

Fig. 1. Normalized scattering curves for bond charges in the direction of the bond. 1 (Full), C—C bond (Fritchie, 1966). 2 (Dashed) C—N bond (Cromer & Larson, 1974). 3 (Dotted) C—N bond, urea, experimental at 123 K. 4 (Dash-dotted) C—N bond, thiourea, experimental at 123 K.

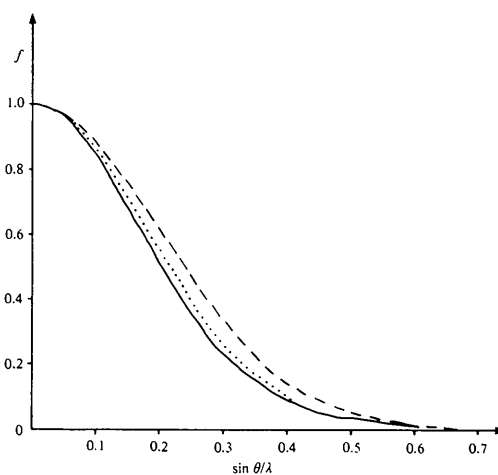


Fig. 2. Normalized scattering curves for bond charges perpendicular to the bond. Otherwise like Fig. 1. Curves 2 and 4 are indistinguishable in the scale of the drawing and are represented as one line (dashed).

electron. It can be seen that, in general, there is good agreement between the various scattering curves, which the authors consider underlines the usefulness and the physical sense of the proposed density model.

#### References

CROMER, D. T. & LARSON, A. C. (1974). *J. Chem. Phys.* **60**, 176–184.

FRITCHIE, C. J. (1966). *Acta Cryst.* **20**, 27–36.

HELLNER, E. (1977). *Acta Cryst.* **B33**, 3813–3816.

MULLEN, D. & HELLNER, E. (1978). *Acta Cryst.* **B34**. In the press.

SCHERINGER, C., MULLEN, D. & HELLNER, E. (1978). *Acta Cryst.* **B34**. In the press.

STEWART, R. F. (1969). *J. Chem. Phys.* **51**, 4569–4577.

*Acta Cryst.* (1978). **A34**, 476–477

**Effects of incorrect phases on difference density distributions.** By D. MULLEN and C. SCHERINGER, *Institut für Mineralogie der Universität Marburg, D-3550 Marburg/Lahn, Federal Republic of Germany*

(Received 3 January 1978; accepted 21 January 1978)

The effect of incorrect phases on difference density distributions is illustrated with the example of thiourea (space group  $P2_1ma$ ). Two difference density maps with phases from the free-atom model ( $R = 0.030$ ) and a molecular model of the charge distribution ( $R = 0.017$ ) are calculated. These maps show deviations as large as  $0.2 \text{ e } \text{Å}^{-3}$  in the peak heights.

The effect of incorrect phases on  $X-N$  maps of acentric structures was first discussed by Coppens (1974), who pointed out that a small phase error in the structure factors  $F_X$ , as is given by the use of phases  $\varphi_N$ , can lead to large errors in the amplitudes and phases of  $F_X - F_N$ . In the structure investigation of lithium formate monohydrate, Thomas, Tellgren & Almlöf found significant differences in two  $X-N$  maps with phases  $\varphi_N$ , on the one hand, and phases  $\varphi_X$ , on the other, where the phases  $\varphi_X$  were calculated from a fully refined free-atom model (room-temperature data without TDS correction). Recently Ito & Shibuya (1977) described a method for refining phases by a numerical Fourier transformation of difference electron density peaks. The method was applied to an artificial two-dimensional

structure, where the phases from a spherical free-atom model were used as a starting set. After 10 cycles of phase refinement the difference density could be significantly improved. In this paper we consider the effects of incorrect phases for the non-centrosymmetric structure of thiourea (space group  $P2_1ma$ , 1122 X-ray data at 123 K).

Two deformation density maps were calculated with identical scale factors but different phases  $\varphi_X$  for the observed  $F$ 's. In the first map (Fig. 1), the phases were those from the free-atom model ( $R = 0.030$ ). In the second (Fig. 2), the phases were those from a molecular model of the density distribution in which core and valence electron distributions were refined separately, and a better agreement between observed and calculated  $F$ 's was obtained ( $R =$

0.017), cf. Hellner (1977) and Mullen & Hellner (1978). In the phase (structure-factor) calculation the same positional and thermal parameters of the nuclei were used for both models. Since the molecular model appears to represent the true density distribution more closely, we classify the phases from the free atom model as 'incorrect' and those from the molecular model as nearly 'correct'.

