SHORT COMMUNICATIONS

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The crystal structure of *p*-chloroiodobenzene.

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p-Chloroiodobenzene, C_6H_4ClI, is monoclinic, $a=15{\cdot}772\ (23)$, $b=5{\cdot}922\ (11)$, $c=4{\cdot}220\ (5)$ Å, $\beta=113{\cdot}64\ (10)°$, space group $P2_1/a$, $Z=2$. It is isomorphous with $C_6H_4Cl_2$, $C_6H_4Br_2$, and C_6H_4BrCl.

Crystalline *p*-bromochlorobenzene is disordered with chlorine and bromine crystallographically equivalent. The structure of *p*-chloroiodobenzene has been examined to see whether the greater differences in size and chemical properties between iodine and chlorine (*versus* bromine and chlorine) lead to ordering of the molecules in the crystal.

Thick needles, elongated along *c*, were grown by sublimation of Eastman Kodak *p*-chloroiodobenzene. Precession photographs showed the crystals to be monoclinic with space group $P2_1/a$ (systematic extinctions: $0k0$, $k=2n+1$; $h0l$, $h=2n+1$). Unit-cell dimensions were determined from the Bragg angles of 13 reflections measured on a Hilger–Watts automatic diffractometer, using Mo $K\alpha$ radiation ($\lambda=0{\cdot}7107$ Å), and are given in Table 1.

Table 1. *Crystal data for* p-C_6H_4XY

X	Cl	Cl	Br	Cl
Y	Cl	Br	Br	I
a (Å)	14·80	15·2	15·36	15·772 (23)
b (Å)	5·78	5·86	5·75	5·922 (11)
c (Å)	3·99	4·11	4·10	4·220 (5)
β (°)	113	113	112·5	113·64 (10)
Molecular volume (Å^3)	157	168	167	181
Reference	(*a*)	(*b*)	(*c*)	this work

(*a*) Croatto, Bezzi & Bua (1952), (*b*) Klug (1947), (*c*) Bezzi & Croatto (1942).

As can be seen from Table 1, the chloroiodobenzene is isomorphous with dichloro-, dibromo-, and bromochlorobenzene. The structures of all three of these molecules have been determined completely and all require the molecule to lie on a crystallographic center of symmetry. Therefore, the chloroiodobenzene must be disordered, with Cl and I atoms occupying equivalent positions at random in the crystal, in spite of the appreciable size difference between the Cl and I atoms.

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References

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