

4,4'-Dibromo-2,2',3,3',5,5',6,6'-octa-
fluorobiphenylTullio Pilati,^{a*} Pierangelo Metrangolo^b and Giuseppe
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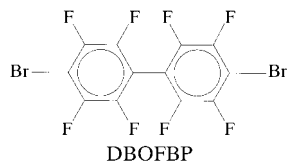
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The molecule of the title compound, C₁₂Br₂F₈, shows approximate D₂ symmetry. The dihedral angle formed by the two rings is 60.2 (1)°.

Comment

Our earlier work on halogen bonding shows that I··O and especially I··N interactions are strong and can successfully be used in supramolecular assembly (Cardillo *et al.*, 2000). We expect that highly polarizable Br atoms bonded to an electron-poor aromatic ring, as in the commercially available title compound, (I), would be used as building blocks for supramolecular assembly, notwithstanding that Br··N/O interactions are weaker than the corresponding I··N/O halogen bonds. We decided to study (I) in order to have a yardstick for evaluating the effect of supramolecular assembly involving such a compound.



The molecule of (I) crystallizes in a general position but presents approximate D₂ symmetry, with a molecular r.m.s. of 0.0277 Å (Pilati & Forni, 1999, 2000). Bond distances and angles are in the normal ranges [C—Br 1.872 (3) and 1.876 (3) Å, C—F 1.334 (4)–1.344 (4) Å, and aromatic C—C 1.370 (4)–1.386 (4) Å]. The length of the C—C bond between the rings is 1.483 (4) Å.

The main feature of biphenyl derivatives is the dihedral angle between the two rings. These molecules reach a compromise between conjugation of π-orbitals of the aromatic system and repulsion between the transannular *ortho*-bonded atoms. In (I), the contacts between the substituents at the 2- and 6-positions, F1··F5 and F4··F8, are 2.884 (4) and

2.881 (3) Å, respectively, with a dihedral angle between the phenyl rings of 60.2 (1)°; such values are identical (to within one s.u.) to those found in perfluorobiphenyl (Gleason & Britton, 1976). This dihedral angle is sometimes smaller in other similar compounds; for example, the same perfluorobiphenyl, when cocrystallized with biphenyl (Naae, 1979), presents an angle of 50.5°. These values are much larger and differ less than those found for 2,2',6,6'-unsubstituted biphenyls; for example, in the previously cited work of Naae (1979), biphenyl shows a dihedral angle of 36.4°, while in *p*-terphenyl (Hori & Nishiura, 1996), the same angle is near 0°.

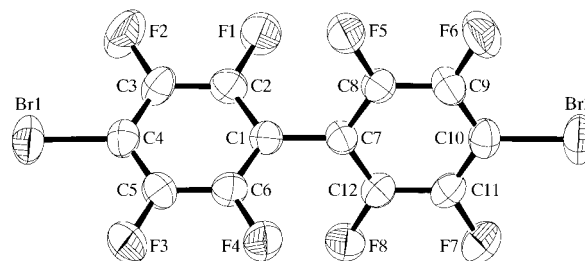


Figure 1

The molecular structure of (I) with the atom-numbering scheme, showing 50% probability displacement ellipsoids.

The packing of (I) is characterized by a pair of molecules linked through a centre of symmetry; rings C1–C6 and C1ⁱ–C6ⁱ [symmetry code: (i) $-x, -y, 1 - z$] are placed in such a way that there is a significant interaction between the π orbital of the C5–C6 bond and Br1ⁱ, with C··Br distances of 3.598 (4) and 3.699 (4) Å. The molecular minimum-inertia axes are parallel or, if related by a screw axis or a glide plane, nearly parallel. The molecules show a head-to-tail Br2··Br1ⁱⁱ contact [symmetry code: (ii) $x, y, 1 + z$] of 3.654 (1) Å, with Br··Br—C angles of 134.2 (1) and 136.0 (1)°.

Experimental

Compound (I) was obtained as a commercial product *ex* Aldrich. Suitable crystals of (I) were obtained from a solution in acetone.

Crystal data

C₁₂Br₂F₈
M_r = 455.94
Monoclinic, P2₁/n
a = 13.5489 (13) Å
b = 7.4975 (10) Å
c = 13.6783 (12) Å
β = 110.309 (8)°
V = 1303.1 (2) Å³
Z = 4

D_x = 2.324 Mg m⁻³
Mo Kα radiation
Cell parameters from 40
reflections
θ = 5.43–12.87°
μ = 6.308 mm⁻¹
T = 291 (1) K
Wedge, colourless
0.32 × 0.20 × 0.16 mm

Data collection

Siemens P4 diffractometer
2θ/ω scans
Absorption correction: ψ scan
(North *et al.*, 1968)
T_{min} = 0.253, T_{max} = 0.364
5995 measured reflections
2993 independent reflections
1594 reflections with I > 2σ(I)

R_{int} = 0.042
θ_{max} = 27.5°
h = 0 → 17
k = -9 → 9
l = -17 → 16
3 standard reflections
every 197 reflections
intensity decay: none

Refinement

Refinement on F^2

$$R[F^2 > 2\sigma(F^2)] = 0.034$$

$$wR(F^2) = 0.063$$

$$S = 0.830$$

2993 reflections

200 parameters

$$w = 1/[\sigma^2(F_o^2) + (0.0237P)^2]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.002$$

$$\Delta\rho_{\max} = 0.32 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.37 \text{ e } \text{\AA}^{-3}$$

Extinction correction: *SHELXL97*
(Sheldrick, 1997)

Extinction coefficient: 0.0015 (3)

Data collection: *XSCANS* (Siemens, 1991); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1983).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: NA1487). Services for accessing these data are described at the back of the journal.

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