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Decabromodiphenylethane

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.010 Å
R factor = 0.043
wR factor = 0.121
Data-to-parameter ratio = 20.4

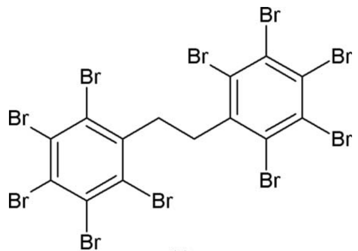
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Decabromodiphenylethane [systematic name: 1,1′-ethane-1,2-diylbis(pentabromobenzene)], $C_{14}H_4Br_{10}$ (DBDPE), was crystallized from toluene. The molecule shows crystallographic inversion symmetry. The C—Br distances are in the range 1.873 (7)–1.891 (6) Å; intermolecular Br$\cdots$Br contacts contribute to the formation of ribbons.

Comment

The title compound is a novel additive brominated flame retardant, introduced as a non-diphenyl oxide-based alternative to brominated diphenyl ethers (BDE). In contrast to BDE, DBDPE produces under pyrolysis conditions no polybrominated dibenzo-*p*-dioxins (Kierkegaard *et al.*, 2004) and during thermal decomposition no formation of furans was observed (Jakab *et al.*, 2003). Until now, DBDPE is not as widely used as the decabromodiphenylether (BDE 209), because of its higher costs. Thus, DBDPE is still expected to become one of the major brominated flame retardants. It is used by the thermoplastics industry since current restrictions on the use of certain hazardous substances in electrical and electronic equipment prevent further use of PBDE-containing materials in the European Union (EU Directive 2002/95/EC).

The occurrence of DBDPE in environmental samples has been the subject of intensive studies, whereas the crystal structure has not been reported so far. A knowledge of the three-dimensional structure is necessary for the understanding of the degradation process and potential accumulation in the environment.



(I)

The average C—Br distance in the centrosymmetric title compound, (I) (Fig. 1), is 1.880 (8) Å, in good agreement with those in BDE [1.893 (10) Å] and comparable compounds in the Cambridge Structural Database (Version 5.27; Allen, 2002) [for example 1.914 (7) Å (BAJVOX; Capon *et al.*, 1981) and 1.867 (14) Å (TEDDIP; Ilin *et al.*, 1996)]. The packing of the molecules is mainly influenced by Br$\cdots$Br interactions. The observed Br$\cdots$Br contacts range from 3.659 (3) to 3.699 (3) Å and can be classified as type II contacts which are polarization-induced and contribute actively to crystal structure stabilization (Pedireddi *et al.*, 1994), leading to the formation of ribbons of DBDPE molecules running along the *c* axis and arranged parallel to the ($3\overline{2}0$) plane.

Weak π–π interactions between aromatic rings of neighboring molecules (symmetry operator for the second molecule: $1 - x$, $-y$, $1 - z$) with a centroid–centroid distance of 4.037 (5) Å, a perpendicular distance from the centroid of one ring to the plane of the other ring of 3.615 (5) Å and an interplanar angle of α = 0° between adjacent rings can be observed (Fig. 2).

Experimental

Decabromodiphenylethane was obtained commercially and was, according to its poor solubility in solvents, purified by pressurized fluid extraction. The purified compound was handled in the absence of light to prevent photodegradation. Colourless crystals of this material were grown by solvent evaporation from toluene at ambient temperature. M.p. 622.1 K (DSC, onset, 5 mg).

Crystal data

$C_{14}H_4Br_{10}$
M_r = 971.17
Triclinic, $P\overline{1}$
a = 7.864 (5) Å
b = 7.970 (4) Å
c = 9.116 (5) Å
α = 94.095 (7)°
β = 107.198 (8)°
γ = 112.263 (8)°
V = 494.1 (5) Å^3
Z = 1
D_x = 3.264 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 20.27 mm^{-1}
T = 273 (2) K
Block, colorless
0.12 × 0.10 × 0.10 mm

Data collection

Bruker APEX CCD area-detector diffractometer
ω scan
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{\min}$ = 0.108, $T_{\max}$ = 0.132
3366 measured reflections
2247 independent reflections
1491 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.021
$\theta_{\max}$ = 27.6°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.121
S = 1.02
2247 reflections
110 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 1.2587P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max}$ = 0.94 e Å^{-3}
$\Delta\rho_{\min}$ = −0.97 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0022 (6)

The H atoms were located in difference maps but positioned with idealized geometry and refined using a riding model, with C—H = 0.97 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *SHELXTL* (Bruker 1997); software used to prepare material for publication: *SHELXL97*.

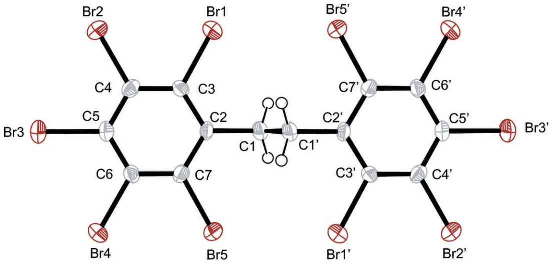


Figure 1
The molecular structure of DBDPE with the atom labeling; displacement ellipsoids are drawn at the 50% probability level. (Symmetry operator for primed atoms: $1 - x$, $1 - y$, $1 - z$.)

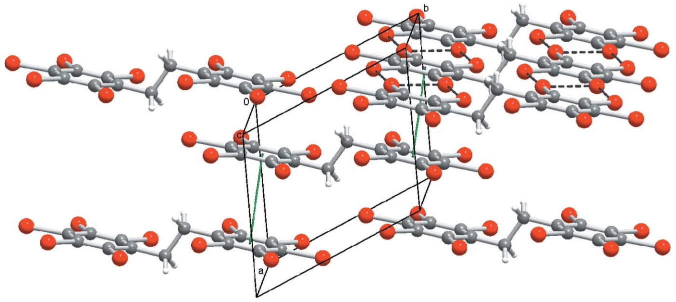


Figure 2
The crystal packing, showing the ribbons of DBDPE molecules running along the *c* axis, connected by Br···Br contacts (dashed lines). The weak π–π interactions are indicated by thin green lines.

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