Short Communications

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An X-ray study of hydrazine hydrate, $N_2H_4.H_2O$.

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In the course of a neutron diffraction study of the configuration of the N_2H_4 molecule in the solid state, the crystal structure of $N_2H_4.H_2O$ has been investigated with X-rays. Crystals (melting point $-46{\cdot}8$ °C., Semishin, 1938) were grown and kept at about -60 °C. for the period of the experiment using an apparatus similar to that described by others (see, for example, Post, Schwartz & Fankuchen, 1951). Zero and first-layer precession photographs were taken using Mo $K\alpha$ radiation, and the intensities of ten reflections were estimated visually by comparison of several films of different exposures. Lorentz and polarization corrections were made in the usual way, and the resulting squares of the structure factors are listed in Table 1, together with their estimated standard errors. These values have been scaled by a factor which is an average of those obtained from the least squares refinements described below.

Table 1. *Observed squares of structure factors with their estimated standard errors*

hkl	F_o^2	σ	*hkl*	F_o^2	σ
111	73	12	400	71	14
200	2367	355	331	17	5
220	615	92	420	59	14
113	21	5	224	12	2
222	187	38	115	33	9

The lattice is face-centered cubic with $a_0 = 6{\cdot}76 \pm 0{\cdot}02$ Å. Assuming $4\ N_2H_4.H_2O$ units per cell the calculated density is 1·075 g.cm.$^{-3}$, in reasonable agreement with the density 1·048 g.cm.$^{-3}$ of the liquid at 0 °C. (Semishin, 1938). The structure appears to be that of NaCl with disordered or rotating H_2O and N_2H_4 molecules replacing Na^+ and Cl^- ions, respectively.

Of the possible models with disorder of this type, four were chosen for least-squares refinement. Three of these models are described by locating fractional nitrogen atoms at positions of point symmetry *4mm*, *3m*, or *mm*, respectively, (positions *e*, *f*, or *h* of space group *Fm3m*), while in the fourth model freely rotating hydrazine molecules were assumed. The observations were assigned weights $w = 1/\sigma^2$, (Table 1) and four parameters were varied: the scale factor, isotropic temperature factor coefficients for nitrogen and oxygen, and a nitrogen position parameter which corresponds to the N–N distance (i.e., the distance between centrosymmetrically related nitrogen positions).

Table 2. *Results of least-squares refinements of four models of* $N_2H_4.H_2O$

Model	B_O (Å^2)	B_N (Å^2)	d_{N-N} (Å)	Fit*
4mm	$12{\cdot}0 \pm 1{\cdot}7$	19 ± 7	$1{\cdot}15 \pm 0{\cdot}31$	1·72
3m	$9{\cdot}8 \pm 1{\cdot}4$	9 ± 3	$1{\cdot}45 \pm 0{\cdot}07$	1·52
mm	$9{\cdot}8 \pm 1{\cdot}5$	8 ± 4	$1{\cdot}45 \pm 0{\cdot}08$	1·48
Free rotation	$10{\cdot}3 \pm 1{\cdot}8$	11 ± 5	$1{\cdot}41 \pm 0{\cdot}11$	1·51

* $\text{Fit} = [\Sigma w(F_o^2 - F_c^2)^2/(10-4)]^{1/2}$.

The results of these refinements are given in Table 2. The *3m*, *mm*, and free rotation models gave equally good agreement, and the N–N distance for these models is consistent with the value of 1·46 Å reported for solid hydrazine (Collin & Lipscomb, 1951). The agreement is not so good for the *4mm* model, and the parameters appear to be less reasonable.

A powder sample of this material showed a transformation to a phase of lower symmetry at about -80 °C.

References

Collin, R. L. & Lipscomb, W. N. (1951). *Acta Cryst.* **4**, 10.

Post, B., Schwartz, R. S. & Fankuchen, I. (1951). *Rev. Sci. Instrum.* **22**, 218.

Semishin, V. I. (1938). *J. Gen. Chem.* (*USSR*), **8**, 654.

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A unified system of nomenclature in micro- and macrocrystallography for points, rows, faces, planes and sets of them related by symmetry.

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In modern crystallography there is no unique notation for faces, lines and points and sets of them related by symmetry. This creates considerable difficulties, particularly for those trained in related sciences when they have to deal with crystallographic data. The problem of the notation of the symmetry properties of crystals may