NMR IN SOLID H2 AND D2 UNDER HIGH PRESSURE

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instance Fig. 7 <sup>1</sup> and H<sub>s</sub><sup>11</sup>. 21,459 (1936); proceed more slowly because the remaining ortho molecules are far away from the impurity. We have not been able to observe such a rapid initial conversion for the normal density, where the scatter in c is smallest. The concentration as a function of time could always be expressed by integration of Eq. (7) and hence is plotted as 1/c versus time in Fig. 3. At normal density several experiments give  $k=6\times10^{-6}$  (% per min)<sup>-1</sup>. This is about twice the rate found by several previous experimenters,<sup>7,40,41</sup> although Sugawara and co-workers<sup>4</sup> also report approximately the same conversion rate. The reason for this result, which was reproducible, is unclear at present.

The dependence of k on density can be predicted in principle from Motizuki and Nagamiya's paper<sup>9</sup> and is rather complicated. This is partly because such quantities as the sound velocity and the Debye temperature  $(\Theta_D)$  occurring in Motizuki and Nagamiya's expression

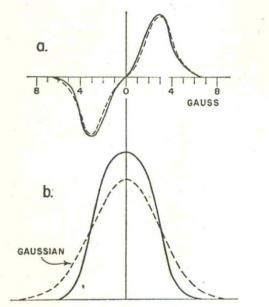


FIG. 5. (a) Derivative of an  $H_2$  line at 4.2°K for c=0.71 and normal density compared to a line of the same ortho concentration recorded by Sugawara,<sup>5</sup> dashed curve. (b) The same line integrated and compared to a Gaussian line of approximately the same area.

are also dependent on density. The assumption of a Debye solid may not be justified for solid  $H_2$ , and so far no experimental determinations of these quantities as a function of density have been made.

Figure 4 gives the data for k plotted versus  $(\rho/\rho_0)$  on a logarithmic scale, and it is seen from the slope that k is approximately proportional to  $(\rho/\rho_0)$ .<sup>2,4</sup> The values from this figure were used to compute c in the rest of the experiments where c enters as a parameter of the quantities being measured. The error in c is about  $2C_{c}$ . We found that the conversion rate for  $(\rho/\rho_0) = 1.65$ (which corresponds to a pressure of about 4800 atm)

41 G. Ahlers, J. Chem. Phys. 40, 3123 (1964).

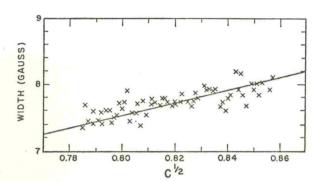


FIG. 6. Linewidth for H<sub>2</sub> at 4.2°K with  $(\rho/\rho_0) = 1.34$  plotted versus  $c^{1/2}$ . The straight line is the best fit consistent with the condition that  $\Delta II = 0$  for c = 0. Each width is measured to  $\pm 0.4$  G.

is 6.7%/h. This compares with 7.5%/h found by McCormick<sup>15</sup> at this same density. Considering the errors involved, the agreement is satisfactory.

It is interesting to note that while the absolute value of the conversion rate is higher than that of Ahlers,<sup>41</sup> the density dependence we find is approximately the same as that obtained by Ahlers, who finds  $k \propto (\rho/\rho_0)^{8/3}$  and who gives a detailed discussion of the expected density dependence.

## (b) The Shape of the Unsplit Line

The parameter usually reported in previous work has been the linewidth  $\Delta H$ , which is the distance, in G, between two points of maximum slope. It has usually been tacitly assumed that the line was Gaussian. Figure 5 shows the derivative for a typical line at 4.2°K compared to a nearly identical line at the same concentration presented by Sugawara.<sup>5</sup> The integrated curve is compared to a Gaussian one of the same area and same width. It is seen that the experimental curve is narrower, perhaps because of exchange, and drops to noise level within 7 G from the center. For this particular density and concentration we believe that the wings are so

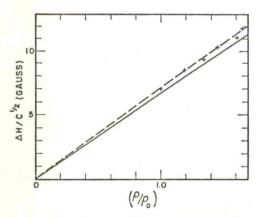


FIG. 7. Plot of the ratio of  $\Delta II/c^{1.2}$  versus relative density for H<sub>2</sub> at 4.2°K. The solid line is that calculated for hcp lattice (Ref. 25) according to the theory of second moments and the empirical relation 8.

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