formation of ice Ih, it has been considered that the impurity of hexagonal ice represents the small amount which did not transform under the experimental conditions employed. Perhaps a period of about 1 h at −40°C might be a more appropriate length of time to allow for the phase transformation if it is desired to essentially eliminate small amounts of hexagonal ice from the sample.

Kamb[6] has pointed out that the unit cell of ice II is rhombohedral. There are 12 water molecules in the unit cell with the oxygen atoms located in two sets of six equivalent positions. Two six-membered rings of oxygen atoms similar to those found in ices Ih and Ic are present; in one the atoms are nearly planar, and in the other there is considerable puckering. In the larger hexagonal cell there are 36 molecules with the oxygens in two sets of 18 equivalent positions.

A Gaussian line-fitting procedure which has been described in a previous study[2] was used to obtain the peak centroids, intensities, and half-widths for the 55 ice II peaks in the 2θ range between 10° and 57.3°. The results are listed in Table I. As indicated, centroid posititons of the weaker peaks were held fixed at the values calculated from the cell lattice parameters in order that a more reliable estimate of their intensities could be made.

Values of the rhombohedral lattice parameters obtained in this work are $a_R=7.743\pm0.002$ Å, $\alpha_R=113.09°\pm0.03°$. For the corresponding hexagonal cell, the parameters are $a_H=12.920\pm0.003$ A and $c_H=6.234\pm0.002$ Å. These results are in excellent agreement with the values reported by Bertie *et al.*[9] In Fig. 1, the centroids of the peaks which were calculated on the basis of these lattice parameters are marked with short vertical lines above the indicated hexagonal indices. Only the more prominent peaks have been indexed in the figure.

An ordered-proton arrangement in ice II has been suggested[5,6] on the basis of dielectric relaxation and residual entropy considerations and infrared and x-ray spectra. There are four nonequivalent hydrogen atoms in the ice II lattice. The coordinates of these atoms together with the positions of the two nonequivalent oxygen atoms given in Table II represent the initial estimate of the spatial arrangement of the atoms. Since the oxygens had been located with such a high degree of precision, no attempt was made to further refine these positions. To simplify calculations in this work, hexagonal coordinates have been used throughout. Rhombohedral coordinates[6] were transformed to hexagonal coordinates with the appropriate transformation matrices.[13]

In the initial estimate of the deuteron coordinates which are given in Table II, each O–D bond distance was chosen to be 1.01 Å as is found in ice Ih. In the selection of the D–O–D bond angles, one choice would

[13] *International Tables for X-Ray Crystallography*, K. Lonsdale *et al.*, Eds. (Kynoch Press, Birmingham, England, 1962), Vol. 2.

TABLE I. Neutron-diffraction line centroids and intensities in ice II at 80°K.

	Experimental		Calculated
hkl	$2\theta°$	$I_0\pm\sigma$	I_c
110	10.12	8.29 0.11	8.00
101	Fixed	0.00 0.20	0.00
021	Fixed	0.00 0.20	0.08
030	17.61	4.55 0.07	4.47
211	18.79	1.52 0.06	1.62
220	20.37	5.67 0.14	5.45
012	21.92	10.53 0.17	10.38
131	23.73	11.03 0.27	10.68
202	24.10	1.78 0.55	1.26
401	Fixed	0.00 0.09	0.20
122	Fixed	9.17 0.21	9.44
410	27.08	12.81 0.20	13.25
321	Fixed	4.81 0.20	5.03
312	30.11	2.94 0.10	2.93
330	30.76	0.03 0.20	0.01
051	Fixed	2.30 0.15	2.27
042	Fixed	0.15 0.50	0.16
003	Fixed	1.00 0.50	1.28
241	Fixed	1.50 0.16	1.98
232	Fixed	3.94 0.80	4.14
113	Fixed	0.57 0.72	1.21
511	34.77	2.65 0.10	2.67
600	Fixed	0.14 0.20	0.26
502	Fixed	0.19 0.20	0.22
033	Fixed	0.05 0.20	0.02
250	Fixed	0.09 0.20	0.09
431	Fixed	1.99 0.20	2.03
422	Fixed	1.53 0.90	1.77
223	Fixed	0.44 0.80	0.15
152	Fixed	1.54 0.05	1.56
161	Fixed	1.29 0.05	1.27
440	Fixed	0.03 0.80	0.01
342	Fixed	0.96 0.80	0.75
413	Fixed	0.31 0.86	0.79
351	Fixed	1.48 0.39	1.37
104	Fixed	1.96 0.36	2.74
621	Fixed	2.86 0.40	3.60
024	Fixed	0.36 0.40	0.51
612	Fixed	0.95 0.50	1.87
333	Fixed	0.55 0.34	0.44
170	Fixed	2.30 0.34	2.18
214	Fixed	1.41 0.20	1.55
532	Fixed	3.16 0.20	3.70
630	Fixed	0.16 0.14	0.20
541	Fixed	1.60 1.50	2.33
134	Fixed	2.00 1.50	3.06
262	Fixed	0.07 0.25	0.29
063	Fixed	2.66 1.50	2.30
081	Fixed	0.06 0.50	0.17
404	Fixed	0.50 0.75	0.74
523	Fixed	1.00 1.00	1.74
271	Fixed	0.75 0.50	0.74
324	Fixed	0.51 0.50	0.92
452	Fixed	0.92 0.60	1.13
550	Fixed	0.39 0.34	0.58