

C3a—C9a	1.555 (3)	1.557 (3)	1.542 (6)
C3a—C12	1.533 (4)	1.543 (4)	1.540 (6)
C3a—C4	1.563 (3)	1.562 (3)	1.568 (6)
C4—C5	1.542 (4)	1.548 (4)	1.531 (6)
C4—C13	1.545 (4)	1.542 (4)	1.537 (7)
C5—C6	1.560 (4)	1.556 (3)	1.559 (6)
C6—C7	1.537 (4)	1.549 (4)	1.526 (7)
C6—C14	1.540 (5)	1.544 (4)	1.544 (7)
C6—C15	1.523 (4)	1.511 (4)	1.526 (7)
C7—C8	1.534 (4)	1.543 (4)	1.543 (8)
C8—C9	1.564 (4)	1.557 (3)	1.573 (8)
C9—C9a	1.556 (3)	1.558 (3)	1.550 (6)
C9—C10	1.552 (4)	1.557 (4)	1.538 (7)
C9—C17	1.541 (4)	1.536 (4)	1.536 (6)
C10—C11	1.532 (4)	1.529 (4)	1.531 (7)
C10—C18	1.529 (4)	1.528 (4)	1.545 (8)
C11—C12	1.513 (4)	1.512 (4)	1.519 (8)
C15—C16	1.260 (4)	1.313 (5)	1.212 (8)
C2—C1—C9a	109.5 (2)	109.1 (2)	106.4 (4)
C1—C2—C3	105.5 (3)	105.7 (2)	107.2 (4)
C2—C3—C3a	105.9 (2)	106.1 (2)	105.5 (4)
C3—C3a—C9a	102.7 (2)	102.9 (2)	103.1 (3)
C4—C3a—C9a	115.2 (2)	116.3 (2)	116.9 (3)
C9a—C3a—C12	106.8 (2)	106.5 (2)	105.7 (3)
C3a—C4—C5	113.1 (2)	112.7 (2)	113.2 (3)
C4—C5—C6	114.7 (2)	116.0 (2)	117.3 (4)
C5—C6—C7	114.0 (2)	111.6 (2)	111.7 (4)
C6—C7—C8	120.3 (2)	119.5 (2)	120.9 (4)
C7—C8—C9	115.2 (2)	115.1 (2)	117.3 (4)
C9a—C9—C10	106.8 (2)	106.8 (2)	105.9 (4)
C8—C9—C9a	109.3 (2)	109.6 (2)	110.1 (4)
C1—C9a—C3a	101.6 (2)	101.9 (2)	102.4 (3)
C3a—C9a—C9	117.6 (2)	118.1 (2)	119.3 (3)
C9—C10—C11	111.3 (2)	111.3 (2)	113.1 (4)
C10—C11—C12	113.1 (2)	114.1 (2)	112.7 (4)
C3a—C12—C11	113.5 (2)	114.0 (2)	114.5 (4)
C3—C3a—C4—C13	-55.6 (3)	-53.0 (3)	-52.5 (5)
C13—C4—C5—O2	-10.5 (3)	-11.1 (3)	-12.7 (5)
C3a—C4—C5—C6	104.1 (3)	104.5 (2)	102.8 (4)
C4—C5—C6—C7	-63.3 (3)	-67.5 (3)	-65.9 (5)
O2—C5—C6—C14	55.2 (4)	55.3 (3)	55.5 (5)
C5—C6—C7—C8	63.7 (3)	66.8 (3)	66.6 (6)
C6—C7—C8—C9	-107.1 (3)	-108.8 (3)	-108.3 (5)
C3—C3a—C9a—C1	37.4 (3)	36.9 (3)	38.8 (4)
C4—C3a—C9a—C9	-70.9 (3)	-70.9 (3)	-69.8 (5)
C1—C9a—C9—C17	-52.6 (3)	-51.9 (3)	-52.8 (5)
C3a—C9a—C9—C8	66.4 (3)	65.4 (3)	64.6 (5)
O3—C8—C9—C17	48.7 (3)	50.5 (3)	46.4 (5)
C7—C8—C9—C9a	46.2 (3)	46.5 (3)	45.6 (5)
C17—C9—C10—C18	-60.7 (3)	-61.1 (3)	-58.5 (6)
C9a—C9—C10—C11	53.5 (3)	52.9 (3)	52.2 (5)
C8—C9—C10—C11	-66.4 (3)	-66.9 (3)	-67.5 (5)
C9—C10—C11—C12	-57.1 (3)	-55.8 (3)	-54.8 (6)
C10—C11—C12—C3a	56.6 (3)	54.9 (3)	54.2 (6)
C9a—C3a—C12—C11	-51.6 (3)	-49.9 (3)	-50.6 (5)

