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**Hydrogen bonding in zirconium sulfate tetrahydrate.\*** By DAVID H. TEMPLETON, *Department of Chemistry and Lawrence Radiation Laboratory, University of California, Berkeley, California, U.S.A.*

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In reporting the structure of zirconium sulfate tetrahydrate, Singer & 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.,  $\text{NiSO}_4 \cdot 6\text{H}_2\text{O}$  (Beevers & Lipson, 1932),  $\text{NiSO}_4 \cdot 7\text{H}_2\text{O}$  (Beevers & Schwartz, 1935),  $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$  (Beevers & Lipson, 1934), and  $\text{KAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$  (Lipson & Beevers, 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 & Cromer (1959), reveals a more plausible assignment. Each water oxygen,  $\text{O}_3$ , has four close neighbors in the same square antiprism,  $\text{O}_2$  at 2.53, 2.62, and 2.86 Å and  $\text{O}_3$  at 2.72 Å. It has three

other neighbors,  $\text{O}_1$  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  $88^\circ$ , and the bisector of this angle, within experimental error, is  $180^\circ$  from the line from  $\text{O}_3$  to Zr.

#### References

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