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David H. Templeton

January 1960

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In reporting the structure of zirconium sulfate tetrahydrate, Singer and Cromer (1959) suggested a configuration for the hydrogen bonds which placed a hydrogen atom between two oxygen atoms in the same coordination polyhedron of zirconium. It is expected that a water molecule coordinated to a cation will have its hydrogen atoms on the side away from the cation. In several hydrated sulfates, e.g., $\text{NiSO}_4 \cdot 6 \text{H}_2\text{O}$ (Beever and Lipson, 1932), $\text{NiSO}_4 \cdot 7 \text{H}_2\text{O}$ (Beever and Schwartz, 1935), $\text{CuSO}_4 \cdot 5 \text{H}_2\text{O}$ (Beever and Lipson, 1934), and $\text{KAl}(\text{SO}_4)_2 \cdot 12 \text{H}_2\text{O}$ (Lipson and Beever, 1935), there are just enough short oxygen-oxygen distances to account for all of the hydrogen bonds, if one excludes from consideration the short distances between oxygen atoms in the same coordination polyhedron or in the same sulfate group.

An examination of the structure of $\text{Zr}(\text{SO}_4)_2 \cdot 4 \text{H}_2\text{O}$, as reported by Singer and Cromer (1959), reveals a more plausible assignment. Each water oxygen, O_3 , has four close neighbors in the same square antiprism, O_2 at 2.53, 2.62, and 2.86 Å and O_3 at 2.72 Å. It has three other neighbors, O_1 at 2.69, 2.75, and 2.93 Å. It is reasonable to assign the hydrogen bonds to the 2.69 and 2.75 Å distances. The angle between these two bonds is 88° , and the bisector of this angle, within experimental error, is 180° from the line from O_3 to zirconium.

Beever, C. A. and Lipson, H. (1932). Z. Krist. 83, 123.

Beever, C. A. and Lipson, H. (1934). Proc. Roy. Soc. London A146, 570.

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Singer, J. and Cromer, D. T. (1959). Acta Cryst. 12, 719.

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