The interpretation of such a model is that the effective shape of atoms in the crystal can be considered spherical, but the centre of the sphere is displaced along the C–X bond. The magnitude of the shift is a parameter close to $2(r_a - r_b)$. Our model lends support to the use of isotropic atom–atom potentials for the description of the physical properties of molecular crystals, but the centre of interaction should be shifted along the C–X bond. The effects of bond foreshortening were noted in the calculations of intermolecular potential for the hydrogen dimer (Williams, 1965; Starr & Williams, 1977). The calculations indicated a bond foreshortening of the order of 0·10–0·16 Å, which reflects the shift of electron density into the bonding region. Similar effects were recently noted in the calculations of static and dynamic properties of solid chlorine (Burgos, Murthy & Righini, 1982) and fluorine (Kirin & Etters, 1986). In those systems it was possible to obtain a reasonable fit for the static properties of the crystal lattice (within the famework of a simple isotropic atom–atom model) by shifting the centre of interaction along the bond by 0·186 and 0·055 Å, respectively. The effective 'bond length' was 1·618 Å for chlorine and 1·30 Å for fluorine. Of course, our interpretation is approximate and it is quite likely that anisotropy plays an important role in intermolecular interactions. Especially in the calculations of the physical properties of halogen solids (Cl_2, Br_2 and I_2) it was noted that very accurate static properties of crystal lattices could not be obtained without assuming intermolecular bonding of a special type or an angular-dependent potential (Nyburg & Wong-Ng, 1979; Williams & Hsu, 1985; Burgos *et al.*, 1982; Price & Stone, 1982). There is no doubt that for higher accuracy the anisotropic-potential model is needed, but it remains an open question whether all physical properties can be reproduced with reasonable accuracy even within the framework of such a model. Most of the sophisticated anisotropic intermolecular potentials are fitted only to a small number of physical quantities; it would be useful to examine if such potentials are transferable and if they can reproduce with reasonable accuracy such physical quantities as lattice-vibrational frequencies, high-pressure structural data, pressure dependence of vibrational frequencies *etc.*

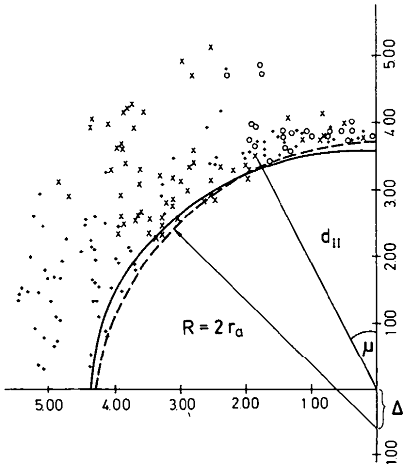

Fig. 1. Polar scatterplot of intermolecular iodine–iodine distance d_{II} (Å) *versus* polar angle μ (μ is the smaller of the two angles μ_1 and μ_2 defined by C–I bonds and intermolecular distance d_{II}). The larger μ value is designated according to its magnitude, 0–30° circles, 30–60° crosses, 60–90° arrows. The data are taken from Fig. 1 of Nyburg & Faerman (1985) and were obtained by examining the large number of crystal structures containing iodine attached to a carbon atom. The full curve is the NF ellipse and the dashed one is the proposed circle.

Since the ultimate goal is to produce a simple and transferable potential for the description of the physical properties of molecular solids, it would be interesting to see if the shift of centre of interaction could lead to satisfactory atom–atom potentials for a broader class of molecular crystals.

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Optical, pyroelectric and X-ray topographic studies of twin domains and twin boundaries in $KLiSO_4$. Erratum.

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Abstract

In the paper by Klapper, Hahn & Chung [*Acta Cryst.* (1987), **B43**, 147–159] figures have been transposed in two cases. In Fig. 2 on page 150, (*b*) is labeled (*c*) and (*c*) is labeled (*b*). In Fig. 5 on page 153, (*a*) is labeled (*b*) and (*b*) is labeled (*a*). In both cases the labels in the figure captions are correct.

All information is given in the *Abstract.*

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