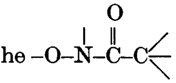
bond exists here', is clearly impossible unless this group has (unexpectedly) assumed the enol configuration, a situation which was not mentioned by those authors, and moreover, is not supported by the observed bond distances. Since the imino nitrogen atom is a hydrogen-bond donor, its presumed acceptor, the carbonyl oxygen atom, is expected to lie on or near the N–H axis. Calculations show that this oxygen atom lies within 0·05 Å of the plane of the  $-\text{O}-\overset{|}{\text{N}}-\overset{\overset{\text{O}}{\|}}{\text{C}}-\text{C}\!<$ group, but that the angles C–N · · · O (of 165°) and O–N · · · O (of 78°) represent a great deviation from the linearity expected for the atoms N–H · · · O in a good hydrogen bond. (It is not possible to predict accurately just what the angles C–N–H and O–N–H would be in a heterocyclic system of this sort, but presumably they would both be within about 10° of 120°.) We accordingly conclude that the imino nitrogen is involved in a rather weak hydrogen bond, and that the O · · · O distance of 2·92 Å is *not* indicative of a bifurcated hydrogen bond, but an entirely normal van der Waals contact. The rarity of bifurcated hydrogen bonds has been emphasized previously (Pauling, 1940; Wells, 1949; Donohue, 1952).

With regard to the $-NH_3^+$ group, which has three close chloride ion neighbors, at 3·15, 3·18 and 3·23 Å, Turley & Pepinsky remark that 'these distances indicate weak hydrogen bonds, and the calculations of the N–Cl–N angles show that the four atoms lie nearly in a plane'. The existence of these short N · · · Cl distances does not, of course, ensure the presence of hydrogen bonds. Moreover, the fact that the arrangement of the hydrogen-bond donors about the chloride-ion acceptor is planar is irrelevant, for the question to be asked is whether or not C–N · · · Cl and Cl · · · N · · · Cl angles are compatible with a tetrahedral nitrogen atom. A convenient method for depicting the situation about an $-NH_3^+$ group is that of the stereographic projection, using the C–N bond as the polar axis. The projection for this group of cycloserine hydrochloride is shown in Fig. 1, where, happily, it is seen that a satisfactory hydrogen-bond situation obtains. It seems probable, from the lengths of the N · · · Cl distances here as compared with other hydrochlorides, that these three N–H · · · Cl hydrogen bonds are of such strength as to dominate the structure of this substance and largely determine the molecular arrangement.

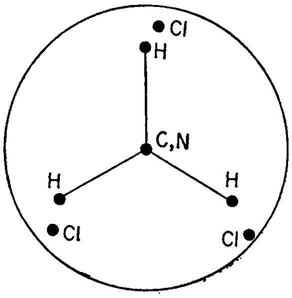


Fig. 1. Stereographic projection of the environment of the NH_3^+ group, viewed down the C–N bond. The bond angles involving the hydrogen atoms have been assumed to be tetrahedral.

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Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. Copy should be sent direct to the British Co-editor (R. C. Evans, Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England).

Acta Crystallographica

The Editors regret that the publication of this and the next few issues of *Acta Crystallographica* may be somewhat delayed owing to pressure of work in connexion with the preparation and printing of the abstracts of the communications to be read at the Fourth General Assembly of the Union.

The Use of the IBM 650 for Crystal Structure Analysis Computations

A conference was held at the University of Pittsburgh on 6 February 1957 for the purpose of exchanging information on IBM 650 programs which were already available or in the process of development for crystal structure analysis computations. There were seven principal speakers and fifty persons attended the conference. In the morning session the speakers gave a general account of their programs, with emphasis on the range of application and performance. The following is a summary of this information.

Prof. Preston M. Harris (Ohio State University) described an *hkl*, non-centric structure-factor program for up to 32 unique atoms of four different kinds in the asymmetric unit. The scattering factors were interpolated to an accuracy of 0·6% and individual isotropic temperature factors for each of the four atom kinds could be included. The program was not applicable to the triclinic case, since it required at least one orthogonal axis. It had been tested on trinitrotoluene, *Pca*, 32 unique atoms, for which it computed at the rate of 9·0 sec./structure factor. The program had 500 instructions and had not been optimized.

