

served resonance spectrum to a theoretical lineshape function first given by Pake (1948). This technique has recently been utilized and described in detail by Pedersen (1968).

The shape of the first derivative of the absorption spectrum is given by

$$F(h) = \int_{-\infty}^{\infty} (h-h')[g(h')+f(h')] \exp[-(h-h')^2/2\beta^2] dh' \quad (1)$$

where $g(h')$ is given by $(1-h'/\alpha)^{-1/2}$ in its non-zero range from -2α to $+\alpha$ and $f(h')$ is given by $(1+h'/\alpha)^{-1/2}$ in its non-zero range from $-\alpha$ to $+2\alpha$. The variable parameters to be determined are α and β where

$$\alpha = \frac{3\mu}{2R^3} \quad (2)$$

and

$$\beta^2 = \frac{9}{5} \mu^2 \sum_i r_i^{-6} + \frac{4}{15} \sum_k \mu_k^2 \frac{I_{k+1}}{I_k} r_k^{-6}. \quad (3)$$

Here μ is the magnetic moment of the proton, R is the H-H distance, r_i is the internuclear distance between any two protons not in the same pair and, r_k is the distance between one proton and any other nucleus in the structure carrying a magnetic moment μ_k and spin I_k . The above definitions of α and β assume the absence of significant molecular motion such as 180° flips of the water molecules.

Four of the many resonance spectra obtained at room temperature were fitted to the theoretical line-shape function using a general Fortran least-squares program *ORGLS* written by Busing & Levy (1962) (Fig. 1). The average value of α is found to be 5.25 ± 0.1 gauss. This gives a value of 1.59 ± 0.01 Å for the H-H distance which is not unlike other values of the H-H distance obtained by p.m.r. in hydrates (El Saffar, 1966). The average value of β is found to be 2.6 ± 0.1 gauss which is in agreement with the value 2.41 gauss calculated from equation (3) using the structure of Buchanan & Harris. Our assumption concerning the

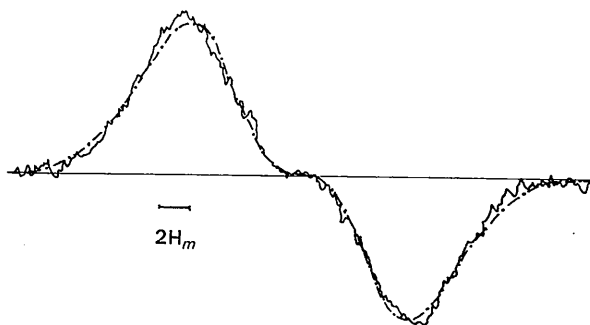


Fig. 1. The observed line shape (solid line) and the theoretical line shape (broken line) fitted by the method of least-squares. $2H_m$ stands for the peak-peak modulation.

absence of twofold motion of the water molecules at room temperature was confirmed by spin-lattice relaxation measurements (El Saffar, Mulcahy & Rochau, 1971).

In conclusion it appears that neutron diffraction studies utilizing a limited number of reflections such as the one reported by Buchanan & Harris (1968) should be viewed with caution.

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The crystal structure of K_2SeO_4 . By A. KÁLMÁN, J. S. STEPHENS and D. W. J. CRUICKSHANK, *Department of Chemistry, U.M.I.S.T., Manchester M60 1QD, England*

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In our paper (Kálmán, Stephens & Cruickshank, 1970) on K_2SeO_4 we referred to 'a slight but systematic error in the geometry of the (Hilger & Watts) four-circle goniometer'. We regret that we did not make it clear that this slight fault was due to accidental disturbance of the alignment of the

instrument, which had not been corrected at the time of use.

References

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