

Short Communications

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An X-ray study of hydrazine hydrate, $N_2H_4 \cdot H_2O$. By M. ZOCCHI,* W. R. BUSING, R. D. ELLISON and H. A. LEVY, *Chemistry Division, Oak Ridge National Laboratory,† Oak Ridge, Tennessee, U.S.A.*

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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 $N_2H_4 \cdot H_2O$ has been investigated with X-rays. Crystals (melting point -46.8 °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

<i>hkl</i>	F_o^2	σ	<i>hkl</i>	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 $a_0 = 6.76 \pm 0.02$ Å. Assuming 4 $N_2H_4 \cdot H_2O$ 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.

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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. By V. A. FRANK-KAMENECKIJ, *Department of Crystallography, Leningrad State University, Leningrad, USSR*

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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, par-

ticularly 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

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 $Fm\bar{3}m$), 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 $N_2H_4 \cdot H_2O$

Model	B_O (Å ²)	B_N (Å ²)	d_{N-N} (Å)	Fit*
$4mm$	12.0 ± 1.7	19 ± 7	1.15 ± 0.31	1.72
$3m$	9.8 ± 1.4	9 ± 3	1.45 ± 0.07	1.52
mm	9.8 ± 1.5	8 ± 4	1.45 ± 0.08	1.48
Free rotation	10.3 ± 1.8	11 ± 5	1.41 ± 0.11	1.51

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

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

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Table 1. Proposed nomenclature for points, faces (planes) and lines (rows, directions) in crystallography

Element	In structure		In diffraction pattern		In polyhedron
	In lattice	In structure	Reciprocal lattice	Direct lattice	
Point <i>·nmp·</i>	Point <i>·nmp·</i>	Base { <i>n_im_ip_i</i> }	Point <i>hkl</i>	Single reflexion from plane <i>hkl</i>	Apex
Set of points <i>:nmp:</i>	Set of points <i>:nmp:</i>	Set of bases { <i>n_im_ip_i</i> }	Set of apices
Line <i>[rst]</i>	Row <i>[rst]</i>	Repeated row { <i>[rst]</i> }	Line <i>-hkl-</i>	Set of reflexions from plane <i>-hkl-</i>	Edge <i>[rst]</i>
Set of lines <i>[[rst]]</i>	Set of rows <i>[[rst]]</i>	Set of repeated rows { <i>[[rst]]</i> }	Edge form <i>[[rst]]</i>
Plane <i>(hkl)</i>	Net <i>(hkl)</i>	Repeated net { <i>(hkl)</i> }	Plane <i>=hkl=</i>	Set of reflexions from zone of planes <i>=hkl=</i>	Face <i>(hkl)</i>
Set of planes <i>((hkl))</i>	Set of nets <i>((hkl))</i>	Set of repeated nets { <i>((hkl))</i> }	Face form <i>((hkl))</i>

be considered as solved in an adequate fashion by the work of Hermann & Mauguin.

A unified system of nomenclature for points, lines, and faces is proposed here, for each of the three ways in which they may appear: as an atomic structure, as a diffraction pattern, and as a polyhedron. Each possibility is examined separately, the crystal structure being taken as basic. In crystalline structure considered as a space lattice both isolated elements (points, rows, nets) and systems of these (systems of rows, points, and nets) may be distinguished. The real structure of a crystal usually requires distinguishing the repeating elements (bases) and sets of them. It is clear that the sets of lattice elements and the repeating elements of a real structure may give different combinations when combined in one, two, or three dimensions (infinite) or zero dimension (finite). In this last case they correspond to the point groups of the crystalline polyhedron and determine the position of its apices, edges and faces. When dealing with the diffraction pattern it is most convenient to use the reciprocal lattice elements (points, lines of points, and planes of points); this is discussed separately.

All these elements of a crystal, considered as a structure (space lattice, and the structure itself) as a diffraction pattern, and as a polyhedron, are represented by names and notations of corresponding kind in Table 1.

In addition we have inserted symbols describing the indices of single faces, forms, and of symmetrical sets related to them by symmetry, using the particularly convenient and rational system proposed by Buerger (1956).

The new system which is proposed here includes all elements in a lattice or in a crystal (point, line, or plane). Considered as single elements these are marked *·nmp·*, *[rst]* and *(hkl)* respectively. As a set of elements of a

lattice or a crystal they are denoted by *:nmp:*, *[[rst]]*, and *((hkl))*. To represent the system of repeating elements in a real structure the same symbols are enclosed in curly brackets, for example *{[rst]}* means the repeated set of rows.

The indices of diffraction are usually denoted by *hkl*, without brackets or parentheses. In our system this notation would remain to represent a single point of the reciprocal lattice, but for a set of reflexions from a plane we should use the notation *-hkl-*, and for a set of reflexions from a zone of planes we should use *=hkl=*. The class of symmetry may be placed before the symbol, and the number of equivalent elements may be indicated by a subscript following the symbol, for example

$$\frac{0}{\infty}((111))_8, \frac{2}{\infty}[[100]]_2, \frac{3}{\infty}\{((110))\}_{12}$$

In the table the column headed 'Polyhedron' gives symbols for the indices of an edge (or, what is the same thing, of a direction in the polyhedron), of an edge form (that is, the combination of edges repeated by the symmetry elements of the point group), a face (or a plane, for example a cleavage plane or a twin plane), and a form (that is, a combination of all the faces or planes related by symmetry elements of the point group). It should be noted that the meaning of 'edge form' is here not the same as in the work of Šafranovskij (1961).

References

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