Miss Dorothy Booth (Bell Telephone Laboratories) described programs for (i) θ functions, (ii) *hkl* structure factors, (iii) two-dimensional Fourier syntheses.

Program (i) included *d*-spacings (except triclinic), $\sin\theta/\lambda$, $\sin\theta$, and atomic scattering factor or Lorentz factors or both. The time for these computations is of the order of 10 min. for $\beta \neq 90°$, $d_{\text{min.}} = 1·0$ Å.

Program (ii) computes the *A* and *B* parts of the general form of the structure factor separately and can accommodate up to 200 atoms. A supplementary program gives

$|F|$ and $\sin\alpha$, $\cos\alpha$. The approximate rate for $(hk0)$ structure factors with 80 atoms was 30 sec./structure factor.

The Fourier program (iii) computes two-dimensional syntheses in the product form. With h to 15, k to 30, at 6° intervals, the cos. cos and sin. sin syntheses were computed in 2 hr.

Dr M. E. Senko (I. B. M. Research Center, Poughkeepsie, N.Y.) described the programs which he, Dr Allan Zalkin, and Prof. D. H. Templeton had developed at the University of California, Berkeley. These were programs for (i) θ functions and intensity to structure amplitude reduction, (ii) hkl structure factors and least-squares refinement, (iii) interatomic distances.

Program (i) could be used to correct the intensity data obtained directly from Weissenberg photographs. It would also compute the f_0 for five different kinds of atoms and a Hughes-type weighting function for the least-squares refinement. The output from this program, in the form of one card for each reflection, contained the necessary information and instructions for the input to program (ii).

Program (ii) was of general application. The structure-factor and derivative formulas must be programmed for each space group. A sub-routine for this purpose was written which, with address changes, is adaptable to all orthorhombic and lower-symmetry space groups. The maximum number of atoms in the asymmetric unit was 20, but for structures exceeding 20 atoms it is possible to carry out the structure refinement in 20 atom groups. The structure factors are computed in the product form. The least-squares part of the program permits the refinement of coordinates, individual isotropic temperature factors and adjustment of scale factors. The output also includes $|F_o|-|F_c|$, three different R factors, and standard deviations of the coordinates and temperature factors. The computing time for a non-centric orthorhombic structure is given approximately by the product of the number of atoms and the number of reflections, in seconds, for each least-squares refinement cycle. Calculation of the structure factors alone proceeds at approximately twice this rate.

Program (iii) computes interatomic distances from the input of atomic parameters, unit-cell dimensions, space-group symmetry, and the maximum distance to be computed. For 8 atoms, $P2_12_12_1$, up to 4 Å, the total time was 5 min.

Mr D. R. Fitzwater (Iowa State College) described a program for three-dimensional Fourier syntheses, which was computed from the general unexpanded formula. The program can handle triclinic through orthorhombic space groups without redundancy in the reflections. It had the advantage that it could be used to evaluate the electron density in restricted regions of the unit cell, e.g. individual points, sections, lines or blocks. The electron density resulting from a change of a few reflections can be recalculated, using only the correction terms, in approximately one-tenth of the time required for the first calculation. The program had not been tested. The following estimated times were given: two-dimensional section (or projection) at 1/40th with 200 reflections, 0·55 hr.; three-dimensional at 1/40th with 1000 reflections, 3·5 hr. per section. With intervals of 1/80th of the cell, these times were increased by factors of about six. A block synthesis of 64 points, $(4\times4\times4)$, with 500 reflections could be computed in 0·3 hr.

Mr R. Shiono (University of Pittsburgh) described programs for (i) structure factors, and (ii) differential Fourier synthesis, for the space groups $P1$, $P2_1/c$ and $P2_12_12_1$. These separate programs form the basis for simple modifications for other space groups.

