



Fig. 1. X-N difference ellipsoids. The hydrogen atoms are indicated by circles. (a) *s*-Triazine viewed along the *c* axis, 70% probability ellipsoids. (b) α -Deuterooxalic acid dideuterate viewed along *b*, 80% probability ellipsoids.

dicular to the molecular plane and in the plane bisecting two bonds. The O(3) thermal parameters are obviously affected by the lone pair electrons, like the *s*-triazine nitrogen, while the carbon atom shows the effect of π density and the C-C bond, but not the C-O bonds. The atom O(1) is extended in a direction tangential to the lone pair and the C-O bond while the effect on O(2) which has two lone pairs and density in the C-O bond is fairly symmetric.

Conclusion

Comparison of X-ray and neutron data confirms that X-ray thermal parameters are affected by bonding. X-ray difference maps calculated with such parameters will show an unreasonably good agreement with the spherical atom model. Temperature parameters obtained with free-atom form factors are of limited usefulness in detailed studies of molecular motion. It seems doubtful that a sufficiently reliable correction formula can be derived. Therefore further improvements in the thermal motion treatment to include

effects such as anharmonicity will only yield meaningful results if bonding is properly taken into account.

References

- COPPENS, P. (1967). *Science*, **158**, 1577.
 COPPENS, P. & COULSON, C. A. (1967). *Acta Cryst.* **23**, 18.
 COULSON, C. A. (1961). *Valence*. 2nd ed., p.150. Oxford Univ. Press.
 HALL, S. R. & MASLEN, E. N. (1967). *Acta Cryst.* **22**, 216.
 HALL, S. R. & MASLEN, E. N. (1968). *Private communication*.
 IWASAKI, F. F. & SAITO, Y. (1967). *Acta Cryst.* **23**, 56.
 JOHNSON, C. K. (1965). *A Fortran Thermal-Ellipsoid Plot Program ORNL-3794*. Oak Ridge National Laboratory, Tennessee.
 POPE, J. A., SANTRY, D. P. & SEGAL, G. A. (1965). *J. Chem. Phys.* **43**, S129.
 STEWART, R. F. (1968). *Private communication*.
 STEWART, R. F. & COPPENS, P. (1968). Abstracts ACA Winter Conference Tucson, Paper G5.

Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the General Secretary of the International Union of Crystallography (G. Boom, Laboratorium voor Fysische Metaalkunde der Rijksuniversiteit, Universiteitscomplex Paddepoel, Groningen, The Netherlands). Publication of an item in a particular issue cannot be guaranteed unless the draft is received 8 weeks before the date of publication.

International Union of Crystallography

Eighth General Assembly and International Congress of Crystallography. Buffalo, N.Y.; Stony Brook, N.Y.; Washington, D.C.; U.S.A. August 7-27, 1967

The attention of those persons interested in attending the Congress is directed to the announcement of the Congress in 'Notes and News', *Acta Cryst.* (1968), A**24**, 251 and B**24**,

159, and to a preliminary announcement already mailed to all known crystallographers. Those interested persons who have not responded to the preliminary announcement are requested to write immediately to

Mrs Emily Wolf
 American Institute of Physics
 335 East 45 Street
 New York, N.Y. 10017, U.S.A.

in order to be placed on the mailing list for the Congress information booklet to be distributed this Fall.

International Union of Crystallography

The Ångström unit in the SI system

At their recent meeting in Cambridge, England, the Executive Committee of the International Union of Crystallography resolved that the Ångström unit should be a permitted unit in the SI system.

The resolution was passed after a discussion of the fact that in the present SI system, which is a particular version of the metre-kilogram-second system, the Ångström unit was mentioned as a unit contrary to the SI system. This being so, it would have to be replaced by either 0.1 nanometre (nm) or 100 picometre (pm). In the SI system a list of 'units to be allowed in conjunction with the SI system' is indicated, containing the parsec, barn, hectare, litre, bar, tonne, stokes, poise, gauss, curie and electron volt.

