Références

Born, M. (1923). *Atomtheorie des Festen Zustandes.* Leipzig: Teubner.

Born, M. (1942). *Rep. Phys. Soc. Progr. Phys.* **9**, 294.

Begbie, G. H. & Born, M. (1947). *Proc. Roy. Soc.* A, **188**, 186.

Laval, J. (1952). *L'état solide*, p. 273. Rapports et Discussions, Congrès Solvay 1951. Bruxelles: Stoops.

Parodi, M. (1938). Thèse, 116. Paris: Hermann.

Press, D. C. (1950). *Proc. Indian Acad. Sci.* A, **31**, 56.

Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 500 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Publication will be quicker if the contributions are without illustrations.*

Acta Cryst. (1953). **6**, 300

Crystal structure of *n*-aliphatic acid hydrazides.

By L. H. Jensen, *Department of Anatomy, School of Medicine, University of Washington, Seattle* 5, *Wash., U.S.A.* and E. C. Lingafelter, *Department of Chemistry and Chemical Engineering, University of Washington, Seattle* 5, *Wash., U.S.A.*

(*Received* 21 *October* 1952 *and in revised form* 10 *November* 1952)

In the course of investigating the structures of paraffin chain compounds, the *n*-aliphatic acid monosubstituted hydrazides have been studied.

Single crystals of hexanoic, heptanoic, octanoic, and nonanoic acid hydrazides were grown (these will be designated C_6, C_7, C_8 and C_9 hydrazides), and oscillation and Weissenberg photographs about the *a* and *b* axes were taken using Cu $K\alpha$ radiation. Preliminary dimensions of the monoclinic unit cells and densities are listed in Table 1.

The space group is either *Aa* or *A*2/*a*; with 8 molecules in the unit cell, *A*2/*a* is probable. This was confirmed by applying to $\{h0l\}$ of C_7 hydrazide the modification of Wilson's ratio test suggested by Howells, Phillips & Rogers (1950). The distribution of intensities follows fairly well that to be expected from a centrosymmetric projection (Fig. 1).

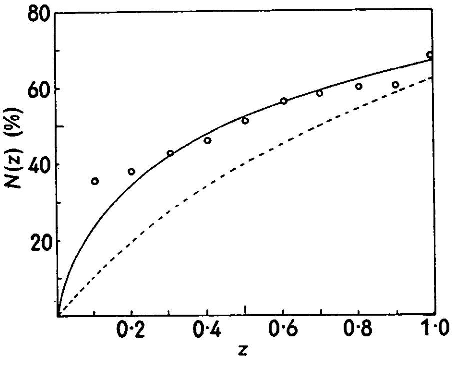
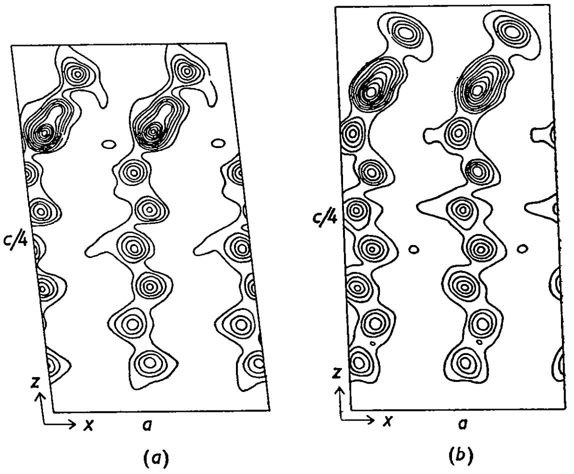


Fig. 1. Plot of $N(z)$ *v.* z for $\{h01\}$ of heptanoic acid hydrazide. Solid line, centrosymmetric; broken line, non-centrosymmetric.

Intensities were estimated by eye for $\{h0l\}$ of C_7 and



(*a*) (*b*)

Fig. 2. Projection on (010) for (*a*) C_7 and (*b*) C_8 hydrazides. Contours at intervals of 1·5 e.Å^{-2}. Origin may be as shown or at ¼, 0. Correct choice will be indicated by F_{hkl} or F_{hk0}.

Table 1. *Dimensions of unit cells and densities*

	a	*b*	*c*	*β*	Density (g.cm.$^{-3}$) Exp.	Density (g.cm.$^{-3}$) Calc.*
$(C_6)C_5H_{11}CONHNH_2$	7·49 Å	4·88 Å	43·47 Å	91° 16′	1·12	1·09
$(C_7)C_6H_{13}CONHNH_2$	7·44	4·88	48·60	96 14	1·09	1·09
$(C_8)C_7H_{15}CONHNH_2$	7·46	4·87	53·47	91 20	1·08	1·08
$(C_9)C_8H_{17}CONHNH_2$	7·44	4·87	58·73	95 4	1·07	1·08

* Assuming 8 molecules per unit cell.