Programs (i) compute structure factors for up to 50 sets of coordinates and eight kinds of atoms, with isotropic temperature factors for each kind. The output data cards are used as input cards for programs (ii). For $P2_1/c$ with nine atoms of two kinds the program computed at the rate of 4·2 sec./structure factor, for 24 atoms of two kinds at 12 sec./structure factor.

Programs (ii) compute electron density, slopes and curvatures at atomic coordinates and solve for parameter shifts for both observed and calculated structure-factor data in one cycle.

Prof. Lynne Merritt (Indiana University) described programs for (i) intensity correction factors and θ functions, and (ii) Fourier syntheses. The program (i), applicable to monoclinic symmetry or higher, calculates the indices of every plane in any octant or octants of the sphere of reflection, the combined correction factors for equi-inclination Weissenberg photographs about each axis, $2\sin\theta$ and $\sin\theta/\lambda$, at the rate of about 20 reflections/min. The Fourier program (ii) computed two- or three-dimensional syntheses for orders H to 50, K to 50, L to 50 at 1/100ths. A Harker section, $25/100\times25/100$, with H to 32, K to 27, 250 reflections, was computed in 3 hr. A projection, $50/100\times50/100$, in $C2$ with K to 7, L to 24, 150 reflections, was computed in 3 hr. A three-dimensional synthesis in $Fdd2$ $50/100\times50/100\times50/100$ with 550 reflections requires 2 hr. to complete the first dimension summation, $2\frac{1}{2}$ hr. for the second dimension and $\frac{1}{2}$–1 hr. for each section desired in the third dimension.

Dr A. Tulinsky (The Protein Structure Project, The Polytechnic Institute of Brooklyn) described programs for (i) conversion of reciprocal-lattice coordinates to spherical coordinates, φ, χ, 2θ, (ii) two-dimensional Fourier synthesis, (iii) three-dimensional Fourier synthesis in $Fd3$, and (iv) hkl structure factors in $Fd3$ with anisotropic temperature factors.

The program (i) had been developed for use with the G. E. goniostat or Eulerian cradle. It had been used for reflections from protein crystals with $2\theta\leq60°$ and computed at the rate of about 6 reflections/min.

The programs (ii) and (iii) computed the syntheses in the Beevers–Lipson form at 1/50 or 1/100. A two-dimensional synthesis at 1300 points with 900 reflections was computed in 45 min. A three-dimensional section, in $Fd3$, at 676 points with 1300 reflections was also computed in 45 min.

In program (iv) the hkl structure factor program for $Fd3$ also included a general anisotropic temperature factor of the form

$$\exp-[\delta_1(h\alpha_1+k\beta_1+\gamma_1)^2+\delta_2(h\alpha_2+k\beta_2+\gamma_2)^2 \\ +\delta_3(h\alpha_3+k\beta_3+\gamma_3)^2]\,,$$

where the δ's are the mean-square displacements along the principal directions of vibration and the α, β, γ's are their direction cosines, referred to the crystallographic axes. Only six of these parameters are independent. This program computed 48 atoms in general positions at the rate 20 sec./structure factor.

Dr J. Kraut* (Department of Biochemistry, University of Washington, Seattle) has prepared a program which tabulates a normalized Lorentz-polarization factor for each reflection appearing on any Buerger precession photograph. It requires as input data the camera settings, the reciprocal-lattice parameters and the orientation of the reciprocal lattice with respect to the camera axis. Results are computed at the rate of 1 sec./reflection unless the lattice vectors are orthogonal, in which case 0·6 sec./reflection is required. The program may be used for precession angles up to 70° and reflection indices up to 999. It occupies drum locations 0000–0549; the instructions have been optimally located. Operation of the program has been checked against tables and charts published by M. Atoji and W. N. Lipscomb (*Acta Cryst.* (1954), **7**, 595).