International Union of Crystallography

Eighth General Assembly and International Congress of Crystallography.

Exhibition of Photographs

During the Eighth General Assembly and International Congress of Crystallography, 13–21 August 1969, Stony Brook, U.S.A., an Exhibition of Photographs of Crystallographic Interest will be organized by the Union's Commission on Crystallographic Apparatus. The first Exhibition was held during the previous Congress in Moscow, 1966, and attracted an international response with exhibits of high quality and both scientific and aesthetic appeal. The Commission on Crystallographic Apparatus has, therefore, decided to organize a similar exhibition during the forthcoming Congress and invites crystallographers and others to participate actively by submitting suitable prints for display.

The exhibition will be divided into two sections:

- (a) photographs of crystals;
- (b) photographs of diffraction patterns from crystals.

The prints should be mounted on standard photographic mounting board (no glass or wooden framing) and may be accompanied by explanatory material if desired. Neither mounted print nor explanatory material should separately exceed 2000 cm² in area (40 × 50 cm format preferred). Each print must have a caption and exhibitor's name and address. Exhibitors may submit more than one print.

The photographs will be judged (by a small committee) in terms of aesthetic appeal rather than technical interest or importance and the best photographs will be awarded certificates of merit and, if possible, published in a suitable journal.

Intending exhibitors (who need not be participants in the Congress) are requested to write to Prof. F. H. Herbstein, Department of Chemistry, Israel Institute of Technology, Haifa, Israel, before 1 March 1969, submitting small prints of their proposed entries. Immediately after that date they will be notified whether their contributions are suitable for the exhibition. Contributions will not be returned unless specific arrangements are made with the organizers; contributors attending the Congress will have to remove their own exhibits.

International Union of Crystallography

Executive Secretary

The Executive Committee of the International Union of Crystallography seek an Executive Secretary to relieve the honorary officers (General Secretary and Treasurer) of the day-to-day administration of the Union and its publications. The office will be in Chester, England. Applicants must have scientific qualifications, administrative and linguistic ability, and preferably be aged under 60. Salary not less than £ 2750 per annum. Details from the I.U.Cr. Hon. Treasurer, Professor D. W. J. Cruickshank, Department of Chemistry, University of Manchester Institute of Science and Technology, P.O. Box No. 88, Sackville Street, Manchester 1, England, to whom applications should be submitted by 31 October 1968.

Book Review

Works intended for notice in this column should be sent direct to the Book-Review Editor (M. M. Woolfson, Physics Department, University of York, Heslington, York, England). As far as practicable books will be reviewed in a country different from that of publication.

Perspectives in structural chemistry, Volume I. Edited by J. D. DUNITZ and J. A. IBERS. Pp. IX + 199. New York: John Wiley, 1967. Price £4.

This is the first volume of a review series which will – in the intention of the editors – provide chemically oriented articles for chemists (not for diffractionists) on various areas of structural chemistry (understood as that branch of chemistry 'dealing with the metrical aspects of molecular structure'). The editors have set themselves high goals: It is their objective to 'weave the results of individual structure determinations into some kind of cohesive pattern'.

This volume contains three articles on widely different subjects: P. J. Wheatley describes π -Complexes of Transition Metals with Aromatic Systems (40 pages, 222 references,

45 molecular diagrams). After introducing the material in tabular form, the author treats systematically the important structural aspects of the complexes: Orientation, planarity and bond lengths of the aromatic systems, metal-ligand interactions, bonding in the complexes *etc.* For each topic he tries to extract the general theme which is apparent (or not yet apparent) behind the experimental results. This paper certainly conveys not only to the expert but also to the non-specialist the present state of the problem in a most concise, well-balanced and understandable fashion.

A similar strategy has been used by D. Britton in his contribution *Structural Chemistry of the C \equiv N Group* (63 pages, 242 references). The structural situation of the C \equiv N group in a wide range of environments is systematically explored: molecules in the vapour phase, ionic solids,