Figs. 1 and 2 show the two deformation density maps through the plane of the molecule. The correct phases  $\phi_x$  give a map which has in general higher and sharper peaks, an effect also noted by Thomas, Tellgren & Almlöf (1975) and by Ito & Shibuya (1977). In particular, the C-S bond peak

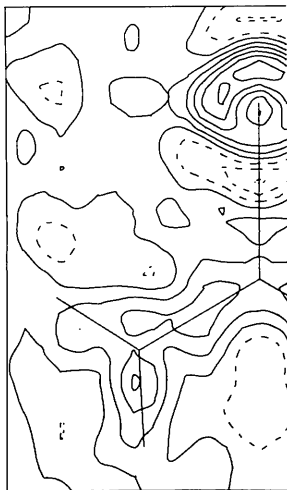


Fig. 1. Difference density map with coefficients  $F(\text{experimental}) - F(\text{free atoms})$  with phases for experimental  $F$ 's from the free-atom model. Contour intervals  $0.1 \text{ e } \text{Å}^{-3}$ , negative contours dashed, zero and positive solid lines.

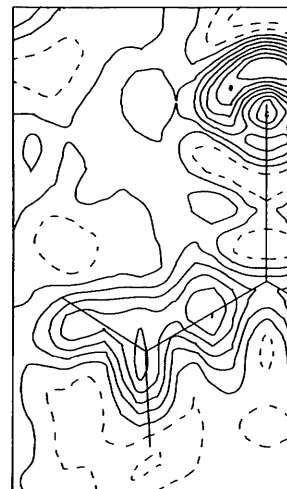


Fig. 2. Phases for experimental  $F$ 's from the molecular model of Mullen & Hellner (1978); otherwise like Fig. 1.

changes from  $0.1$  to  $-0.1 \text{ e } \text{Å}^{-3}$ , and the C-N peak from  $0.25$  to  $0.50 \text{ e } \text{Å}^{-3}$ . These are differences of about  $0.2 \text{ e } \text{Å}^{-3}$ , a significantly large value in the study of bonding densities.

#### References

- COPPENS, P. (1974). *Acta Cryst.* **B30**, 255-261.  
 HELLNER, E. (1977). *Acta Cryst.* **B33**, 3813-3816.  
 ITO, T. & SHIBUYA, I. (1977). *Acta Cryst.* **A33**, 71-74.  
 MULLEN, D. & HELLNER, E. (1978). To be submitted to *Acta Cryst.* **B**.  
 THOMAS, J. O., TELLGREN, R. & ALMLÖF, J. (1975). *Acta Cryst.* **B31**, 1946-1955.

## International Union of Crystallography

### Eleventh International Congress of Crystallography

#### General Lectures

Six General Lectures will be given at the Congress, between 9 a.m. and 10 a.m. on 4, 5, 7, 8, 9, and 10 August 1978. The provisional list of topics and speakers is as follows:

- X-ray studies of the structure and organization of biologically important proteins - T. L. Blundell (UK),
- New intense sources of X-ray and neutron radiation and new detectors - A. Guinier (France),
- Real imperfect crystals - Y. Quéré (France),
- Crystal structure information in chemistry - B. Jeżowska-Trzebiatowska (Poland),
- Three-dimensional reconstruction in electron microscopy - B. K. Vainshtein (USSR),
- Crystallographic contributions to the energy problem - M. K. Wilkinson (USA).

#### Open Meetings of the Commission on Journals

Open meetings of the Commission on Journals will be held in the morning and afternoon of 11 August 1978. Questions such as the following will be discussed with all interested crystallographers. Presentations on the last three questions will be made in the morning plenary session. Ample time will be scheduled for discussion.

- Should the *Journal of Applied Crystallography* be popularized?
- Should *Acta Crystallographica*, Section B become a data handbook?
- Should *Acta Crystallographica*, Section B become a synopsis journal with microfiche back-up?
- Should other changes in journal format, refereeing standards, or coverage be made?
- Should page charges be levied to reduce subscription costs?
- Could the Union cut costs and delays by doing its own composition in house, utilizing advanced technology?
- What are the good and bad features of the new copyright laws and how should the Union best respond to them?