Table 2. *Coordinates for* C_7, C_8 *and* C_9 *hydrazides*

	C_7		C_8		C_9
	x (Å)	z (Å)	x (Å)	z (Å)	y (Å)
C_1	3·56	1·57	0·33	1·57	1·57
C_2	3·13	2·85	0·94	2·87	0·96
C_3	3·88	4·11	0·39	4·12	1·48
C_4	3·46	5·38	0·97	5·37	0·98
C_5	4·21	6·65	0·44	6·64	1·67
C_6	3·78	7·91	1·03	7·92	0·92
C_7	4·28*	9·25*	0·44	9·20	1·60
C_8	—	—	1·13*	10·60*	0·95
C_9	—	—	—	—	1·99*
O	4·28*	9·25*	1·13*	10·60*	1·99*
N_1	5·16	10·00	1·66*	11·29*	0·91
N_2	5·97	11·18	2·41	12·48	1·24

* Not resolved in F projection.

C_8 hydrazides and $\{0kl\}$ for C_9 hydrazide. The Δd_{001} values indicate that the chains are very nearly normal to (001). Bragg–Lipson charts were used to determine the approximate structure. Electron densities were computed at units of $a/60$, $b/30$ and $c/120$ using Patterson–Tunell strips. The third F syntheses on (010) for C_7 and C_8 hydrazides (116 and 98 terms respectively) are shown in Fig. 2, and the first F synthesis on (100) for C_9 hydrazide (50 terms) is shown in Fig. 3. Approximate coordinates derived from these projections are listed in Table 2.

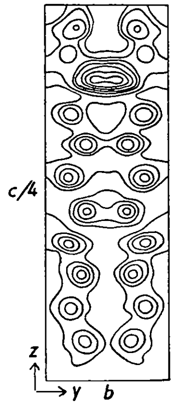


Fig. 3. Projection on (100) for C_9 hydrazide. Contours at arbitrary intervals of electron density.

Although these results are preliminary and not very accurate, some conclusions can be reached. The structures of these compounds with either an even or odd number of carbon atoms in the chain appear almost the same in (010) projection. There seem to be no consistent irregularities in bond lengths along the chains, nor do the rather short chains appear to deviate from linearity.

The C_8 and C_9 hydrazides have been chosen for further study and three-dimensional integrated data have been collected for the C_9 compound.

The authors express appreciation to Mr Clifford Roth and Dr Wayne Chen, who performed most of the numerical work, and to the Agnes H. Anderson Fund for support of the early part of this work.

Reference

Howells, E. R., Phillips, D. C. & Rogers, D. (1950). *Acta Cryst.* 3, 210.

Acta Cryst. (1953). **6**, 301

Anisotropic temperature factors in *hkl* structure-factor calculations.

By D. R. Holmes, *Imperial Chemical Industries Ltd, Plastics Division, Research Department, Welwyn Garden City, Herts., England*

(*Received* 13 *October* 1952 *and in revised form* 1 *December* 1952)

In recent crystal-structure analyses it has been found necessary to apply anisotropic temperature factors, either to the structure factors as a whole (Hughes, 1941) or to the structure-factor contributions of particular atoms (Cochran, 1951*a*). Effects closely similar to those of asymmetric thermal vibrations are produced on the observed structure factors of crystals containing atoms whose electron clouds show appreciable departures from spherical symmetry owing to their bonding arrangements. Difference syntheses (Cochran, 1951*b*) enable one to find the direction of maximum thermal vibration (or maximum departure from spherical electron density) and the magnitude of the constants involved, and Cochran himself has shown how to apply anisotropic temperature factors in two-dimensional structure-factor calculations. The purpose of this note is to show that, by making certain assumptions about the symmetry of the electron-density clouds, such factors may easily be applied to the calculations of general *hkl* structure factors required by accurate crystal-structure analyses. The analysis given applies only to cases in which the vibration ellipsoid of the atom (or electron-density ellipsoid) is an ellipsoid of revolution. The ellipsoid is treated as a linear vibration imposed on a spherically symmetrical vibration, and the effects of both are considered separately. This limitation was imposed so that the final result could be used in a practical case by a simple graphical interpretation.

For the sake of simplicity of explanation the formula