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COMMENTS ON THE ORIENTATION OF THE PROTON-PROTON
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July 1963

Comments on the Orientation of the Proton-Proton Vectors
of Water in Tutton's Salts*

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From proton magnetic resonance data Chidambaram and Rao¹ determined the orientation of the $p-p$ vectors of water molecules in two Tutton's salts and concluded that the results were inconsistent with the crystal structure determined by Hofmann.² At almost the same time a redetermination of the crystal structure by x-ray diffraction in our laboratory³ revealed serious errors in the oxygen coordinates given by Hofmann. This x-ray study also gave coordinates for the hydrogen atoms.

The orientations of the $p-p$ vectors determined by the two methods are in excellent agreement. To facilitate the comparison, we have calculated the angles ϕ_0 and δ (notation of Chidambaram and Rao¹) from the hydrogen coordinates determined in the x-ray work and list them with the other values in Table I. Corresponding angles are expected to be nearly the same in the three salts, and in no case is there any significant difference. Each of the water protons is involved in a normal hydrogen bond, as described for $(NH_4)_2Mg(SO_4) \cdot 6H_2O$ by Margulis and Templeton.³

TABLE I. Orientation of proton-proton vectors.

Salt	K-Zn ^a	K-Mg ^a	NH ₄ -Mg ^b
Method	p-m-r	p-m-r	x-ray
$(\underline{p}-\underline{p})_1$ ^c	113 ± 2°	115 ± 2°	115 ± 6°
0_8 ^d			
$(\underline{p}-\underline{p})_2$	172 ± 5°	170 ± 5°	177 ± 7°
0_9			
$(\underline{p}-\underline{p})_3$	20 ± 2°	18 ± 5°	21 ± 9°
0_7			

^aRef. 1. ^bRef. 3. ^cNotation of Ref. 1. ^dNotation of Ref. 3.

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¹R. Chidambaram and C. R. Rao, J. Chem. Phys. 38, 210 (1963).

²W. Hofmann, Z. Krist. 76, 279 (1931).

³T. N. Margulis and D. H. Templeton, Z. Krist. 117, 344 (1962).

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