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Crystal and Molecular Structures of Alkali Oxalates - First Proof of a Staggered Oxalate Anion in the Solid State

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Beamline: X3B1

Introduction: The molecular and crystal structures of solvent free potassium, rubidium, and cesium oxalates have been determined *ab initio* from high resolution synchrotron (X3B1, NSLS) and x-ray laboratory powder patterns.

Results: In case of potassium oxalate $K_2C_2O_4$, the oxalate anion is planar (*a*= 10.91176(7) Å, *b*= 6.11592(4) Å, *c*= 3.44003(2) Å, orthorhombic, *Pbam*, Z = 2; Fig. 1), whereas in cesium oxalate $Cs_2C_2O_4$ (*a*= 6.62146(5) Å, *b*= 11.00379(9) Å, *c*= 8.61253(7) Å, β= 97.1388(4)°, monoclinic, $P2_1/c$, Z = 4; Fig. 2) it shows a staggered conformation (Fig. 3). For rubidium oxalate at room temperature, two polymorphs exist, one (β-$Rb_2C_2O_4$) isotypic to potassium oxalate (*a*= 11.28797(7) Å, *b*= 6.29475(4) Å, *c*= 3.62210(2) Å, orthorhombic, *Pbam*, Z = 2) and the other (α-$Rb_2C_2O_4$) isotypic to cesium oxalate (*a*= 6.3276(1) Å, *b*= 10.4548(2) Å, *c*= 8.2174(2) Å, β= 98.016(1)°, monoclinic, $P2_1/c$, Z = 4). The potassium oxalate structure can be deduced from the AlB_2 type, whereas the cesium oxalate structure from that of $Hg_{99}As$.

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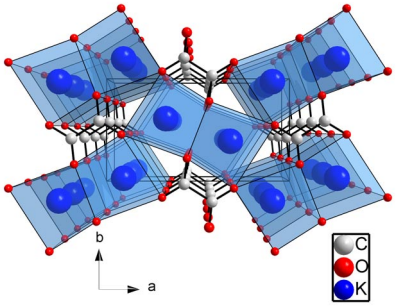

Fig. 1: Crystal structure of $K_2C_2O_4$ in a view along *c*-axis at ambient conditions.

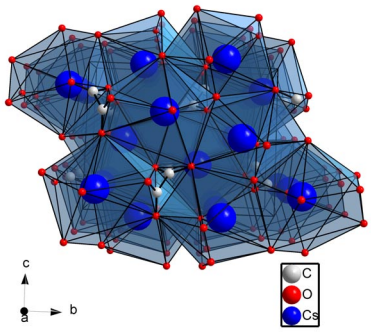

Fig. 2: Crystal structure of $Cs_2C_2O_4$ in a view along *c*-axis at ambient conditions.

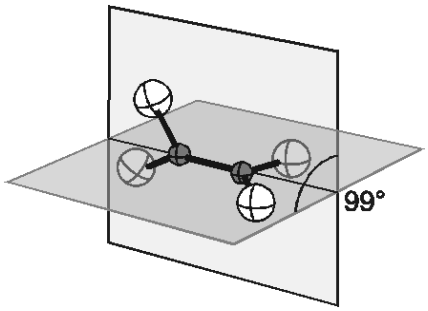

Fig. 3: Scetch of the oxalate ion as found in $Cs_2C_2O_4$.