For all compounds, data collection: *XSCANS* (Fait, 1991); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structures: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structures: *SHELXL93* (Sheldrick, 1993); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL93*.

We thank the Servizio Italiano di Diffusione Dati Cristallografici del CNR (Parma) for the access to the Cambridge Data Files.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: NA1195). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

- Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435–436.
- Arigoni, D. (1968). *Pure Appl. Chem.* **17**, 331–348, and references therein.
- Berner, H., Vypel, H. & Schulz, G. (1987). *Tetrahedron*, **43**, 765–770, and references therein.
- Birch, A. J., Holzappel, C. W. & Rickards, R. W. (1966). *Tetrahedron*, **8**, 359–387.
- Dobler, M. & Dürr, B. G. (1975). *Cryst. Struct. Commun.* **4**, 259–264.
- Fait, J. (1991). *XSCANS Users Manual*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Hogenauer, G. (1979). *Mechanism of Action of Antibacterial Agents*, pp. 334–360. Edited by R. E. Kahn. New York: Springer-Verlag.
- Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
- Kavanagh, F., Hervey, A. & Robbins, W. J. (1951). *Proc. Natl Acad. Sci. USA*, **37**, 570–574.
- Kavanagh, F., Hervey, A. & Robbins, W. J. (1952). *Proc. Natl Acad. Sci. USA*, **38**, 555–560.
- Sheldrick, G. M. (1990). *SHELXL/PC Users Manual*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Sheldrick, G. M. (1993). *SHELXL93. Program for the Refinement of Crystal Structures*. Univ. of Göttingen, Germany.

Acta Cryst. (1995). **C51**, 2680–2683

3-Nitrodibenzofuran and 3-Iododibenzofuran

PENNY A. CHALONER, PETER B. HITCHCOCK AND
PETER G. SUTTON

*School of Chemistry and Molecular Sciences,
University of Sussex, Falmer, Brighton, England*

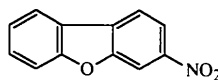
(Received 25 October 1993; accepted 18 July 1995)

Abstract

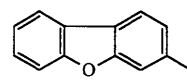
The structures of 3-nitrodibenzofuran, C₁₂H₇NO₃, and 3-iododibenzofuran, C₁₂H₇IO, have been determined. Both molecules are nearly planar and pack in herringbone patterns composed of symmetry related head-to-tail pairs with parallel π systems.

Comment

The title structures, 3-nitrodibenzofuran, (1), and 3-iododibenzofuran, (2), were determined as part of a study of the relationship between NMR spectroscopic parameters and molecular geometry in diphenyl ethers and dibenzofurans.



(1)



(2)

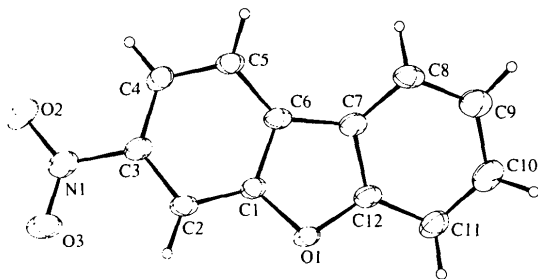


Fig. 1. The molecular structure and atom-numbering scheme for (1). Displacement ellipsoids are plotted at the 20% probability level.

