in this sample prepared by the transformation of ice II, the mean particle size is about 130 Å. It appears that the crystals are of varying thickness depending upon the crystallographic direction examined, as would be expected. However, because of the uncertainties associated with the application of the Scherrer formula, only qualitative differences in thickness are assumed to be indicated.

The ice Ic prepared from ice II was transformed to ice Ih in several stages. The sample was heated from liquid-nitrogen temperature in the *n*-pentane bath (a) for 15 min at −65°C, (b) for 15 min at −55°C, and (c) for 30 min at −52°C. The neutron-diffraction pattern was recorded at 80°K after each heating period. As indicated by the (10·0) linewidth results, the crystal size of ice Ih increased from 310 Å in (a) to 350 Å in (b) and finally to 610 Å in (c). Approximately corresponding increases were also noted from the (00·2), (10·1), and (10·2) reflections. If any particle-size growth occurred at the temperature of liquid nitrogen, it was exceedingly small since linewidths in both the ice Ic and Ih patterns were reproducible even after the lapse of many days at this temperature.

The fact that cubic ice was not produced in significant amounts by the quenching of aqueous (D_2O) solutions of $FeCl_2$ or KCl is of interest. It is possible that the ^{57}Fe nuclei in the Mössbauer experiments[10] were influenced by strains in the crystal lattice induced by quenching the solution in liquid nitrogen. The neutron-diffraction spectrum clearly indicates the lattice is principally hexagonal in character. Although traces of ice Ic conceivably could be formed, if the Mössbauer spectrum is influenced more than a trace of ice Ic would appear to be required. Changes in the field gradient around the ^{57}Fe caused by crystal strains seems more probable in view of this neutron-diffraction analysis.

Weltman[11] has based his conclusion of the induced formation of ice Ic in rapidly cooled aqueous KCl solutions on resistivity changes and on the appearance of lines in the x-ray spectrum which are not found in the ice Ih. It appears that this is in error. A computer analysis of the two ices shows intensity differences for various reflections but no *new* lines in the ice Ic spectrum.

Note added in proof: The possibility of demonstrating the existence of a proton-disordered structure in ice Ic from neutron-diffraction results was suggested by the referee. We have shown that the proton-disordered model (O–H distance = 1.01 Å, and H–O–H angle = 104.5°) reproduces the observed spectrum with an $R = 9.5\%$. A reasonable proton-ordered arrangement, space group I_4-*md*, with the same angle and distance as the disordered structure is in poor agreement ($R = 71\%$) with the experimental pattern. In response to a suggestion that the behavior of the H_2O and D_2O ices may not be the same in the vicinity of the iron nucleus, we have made diffraction measurements on a sample of quenched $0.47M$ $FeCl_2$ in H_2O and find no ice Ic phase present within a detection limit of about 5%.

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LCAO–MO–SCF Calculations Using Gaussian Basis Functions. II. BeH_2

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Results of extensive LCAO–MO–SCF calculations on BeH_2 utilizing Gaussian basis functions are presented. It is established that BeH_2 is linear in its ground state, and the equilibrium bond distance has been determined. Force constants and normal frequencies were obtained. Utilizing an accurate estimate of the correlation energy, the dissociation energy of BeH_2 was determined to within the experimental error of the National Bureau of Standards measurement.

I. INTRODUCTION

In this paper we present the results of an intensive LCAO–MO–SCF study of beryllium hydride, BeH_2, which is of great practical interest because of its potential utility as one of the most energetic of high-energy rocket fuels. This molecule has also posed a difficult enigma to experimentalists because of the immense difficulty of obtaining a sample pure enough to allow measurement of an accurate heat of formation. It was in the framework of this question of obtaining the BeH_2 bond dissociation energy (which has beset thermochemists for the past five years) that we undertook to perform accurate LCAO–MO–SCF