approximately 0·58 for Cl and −0·53 for $n = 2$, is not large and C=C varies only from 1·3130 (3) to 1·3140 (3) Å. For $n = 1$ the C=C values for all refinements are larger than for $n = 2$. This type of correlation is not printed by the computer program, as n is kept constant during the refinement. For $n = 1$ where the value of the slope varies with Pop_C^{Di}, the correlation $\rho[\mathrm{Pop}_C^{Di}, \mathbf{p}_C] \simeq -0{\cdot}75$ is larger than for $n = 2$. Consequently, larger values for σ[C=C] and larger variations in the C=C lengths are found in this case. Finally the table shows that C=C is not determined only by the type of radial function used for the dipole, but also by the radial functions applied for the other multipoles.

According to Table 1(*b*) an increase in the compactness of $R_C^{Mono}(r_C)$ decreases both the population and the thermal parameters of C. High-order (HO) refinements with $\sin\theta/\lambda > 0{\cdot}6$ Å^{-1} have given C=C = 1·3142 (3) Å and U_{eq} = 0·03672 (9) Å^2. From a recent model study on solid N_2 by Braam (1981) it can be deduced that for volatile compounds with $U_{eq} \simeq 0{\cdot}04$ Å^2 HO refinements give small systematic errors ($|\Delta \mathbf{r}| \simeq 3 \times 10^{-4}$ Å) for the positions, whereas systematic errors in the HO thermal parameters can be considerable, $\Delta U_{ii} \simeq 10^{-3}$ Å^2. For C_2H_4 C=C approaches the HO value best if for $R_C^{Di}(r_C)$ either formula (2) with $n = 2$ or Cl is taken. U_{eq} comes closest to the HO values for $R_C^{Mono}(r_C)$ = Cl. Use of this monopole function for C also gives the physically most reasonable values for the monopole populations (Table 1), as in C_2H_4 C is slightly electronegative with respect to H. Not too much value should be attached to the atomic charges, however, as they are not observables (Stewart, 1977; Stewart & Spackman, 1981).

In view of the discussion given above we prefer for the dipoles of first-row elements single exponentials with $n = 2$ above single exponentials with $n = 1$. For the monopoles no decision can be taken on the basis of the present refinements, as the uncertainty in the HO thermal parameters is large for crystals with high U_{eq} values.

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References

BECKER, P. J. & COPPENS, P. (1974). *Acta Cryst.* A**30**, 129–147.

BRAAM, A. W. M. (1981). PhD Thesis, Univ. of Groningen, The Netherlands.

CLEMENTI, E. (1965). *Tables of Atomic Functions*. San José Research Laboratory, International Business Machines Corporation, San José, California, USA.

COPPENS, P., GURU ROW, T. N., STEVENS, E. D., BECKER, P. J. & WANG, Y. W. (1979). *Acta Cryst.* A**35**, 63–72.

DUNCAN, J. L. (1974). *Mol. Phys.* **28**, 1177–1191.

HIRSHFELD, F. L. (1971). *Acta Cryst.* B**27**, 769–781.

NES, G. J. H. VAN & VOS, A. (1979). *Acta Cryst.* B**35**, 2593–2601.

SCHERINGER, C., KUTOGLU, A. & MULLEN, D. (1978). *Acta Cryst.* A**34**, 481–483.

STEWART, R. F. (1974). *VALRAY* 1974 system. Department of Chemistry, Carnegie–Mellon Univ., Pittsburgh, Pennsylvania 15213, USA.

STEWART, R. F. (1977). *Isr. J. Chem.* **16**, 124–131.

STEWART, R. F. (1980). In *Electron and Magnetization Densities in Molecules and Crystals*, edited by P. BECKER, pp. 439–441. New York and London: Plenum.

STEWART, R. F., BENTLEY, J. & GOODMAN, B. (1975). *J. Chem. Phys.* **63**, 3786–3793.

STEWART, R. F. & SPACKMAN, M. A. (1981). *Structure and Bonding in Crystals*. Vol. I, edited by M. O'KEEFFE & A. NAVROTSKY, pp. 279–283. New York: Academic Press.

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Suggested guidelines for the publication of Rietveld analyses and pattern decomposition studies

A letter from R. A. Young, E. Prince and R. A. Sparks to the Editor of *Journal of Applied Crystallography* has been published [*J. Appl Cryst.* (1982), **15**, 357–359] with the above title. The first paragraph read as follows:

At the request of the Commission on Journals, we drew up some draft guidelines for the publication of Rietveld analyses and of pattern decomposition studies with powder diffraction patterns. The draft was sent for comment to some 25 persons in Europe, Australia, Japan, and the USA. We are grateful for their responses, which both were generally supportive of the idea that there be guidelines and were most helpful in illuminating oversights and other deficiencies. Not all suggestions were incorporated in the revised draft, of course (in fact, a number were mutually contradictory), but all were carefully considered and many were incorporated in the version which follows.

In presenting these suggested guidelines, we emphasize that we offer them as guidelines, not rigid rules. They are intended primarily to be helpful to the co-editors; they are not intended to infringe on a co-editor's judgement of scientific worth of a submitted manuscript, nor should they be allowed to do so. For the most part, these suggested guidelines address matters of format and presentation of details, and not the fundamental question of scientific interest and worth of the submission. It is primarily for the making of such fundamental judgements that the co-editor system exists; for the health of our science it cannot and should not be replaced with a system of blind rules on a check-off sheet. It is against this background of more overreaching considerations that we offer the following suggestions for guidelines to assist, but not to control or coerce, the co-editors in their acceptance decisions.