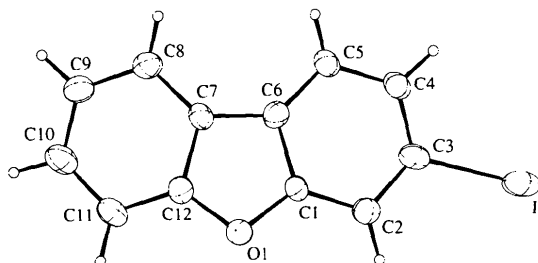


Fig. 2. The molecular structure and atom-numbering scheme for (2). Displacement ellipsoids are plotted at the 20% probability level.

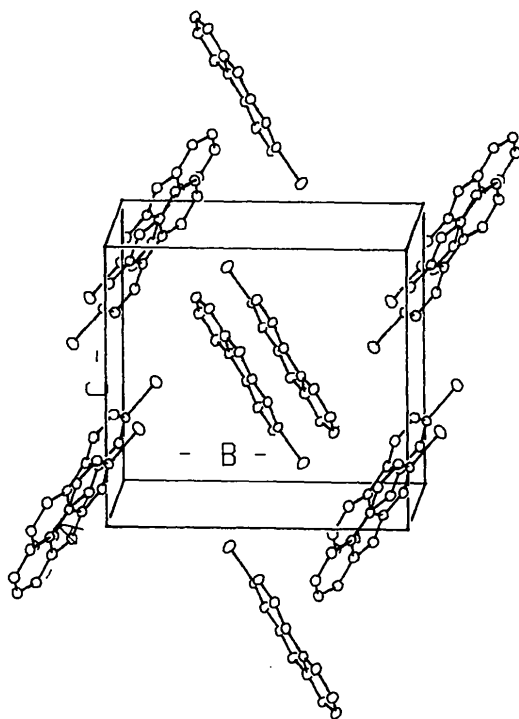


Fig. 3. Packing diagram for compound (2).

The structure of the parent dibenzofuran has been determined several times. The most reliable study was conducted at low temperature and indicated 9% disorder (Reppart, Gallucci, Lundstedt & Gerkin, 1984). The study reinterpreted the data published earlier in terms of similar disorder found in other samples investigated. The dibenzofuran molecule is nearly planar, as noted for both our structures and also for a number of dibenzofuran derivatives with increased substitution (Berg, Karlsson, Pilotti & Söderholm, 1978; Wagner & Malmros, 1979; Burden, Kemp, Wiltshire & Owen, 1984). Stacking has been noted for other related structures, including 3,4,7,8-tetrachlorodibenzofuran (Hubbard, Mighell & Pomerantz, 1978), but the most closely related structure is that of dibenzofuran-2-carbaldehyde, which packs in pairs related by inversion centres, with these pairs arranged in a close herringbone array (Fitzgerald, Gallucci, Gerkin & Rawal, 1991). This is the packing arrangement seen for both the title compounds, that for compound (2) being depicted in Fig. 3.

Experimental

3-Nitrodibenzofuran, (1) (m.p. 454–455 K), was prepared as essentially the sole product of the nitration of dibenzofuran with $\text{HNO}_3/\text{CF}_3\text{COOH}$ at 273 K (Keumi, Yamada, Takahashi & Kitajima, 1982) and recrystallized from trichloromethane. Reduction of the nitro compound using Fe/HCl gave the corresponding amine (Hazlet & Dornfield, 1941). Diazotization followed by reaction with potassium iodide gave 3-iododibenzofuran, (2) (m.p. 420–421.5 K, literature 416–418 K; Keumi, Umeda, Inoue & Kitajima, 1989), which was purified by recrystallization from aqueous ethanol.

