anisotropic component is finite along $\hat{S}_1$ and zero along $\hat{S}_2$ removes the almost complete isotropy of the atom in the plane of the molecule. The entire anisotropy due to σ bonding is then reflected in the imaginary contribution. Moreover, if the imaginary part is ignored, the electron density represented by the scattering factor is centrosymmetric, which is clearly incorrect. The point group symmetry of the graphite atom is $P3m$, but if the real part alone were used, the symmetry would be $P6m$.

Examination of Figs. 1 and 2 shows that the magnitude of the imaginary component of the scattering factor is as great as the total variation in the real part. This result is similar to those obtained by Dawson (1964*b*) for the prepared valence state scattering factors of a number of light elements. The asphericity of bonded carbon is about 30% of that of the prepared state of nitrogen. However, when an atom is symmetrically bonded, as in the case of diamond or graphite, the use of spherical scattering factors does not give rise to errors in position such as those resulting in the case of nitrogen (Dawson 1964*a*). Nevertheless, the use of aspherical scattering factors would be necessary for highly accurate measurements of thermal parameters or the detailed investigation of other features of the electron density.

Experimental application

The refinement of the structure of diphenylbenzene is described by Rietveld & Maslen (1965). Using the scattering curve for the isolated carbon atom evaluated by Freeman (1959), an R index of 9·2% was obtained. A section through the molecular plane of the final difference synthesis is shown in Fig. 3(*a*). Inspection of the distribution of electron density over the molecule shows that there are positive areas on all the carbon–carbon bonds, which are consistent with the evidence of σ-bonding electrons. It was decided to test the effect of using anisotropic scattering factors on the structure accuracy and the appearance of the difference synthesis.

Complex anisotropic scattering factors were evaluated for each reflexion using equation (7) of McWeeny (1954). Structure factors were calculated using first only the real part and then the total complex scattering factor. The R values, after scaling so that $\Sigma|F_o| = \Sigma|F_c|$, were 10·0% and 9·8% respectively. The difference syntheses evaluated using the two sets of structure factors are shown in Figs. 3(*b*) and 3(*c*). Where the real parts only were used, the effects due to σ-bonding have been, if anything, enhanced while, with the use of complex scattering factors, these features have been largely eliminated. There is still some residual electron density on and around the atoms forming the bond between the two rings, and the hollows in the middle of the end rings persist.

Similar calculations were made using the data by Cox, Cruickshank & Smith (1958) for benzene. In this case the structures were actually refined by least-squares using complex, real anisotropic and isotropic curves. The sum of the residuals was slightly lower for the complex than the real anisotropic case, but both refinements were inferior to that using the isotropic curve.

The failure of the use of complex scattering factors to lower the R index and the persistence of some of the anomalous features in the difference map indicate that the scattering factors are still not correct. In some respects the use of the isolated atom scattering factor of Freeman (1959) leads to better results than the use of the complex bonded atom curve. This may be due to the fact that the scattering factors for aromatic compounds are different from those of graphite, owing to the replacement of C by H. In particular there is no π-charge on the C–H bond and the σ-charges may also be affected. However, these would be expected to be second order effects which would, if anything, enhance the asphericity and acentricity of the atoms and it is difficult to see why spherically symmetric scattering factors should then give better values. It is more likely that the results are due to the higher accuracy of the isotropic form factors which were evaluated more recently, and it is clearly necessary for the bonded atom scattering factor to be recalculated before serious attempts are made to apply it to structure analysis.

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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. The notes (in duplicate) should be sent to the General Secretary of the International Union of Crystallography (D. W. Smits, Rekencentrum der Rijksuniversiteit, Grote Appelstraat 11, *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

Seventh General Assembly and International Congress
Moscow, U.S.S.R., 12–21 July 1966

Exhibition of Photographs of Crystallographic Interest

The Commission on Crystallographic Apparatus of the Union is organizing an 'Exhibition of Photographs of Crystallographic Interest' at the Congress. This exhibition will be divided into two sections:

(*a*) Photographs of crystals; and

(*b*) Photographs of diffraction patterns from crystals.

Crystallographers and others are invited to participate actively in this exhibition by submitting suitable prints for display. 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 cm^2 in area (40 × 50 cm format preferred). Each print must have a caption and the exhibitor's name and address. Authors 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. 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 asked to write to Prof. F. H. Herbstein (Department of Chemistry, Israel Institute of Technology, Haifa, Israel) before 1 March 1966, submitting small prints of their proposed entries. Intending exhibitors will be notified immediately thereafter 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.

Books Received

The undermentioned works have been received by the Editors. Mention here does not preclude review at a later date.

Étude de la plasticité et application aux métaux. By B. JAOUL. Pp. xvi+600. Paris: Dunod, 1965. Price 138 F.

This book contains a good summary of theory and experiments bearing on the plastic deformation of metals, both as single crystals and as polycrystalline aggregates. The treatment is not only rheological, but treats fully the modifications of structure introduced by deformation and the role of the structural state in explaining the plastic phenomena. It is very fully illustrated, and there are extensive bibliographies at the end of each chapter. The subject index is fuller than in many French books, but there is no author index.