Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,1,1,3,3,3-Hexafluoro-2,2-bis[4-(4-nitrophenoxy)phenyl]propane

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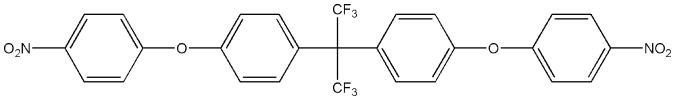
Received 5 July 2008; accepted 15 July 2008

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; R factor = 0.045; wR factor = 0.092; data-to-parameter ratio = 12.5.

In the title compound, $C_{27}H_{16}F_6N_2O_6$, the nitro groups are almost coplanar with the aromatic rings to which they are attached [dihedral angles = 3.5 (5) and 6.2 (3)°]. The dihedral angles between adjacent aromatic rings are 78.07 (8) and 71.11 (8)° for nitrophenyl/phenyl and 69.50 (8)° for phenyl/phenyl. An intermolecular C—H$\cdots\pi$ interaction seems to be effective in the stabilization of the structure.

Related literature

For related literature, see: Liaw *et al.* (2005); Yang *et al.* (2003); Miyagawa *et al.* (2003); Leu *et al.* (2003); Zhou *et al.* (2001.



Experimental

Crystal data

$C_{27}H_{16}F_6N_2O_6$
M_r = 578.42
Monoclinic, $P2_1/c$
a = 25.523 (3) Å
b = 10.5530 (12) Å
c = 9.3869 (8) Å
β = 98.248 (8)°
V = 2502.2 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 173 (2) K
0.23 × 0.10 × 0.10 mm

Data collection

Stoe IPDSII two-circle diffractometer
Absorption correction: none
13020 measured reflections
4653 independent reflections
2651 reflections with $I > 2\sigma(I)$
R_{int} = 0.076

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.092
S = 0.91
4653 reflections
371 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C46—H46$\cdots Cg1^{i}$	0.95	3.04	3.710	129

Symmetry code: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$. $Cg1$ is the centroid of the C31–C36 ring.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

The authors are grateful to the Department of Chemistry, Quaid-I-Azam University, Islamabad, Pakistan, and to the Institute for Inorganic Chemistry, University of Frankfurt, Germany, for providing laboratory and analytical facilities.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2089).

References

Leu, C. M., Chang, Y. T. & Wei, K. H. (2003). *Chem Mater*. **15**, 3721–3727.
Liaw, D. J., Chang, F. C., Leung, M., Chou, M. Y. & Muellen, K. (2005). *Macromolecules*, **38** 4024–4029.
Miyagawa, T., Fukushima, T., Oyama, T., Iijima, T. & Tomoi, M. (2003). *J. Polym. Sci. Part A Polym. Chem*. **41**, 861–871.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Stoe & Cie (2001). *X-AREA*. Stoe & Cie, Darmstadt, Germany.
Yang, C. P., Hsiao, S. H. & Wu, K. L. (2003). *Polymer*, **44**, 7067–7078.
Zhou, H. W., Liu, J. G., Qian, Z. G., Zhang, S. Y. & Yang, S. Y. J. (2001). *J. Polym. Sci. Part A Polym. Chem.* **39**, 2404–2413.