Compound (1)

Crystal data

$\text{C}_{12}\text{H}_7\text{NO}_3$
 $M_r = 213.2$
 Triclinic
 $P\bar{1}$
 $a = 6.886(3) \text{ \AA}$
 $b = 7.106(3) \text{ \AA}$
 $c = 10.591(4) \text{ \AA}$
 $\alpha = 75.23(4)^\circ$
 $\beta = 84.72(3)^\circ$
 $\gamma = 69.46(3)^\circ$
 $V = 469.2(6) \text{ \AA}^3$
 $Z = 2$
 $D_x = 1.51 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation
 $\lambda = 0.71069 \text{ \AA}$
 Cell parameters from 25 reflections
 $\theta = 7\text{--}10^\circ$
 $\mu = 0.1 \text{ mm}^{-1}$
 $T = 293 \text{ K}$
 Needle
 $0.25 \times 0.25 \times 0.1 \text{ mm}$
 Pale yellow

Data collection

Enraf–Nonius CAD-4 diffractometer
 θ – 2θ scans
 Absorption correction: none
 1659 measured reflections
 1659 independent reflections
 1313 observed reflections
 $[F^2 > 2\sigma(F^2)]$

$\theta_{\text{max}} = 25^\circ$
 $h = 0 \rightarrow 8$
 $k = -8 \rightarrow 8$
 $l = -12 \rightarrow 12$
 2 standard reflections
 frequency: 60 min
 intensity decay: 1.2%

Refinement

Refinement on *F**R* = 0.047*wR* = 0.056*S* = 1.8

1313 reflections

173 parameters

All H-atom parameters refined

 $w = 1/\sigma^2(F)$ $(\Delta/\sigma)_{\max} = 0.01$ $\Delta\rho_{\max} = 0.22 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.4 \text{ e } \text{\AA}^{-3}$

Atomic scattering factors

from *MolEN* (Fair, 1990)

Data collection

Enraf-Nonius CAD-4 diffractometer

 θ - 2θ scansAbsorption correction: refined from ΔF

(DIFABS; Walker &

Stuart, 1983)

 $T_{\min} = 0.53$, $T_{\max} = 0.81$

1974 measured reflections

1815 independent reflections

1415 observed reflections

 $[F^2 > 2\sigma(F^2)]$ $R_{\text{int}} = 0.02$ $\theta_{\max} = 25^\circ$ $h = 0 \rightarrow 7$ $k = 0 \rightarrow 15$ $l = -14 \rightarrow 14$

2 standard reflections

frequency: 60 min

intensity decay: 1.0%

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (\AA^2) for (1)

$$U_{\text{eq}} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq}
O1	0.2069 (2)	0.6861 (2)	0.10467 (11)	0.044 (1)
O2	0.2601 (2)	0.7964 (3)	-0.46901 (13)	0.079 (1)
O3	0.5224 (2)	0.7165 (3)	-0.34461 (14)	0.076 (1)
N	0.3370 (2)	0.7569 (2)	-0.36168 (14)	0.051 (1)
C1	0.1511 (2)	0.7227 (2)	-0.02325 (15)	0.035 (1)
C2	0.2880 (2)	0.7153 (2)	-0.12652 (15)	0.039 (1)
C3	0.1998 (2)	0.7584 (2)	-0.24737 (15)	0.039 (1)
C4	-0.0103 (2)	0.8039 (2)	-0.26583 (16)	0.043 (1)
C5	-0.1421 (2)	0.8069 (2)	-0.15935 (16)	0.041 (1)
C6	-0.0614 (2)	0.7674 (2)	-0.03622 (15)	0.035 (1)
C7	-0.1441 (2)	0.7575 (2)	0.09509 (15)	0.036 (1)
C8	-0.3403 (2)	0.7836 (2)	0.15202 (17)	0.046 (1)
C9	-0.3591 (3)	0.7627 (3)	0.28513 (18)	0.053 (1)
C10	-0.1881 (3)	0.7160 (3)	0.36186 (18)	0.055 (1)
C11	0.0078 (3)	0.6889 (3)	0.30884 (17)	0.049 (1)
C12	0.0231 (2)	0.7093 (2)	0.17557 (15)	0.038 (1)