The presentation of these papers was followed in the afternoon by two general discussions led by Mr William Kehl (University of Pittsburgh Computation and Data Processing Center). The first session was concerned mainly with programming and equipment. The advantages of certain auxiliary equipment for the basic, 2000-word storage, machine was discussed. There was interest in the possibility of plotting the data for electron-density maps directly from the punched cards, using an automatic graph plotter (e.g. commercially available equipment from Librascope Inc., Engineering Associates Inc., and others).

In the second session, the problems of the exchange and distribution of programs were discussed. It was agreed that it would be a great advantage to the users to have a central agency through which the programs could be shared. The function of this agency would be to distribute information and to facilitate the exchange of programs between crystallographic laboratories. Mr Kehl described the standardization procedure for program information drawn up for the computing centers of a group of the Mid-Western Universities.

It was agreed that the Computation and Data Processing Center of the University of Pittsburgh should try to provide the services of a central agency for the IBM 650 crystal structure analysis programs. The Center would (i) accept and distribute copies of programs submitted in the standard form; (ii) record the testing of these programs, either by the Center in collaboration with the Crystallographic Laboratory at the University of Pittsburgh or by the first crystallographic re-user; (iii) distribute information obtained relating to (i) and (ii) by newsletter at least biannually to the members of this conference and others who request this information.

Dorothy Booth
D. R. Fitzwater
P. M. Harris
L. Merritt
M. E. Senko
R. Shiono
A. Tulinsky
W. Kehl
G. A. Jeffrey, Conference Chairman

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* Information received after the conference.

Book Reviews

Works intended for notice in this column should be sent direct to the Editor (P. P. Ewald, Polytechnic Institute of Brooklyn, 99 Livingston Street, Brooklyn 2, N.Y., U.S.A.). As far as practicable books will be reviewed in a country different from that of publication.

Théorie et Technique de la Radiocristallographie.

By A. Guinier. Pp. xviii + 736 with 350 figs. and many tables. Paris: Dunod. 2nd ed. 1956. Price 9,500 fr.

It is a great pleasure to welcome this almost completely re-written text-book. Its author has evidently given much original thought to the teaching of a subject of which he is himself a widely acclaimed master, not only as a theoretician but, through the use of artistic fingers, also as an outstanding experimentalist.

Because of poor presentation, and hesitation by many scientists before turning to a French text, the first edition in 1945 was not as widely used as its merits warranted. When in 1952 an English translation by T. L. Tippell (*Acta Cryst.* (1953), **6**, 751) removed the original deficiencies it laid itself open to two other valid criticisms: a new text-book in an active field of science can afford neither to be seven years out of date nor to appear under a title that is liable to misinterpretation (*X-ray Crystallographic Technology* implied a far more practical and scientifically less erudite approach than that used by Guinier).

Fortunately we can now forget most of the past. The French language remains, but owing to an attractive simple style the reviewer became almost unconscious of reading an all too unfamiliar language. The material of the book is now well up to date and the production must be regarded as a triumph of French publishing. Only judged by the highest (mostly American) standards fault can be found, especially with several figures. Fig. IV–35, p. 209, for example, is unsuitable as a half-tone reproduction and should have been re-drawn paying regard to legibility of numbers; Fig. VI–13, p. 267, and many others deserve art paper and Fig. III–11, p. 88, has slight drawing inaccuracies to which the eye is sensitive. Careful attention to detail by a professional proof-reader might have avoided numerous minor inconsistencies such as the three different ways of writing '*Franç.*' in three adjacent lines in reference 22 of chapter 1, p. 48.

The book aims to include all aspects of X-ray crystallography other than the techniques of crystal-structure determination, but the principles and factors influencing the intensities of X-ray reflexions are fully dealt with throughout the volume. It logically excludes also any systematic treatment of known structures. This might have been clearly stated with a reference to such works on crystal chemistry as those by Evans and Wells. Instead the author includes two inadequate tables, one on the structures of the elements and a very meagre one on 'crystallographic data of some common substances'.

Guinier divides his book into five main parts:

The first, on properties and practical sources of X-rays, is a fine exposition with clear descriptions of the fundamental physical principles. The second part, on elementary crystallography and diffraction theory, gives a