The Intermolecular Interactions in the Crystal Structure of Dipotassium Hydrogen Di-iodate Chloride

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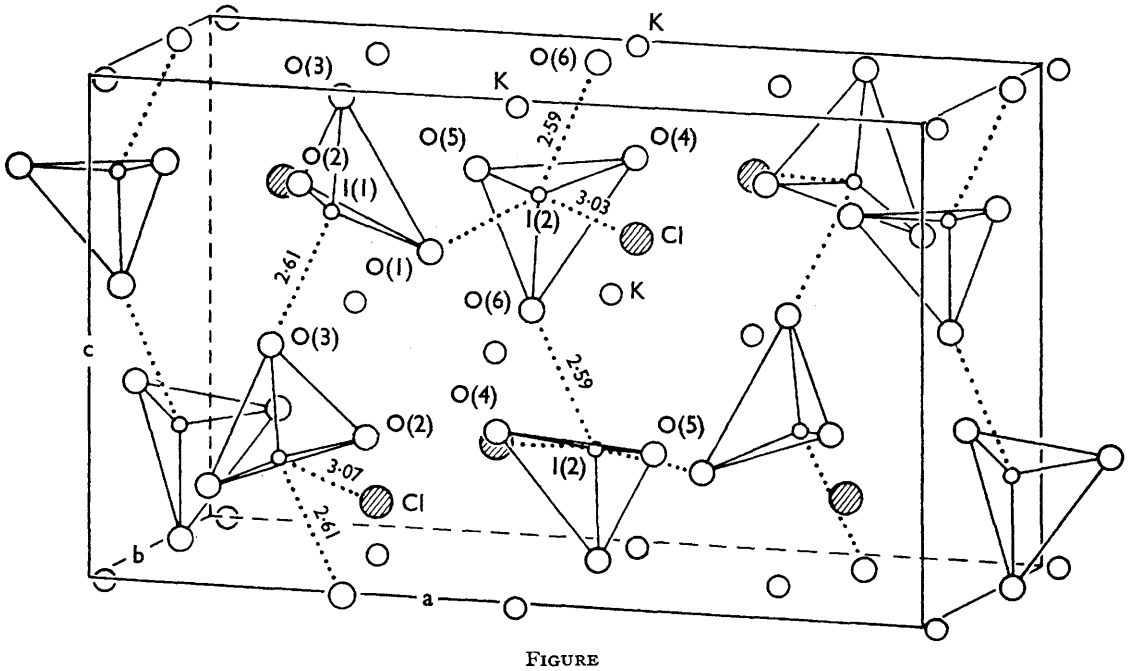
THE crystal structure of dipotassium hydrogen di-iodate chloride, $K_2H(IO_3)_2Cl$, has been investigated by *X*-ray methods. The crystals are orthorhombic and the unit cell parameters, determined by Cu-K_α radiation, are: $a = 15{\cdot}043(17)$, $b = 6{\cdot}556(6)$, $c = 8{\cdot}657(5)$ Å; $U = 845$ Å^3, $M = 464{\cdot}5$, $Z = 4$, $D_m = 3{\cdot}637$, $D_c = 3{\cdot}650$. Space group: $Pca2_1$ (from systematic absences and piezoelectric response).

The structure of this compound has been determined and refined by differential syntheses ($R = 10{\cdot}1\%$) using three-dimensional data (530 reflections) recorded photographically by an integrating Weissenberg camera. The structure consists of chains of pyramidal IO_3^- anions (see Figure) joined to one another through very short intermolecular contacts I(1) · · · O(3′) = 2·61 ± 0·01, I(2) · · · O(6′) = 2·59 ± 0·02 Å. Further inter-chain contacts I(2) · · · O(1′) = 2·47 ± 0·04 Å have been determined. Also chloride ions have been found at short distances from iodine, I(1) · · · Cl = 3·07 ± 0·01, I(2) · · · Cl = 3·03 ± 0·01 Å. These contact distances are much larger than the oxygen–iodine bond distances which are: I(1)–O(1) = 1·89 ± 0·03, I(1)–O(2) = 1·83 ± 0·02, I(1)–O(3) = 1·94 ± 0·01, I(2)–O(4) = 1·94 ± 0·03, I(2)–O(5) = 1·81 ± 0·03, I(2)–O(6) = 1·96 ± 0·02 Å. Similar behaviour has been observed[1] and is in accordance with the spectroscopic data.[2] Whether these short contact distances are real inter-atomic bonds can be questioned. The pyramidal IO_3^- anion should possess a high dipole moment with the positive end at the iodine so that the existence of dipole–dipole interactions seems the more likely interpretation. No theoretical treatment of the problem has yet been reported.



FIGURE

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[1] A. C. Larson and D. T. Cromer, *Acta Cryst.*, 1961, **14**, 128; J. L. de Boer, F. van Bolhuis, R. Olthof-Hazekamp, and A. Vos, *ibid.*, 1966, **21**, 841; D. T. Cromer and A. C. Larson, *ibid.*, 1956, **9**, 1015; J. A. Ibers, *ibid.*, 1956, **9**, 225; Y. D. Feikema and A. Vos, *ibid.*, 1966, **20**, 769.

[2] T. Depuis, *Mikrochim. Acta*, 1962, 289.