Table 2. Selected geometric parameters (\AA , $^\circ$) for (1)

O1—C1	1.377 (2)	O1—C12	1.391 (2)
O2—N	1.223 (2)	O3—N	1.226 (2)
N—C3	1.466 (2)	C1—C2	1.376 (2)
C1—C6	1.396 (2)	C2—C3	1.383 (2)
C3—C4	1.388 (2)	C4—C5	1.381 (2)
C5—C6	1.387 (2)	C6—C7	1.448 (2)
C7—C8	1.398 (2)	C7—C12	1.387 (2)
C8—C9	1.378 (3)	C9—C10	1.387 (3)
C10—C11	1.380 (3)	C11—C12	1.380 (2)
C1—O1—C12	105.2 (1)	O2—N—O3	123.6 (2)
O2—N—C3	118.1 (2)	O3—N—C3	118.3 (1)
O1—C1—C2	124.2 (1)	O1—C1—C6	112.1 (1)
C2—C1—C6	123.7 (2)	C1—C2—C3	115.1 (1)
N—C3—C2	117.7 (1)	N—C3—C4	118.7 (1)
C2—C3—C4	123.6 (1)	C3—C4—C5	119.5 (2)
C4—C5—C6	119.0 (2)	C1—C6—C5	119.1 (1)
C1—C6—C7	105.1 (1)	C5—C6—C7	135.7 (1)
C6—C7—C8	135.4 (2)	C6—C7—C12	106.2 (1)
C8—C7—C12	118.4 (2)	C7—C8—C9	118.5 (2)
C8—C9—C10	121.2 (2)	C9—C10—C11	121.8 (2)
C10—C11—C12	116.0 (2)	O1—C12—C7	111.4 (1)
O1—C12—C11	124.5 (2)	C7—C12—C11	124.1 (2)

Compound (2)

Crystal data

C₁₂H₇IO*M_r* = 294.1

Monoclinic

*P*2₁/*n**a* = 6.245 (2) \AA *b* = 13.399 (5) \AA *c* = 11.899 (3) \AA $\beta = 98.14 (3)^\circ$ *V* = 986 (1) \AA^3 *Z* = 4*D_x* = 1.98 Mg m⁻³Mo *K*α radiation $\lambda = 0.71069 \text{ \AA}$

Cell parameters from 25 reflections

 $\theta = 7-10^\circ$ $\mu = 3.17 \text{ mm}^{-1}$ *T* = 293 K

Elongated cube

0.2 × 0.2 × 0.1 mm

Pale brown

Refinement

Refinement on *F**R* = 0.030*wR* = 0.038*S* = 1.2

1415 reflections

127 parameters

H-atom parameters not refined

 $w = 1/\sigma^2(F)$ $(\Delta/\sigma)_{\max} = 0.03$ $\Delta\rho_{\max} = 0.45 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.58 \text{ e } \text{\AA}^{-3}$

Atomic scattering factors

from *International Tables*for *X-ray Crystallography* (1974, Vol. IV)Table 3. Fractional atomic coordinates and equivalent isotropic displacement parameters (\AA^2) for (2)

