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SHORT COMMUNICATION

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Acta Cryst. (1988). C**44**, 2039

On the structure of 2-hydroxybiphenyl.

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Abstract

The crystal structure of 2-hydroxybiphenyl recently reported in space group *Cc* [Perrin, Bekkouch & Thozet (1987). *Acta Cryst.* C**43**, 980–982] has been refined in *Fdd*2. The increase in Laue symmetry – from 2/*m* to *mmm* – has caused no significant changes in the structural parameters.

The structure of 2-hydroxybiphenyl, $C_{12}H_{10}O$, has been reported (Perrin, Bekkouch & Thozet, 1987) in space group *Cc* [$a = 5{\cdot}882\ (2)$, $b = 12{\cdot}867\ (2)$, $c = 12{\cdot}313\ (3)$ Å, $\beta = 103{\cdot}76\ (3)°$, $Z = 4$] and refined to an R of 0·064 for 751 observed reflections. The vectors [0,1,0], [1,0,2] and [1,0,0] define an orthorhombic cell ($a' = 12{\cdot}867$, $b' = 23{\cdot}919$, $c' = 5{\cdot}882$ Å, $Z = 8$) and the corresponding coordinate transformation $x' = y - 0{\cdot}1250$, $y' = 0{\cdot}5z - 0{\cdot}4692$, $z' = x - 0{\cdot}5z$ led to a structure in space group *Fdd*2 that we have refined based on the original data recovered from SUP 43666. Refinement on F by the *SHELX*77 system of programs (Sheldrick, 1977) converged routinely to $R = 0{\cdot}056$ for 441 averaged reflections and 79 parameters. Final *Fdd*2 coordinates are given in Table 1.*

The change in space group requires the molecule to have an exact twofold axis which bisects the C4—C4′ bond joining the phenyl rings. The oxygen atom was again found to be disordered with occupancies 0·4 and 0·1. Since the space-group change involves only an increase in Laue symmetry, there are no significant alterations in the bond lengths and angles (Schomaker & Marsh, 1979; Marsh & Herbstein, 1988). E.s.d.'s of bonds are usually smaller (by ~0·002 Å) than those originally reported. E.s.d.'s of angles reported by Perrin *et al.* are twice as large as those found for the present refinement.

Table 1. *Final atomic coordinates* ($\times 10^4$) *and* U_{eq} (Å$^2 \times 10^3$) *for the carbon and* O1 *atoms, atomic coordinates* ($\times 10^3$) *and* U_{iso} (Å$^2 \times 10^3$) *for* O2 *and the hydrogen atoms*

$U_{eq} = \frac{1}{3}\sum_i\sum_j[U_{ij}(a_i^* a_j^*)(\mathbf{a}_i.\mathbf{a}_j)]$.

	x	y	z	U_{eq}/U_{iso}
C1	2223 (4)	−877 (2)	4100	78 (1)
C2	2046 (4)	−509 (2)	5883 (14)	75 (1)
C3	1172 (3)	−172 (2)	5864 (15)	65 (1)
C4	466 (3)	−182 (2)	4068 (11)	54 (1)
C5	657 (3)	−558 (2)	2300 (14)	63 (1)
C6	1530 (4)	−893 (2)	2335 (16)	76 (1)
O1*	−56 (5)	−622 (3)	664 (17)	72 (2)
O2†	101 (2)	14 (1)	741 (6)	100 (7)
H1	286 (3)	−113 (1)	404 (8)	57 (10)
H2	256 (4)	−50 (2)	725 (12)	101 (17)
H3†	101 (2)	14 (1)	741 (6)	100 (7)
H6	154 (4)	−117 (2)	152 (12)	110 (23)

* Refined with occupancy of 0·4.

† Refined as an average atom of 0·1 oxygen + 0·9 hydrogen.

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* Anisotropic temperature factors of the non-hydrogen atoms and a list of structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51146 (4 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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