

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 ϕ_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

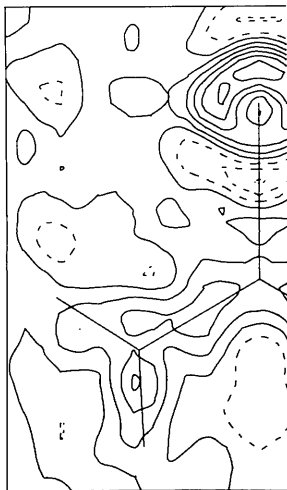


Fig. 1. Difference density map with coefficients $F(\text{experimental}) - F(\text{free atoms})$ with phases for experimental F 's from the free-atom model. Contour intervals $0.1 \text{ e } \text{Å}^{-3}$, negative contours dashed, zero and positive solid lines.

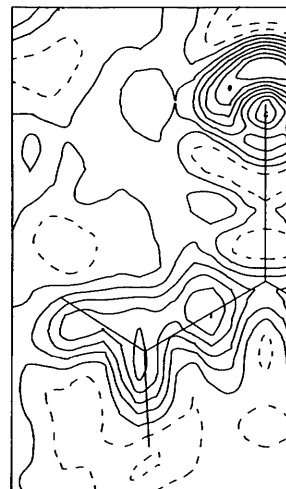


Fig. 2. Phases for experimental F 's from the molecular model of Mullen & Hellner (1978); otherwise like Fig. 1.

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.

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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?