SHORT COMMUNICATIONS

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

Acta Cryst. (1983). A**39**, 422

Conditions for direct structure imaging in silicon carbide polytypes. Erratum.

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Abstract

As a result of a printer's error, Figs. 9(*a*) and 9(*b*) in Smith & O'Keefe [*Acta Cryst.* (1983), A**39**, 139–148] have been transposed, so that (*a*) is labelled (*b*) and (*b*) is labelled (*a*).

All information is given in the *Abstract*.

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A cusp-constrained scattering factor for bonded hydrogen atoms.

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Abstract

A simple one-parameter form factor that satisfies a cusp condition has been developed. A one-parameter form factor, based on a 1*s*-type density function, is more tractable in a least-squares analysis than the corresponding cusp-constrained form factor. Application of both form factors for bonded hydrogen atoms to X-ray diffraction data of sucrose revealed a more contracted density for H bonded to C compared to H bonded to O.

At a NATO-sponsored international school on electron and magnetization densities in molecules and crystals (Becker, 1980) held in Arles, France, in August 1978, a number of exercises were distributed by the participants. One exercise, proposed by Professor Hirshfeld, was to develop an atomic form factor which satisfies the electron–nuclear cusp condition. The present communication is an approximate solution to the problem for a bonded hydrogen atom.

The electron–nuclear cusp condition,

$$\lim_{r_j \to 0} [(\partial\bar{\rho}/\partial \mathbf{r}_j)/\bar{\rho}] = -2Z_j, \qquad (1)$$

is a consequence of satisfying the many-electron *non-relativistic* Schrödinger equation (Kato, 1957; Steiner, 1963; Pack & Brown, 1966). In (1) $\bar{\rho}$ is the one-electron density spherically averaged about the jth nucleus with atomic number Z_j. The $\mathbf{r}_j$ is a scalar radial length in atomic units (1 a.u. = 0·529177 Å). One possible form for ρ is

$$\rho(\mathbf{r}) = A_o e^{-\gamma \mathbf{r}} \sum_{n=0}^{N} (A_n/A_o)\, \mathbf{r}^n/4\pi. \qquad (2)$$

For (2) to satisfy (1),

$$A_1/A_0 = \gamma - 2Z. \qquad (3)$$

For $\rho(\mathbf{r})$ normalized to unity,

$$A_o = 1\Big/\left[(2/\gamma)^3\,(1 - 3Z/2\gamma) + \sum_{n=2}^{N} (A_n/A_0)\,(n+2)!/\gamma^{n+3}\right]. \qquad (4)$$

To maintain simplicity, we set all A_n/A_0 equal to zero for $n \geq 2$. This gives a simple one-parameter function which normalizes to one and satisfies (1):

$$\rho(\gamma, \mathbf{r}) = (\gamma/2)^3\,(1 - 3Z/2\gamma)^{-1}\, e^{-\gamma r}[1 + (\gamma - 2Z)\,\mathbf{r}]/4\pi. \qquad (5)$$

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