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 pubished as speedily as possible.*

Acta Cryst. (1978). B**34**, 2956

Bis(*N*-acetylglycinato)-1,10-phenanthrolinecopper(II): erratum.

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In the paper by Battaglia, Bonamartini Corradi, Marcotrigiano & Pellacani [*Acta Cryst.* (1977), B**33**, 3886–3888] the coordinates of the copper atom are given incorrectly. The correct values are $x = 0, y = 0{\cdot}1424, z = 0$.

All the relevant information is given in the Abstract.

Acta Cryst. (1978). B**34**, 2956–2957

Dibenzo-*p*-dioxin: a refinement.

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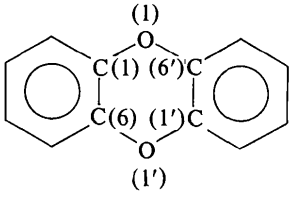
In agreement with Senma, Taira, Taga & Osaki [*Cryst. Struct. Commun.* (1973), **2**, 311–314] we find that the space group of dibenzo-*p*-dioxin is *C*2/*c*, and not *Cc* as reported by Cordes & Fair [*Acta Cryst.* (1974), B**30**, 1621–1623].

Two reports on the structure of dibenzo-*p*-dioxin (DPDO) (I) have appeared



(I)

In the first (Senma, Taira, Taga & Osaki, 1973), the structure was refined in the centrosymmetric space group *C*2/*c* using 948 visually-estimated photographic data, while in the second (Cordes & Fair, 1974; C&F hereinafter) the refinement was carried out in the noncentrosymmetric space group *Cc*, using 233 Mo *Ka* diffractometer data. The latter authors state that the space group *Cc* proved to be correct, presumably because they were unable to refine the structure in the centrosymmetric space group *C*2/*c*. They attribute the large discrepancies in the derived structural parameters (*e.g.* a difference of 7° for two chemically equivalent C—C—O angles) and the large magnitudes of their e.s.d.'s (2° for bond angles and up to 0·04 Å for bond distances) to the presence of a small percentage of intense reflections in their data set.

Structural confirmation of the basic dibenzo-*p*-dioxin nucleus is important since certain halogenated dioxin derivatives are now known to possess extreme toxicity (Schwetz, Norris, Sparchu, Rowe, Gehring, Emerson & Gerbig, 1973; McConnell & Moore, 1976) and biological potency (Poland & Glover, 1973).

We have successfully refined the parameters of C&F using their intensity data in the centrosymmetric space group *C*2/*c*. The resulting internal consistency in bond distances and bond angles and excellent agreement with the values reported in the literature for similar compounds (see below) clearly indicate the space group to be *C*2/*c*, and not *Cc* as assigned by C&F.

In order to refine the structure of DPDO in space group *C*2/*c* the coordinates reported by C&F had to be transformed so as to place the molecular center of inversion at the crystallographic center of inversion at $(\frac{1}{4},\frac{1}{4},0)$, and not at (0,0,0). This was done by adding (0·25,0,−0·25) to the coordinates of the centrosymmetric half of the molecule (non-hydrogen atoms only). The refinement was carried out on *F* by the full-matrix least-squares procedure. The weights were assigned according to the formula $w = 1/\{1 + [(|F_o| -$

Table 1. *Atomic fractional coordinates and thermal parameters with associated e.s.d.'s*

	x	*y*	*z*	*B* (Å²)
O(1)	0·3714 (4)	0·2510 (10)	0·0023 (3)	5·1 (1)
C(1)	0·2018 (6)	0·4176 (15)	0·0530 (5)	4·2 (2)
C(2)	0·1525 (6)	0·5875 (15)	0·1063 (5)	4·6 (2)
C(3)	0·2232 (6)	0·7602 (16)	0·1616 (5)	5·0 (2)
C(4)	0·3419 (6)	0·7616 (16)	0·1640 (5)	5·0 (2)
C(5)	0·3898 (6)	0·5888 (15)	0·1101 (4)	4·7 (2)
C(6)	0·3195 (6)	0·4182 (16)	0·0556 (4)	4·2 (2)
HC(2)	0·064	0·577	0·103	6·0
HC(3)	0·191	0·915	0·199	6·0
HC(4)	0·394	0·932	0·201	6·0
HC(5)	0·477	0·582	0·107	6·0