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In the course of a study on the crystal chemistry of zirconium oxysalts synthesized at low-hydrothermal conditions [1-3] we also prepared the title compounds from $Zr_2O_2(CO_3)(OH)_2$, the respective acids and minor contents of water.

The $Zr_2(OH)_2(XO_4)_3{\cdot}4H_2O$ (*X*=S,Se) salts crystallize isotypic in space group *C*2/*c*, the structure of the sulfate has been described earlier [4]. The present single crystal X-ray data allowed high-quality refinements disclosing the hydrogen bonding system and its role in the framework structure of $Zr^{[8]}{}_2O_{14}$ dimers and XO_4 groups.

For $Zr(SeO_3)_2$, only a microcrystalline precipitate could be extracted so far, hence X-ray powder data were measured on a Bruker D8eco system. A previous description [5] in *Pmmm* (*a*=8.555, *b*=6.479, *c*=15.232 Å) resulted in several unindexed main peaks. The new cell is re-indexed in $P2_1/c$ with *a*=4.9724(3), *b*=8.5992(5), *c*=6.9447(3) Å, *β*=110.128(3)°. The structure obtained from our Rietveld refinement proves isotypism with other $M^{4+}(SeO_3)_2$ compounds, i.e. $Ti(SeO_3)_2$, β-$Sn(SeO_3)_2$ and $Pb(SeO_3)_2$ [6,7]. The $Zr^{[6]}$–O (2.031–2.083 Å) and Se–O (1.710–1.718 Å) bond lengths are in good agreement with values from literature.

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