$$U_{\text{eq}} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq}
I	0.12522 (7)	0.11611 (3)	0.37128 (4)	0.062 (1)
O	0.2667 (6)	-0.1002 (3)	-0.0006 (3)	0.045 (2)
C1	0.3297 (8)	-0.0631 (4)	0.1059 (4)	0.040 (3)
C2	0.2012 (9)	-0.0037 (4)	0.1666 (5)	0.043 (3)
C3	0.3004 (9)	0.0249 (4)	0.2727 (5)	0.043 (3)
C4	0.5082 (9)	-0.0023 (4)	0.3186 (5)	0.047 (3)
C5	0.6351 (9)	-0.0624 (4)	0.2568 (5)	0.047 (3)
C6	0.5465 (9)	-0.0939 (4)	0.1503 (5)	0.042 (3)
C7	0.6135 (8)	-0.1545 (4)	0.0624 (4)	0.040 (2)
C8	0.7989 (9)	-0.2082 (4)	0.0483 (5)	0.050 (3)
C9	0.7975 (9)	-0.2622 (5)	-0.0513 (5)	0.051 (3)
C10	0.6250 (9)	-0.2631 (5)	-0.1355 (5)	0.055 (3)
C11	0.4384 (9)	-0.2091 (4)	-0.1273 (5)	0.048 (3)
C12	0.4349 (9)	-0.1564 (5)	-0.0286 (5)	0.046 (3)

Table 4. Selected geometric parameters (\AA , $^\circ$) for (2)

I—C3	2.104 (6)	O—C1	1.367 (6)
O—C12	1.372 (7)	C1—C2	1.401 (8)
C1—C6	1.442 (7)	C2—C3	1.380 (7)
C3—C4	1.383 (8)	C4—C5	1.408 (8)
C5—C6	1.375 (8)	C6—C7	1.433 (8)
C7—C8	1.394 (8)	C7—C12	1.440 (7)
C8—C9	1.388 (9)	C9—C10	1.363 (8)
C10—C11	1.387 (8)	C11—C12	1.373 (8)
C1—O—C12	107.2 (4)	O—C1—C2	125.0 (4)
O—C1—C6	111.6 (5)	C2—C1—C6	123.4 (5)
C1—C2—C3	114.5 (5)	I—C3—C2	118.0 (4)
I—C3—C4	117.8 (4)	C2—C3—C4	124.2 (5)
C3—C4—C5	120.7 (5)	C4—C5—C6	118.3 (5)
C1—C6—C5	118.9 (5)	C1—C6—C7	104.5 (4)
C5—C6—C7	136.5 (5)	C6—C7—C8	135.5 (5)
C6—C7—C12	106.5 (5)	C8—C7—C12	118.0 (5)
C7—C8—C9	117.8 (5)	C8—C9—C10	122.8 (6)
C9—C10—C11	121.9 (5)	C10—C11—C12	116.4 (5)
O—C12—C7	110.3 (5)	O—C12—C11	126.5 (5)
C7—C12—C11	123.2 (5)		

For both compounds, non-H atoms were located by heavy-atom methods using *SHELXS86* (Sheldrick, 1985). Refinement was by full-matrix least-squares methods using *MolEN* (Fair, 1990). For compound (1), H-atom positions were refined

isotropically; for compound (2), H atoms were fixed in calculated positions with $U_{iso} = 1.3U_{eq}$ of the parent atom and not refined.

We thank the SERC and Zeneca for a SERC CASE award (to PGS).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and least-squares-planes data have been deposited with the IUCr (Reference: HU1087). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

- Berg, J.-E., Karlsson, B., Pilotti, A. M. & Söderholm, A. C. (1978). *Acta Cryst.* **B34**, 2041–2042.
- Burden, R. S., Kemp, M. S., Wiltshire, C. W. & Owen, J. D. (1984). *J. Chem. Soc. Perkin Trans.* 1, pp. 1445–1448.
- Fair, C. K. (1990). *MolEN. An Interactive Intelligent System for Crystal Structure Analysis*. Enraf–Nonius, Delft, The Netherlands.
- Fitzgerald, L. J., Gallucci, J. C., Gerkin, G. E. & Rawal, V. H. (1991). *Acta Cryst.* **C47**, 2134–2137.
- Hazlet, S. E. & Dornfield, C. A. (1941). *J. Am. Chem. Soc.* **66**, 1781–1782.
- Hubbard, C. R., Mighell, A. D. & Pomerantz, I. H. (1978). *Acta Cryst.* **B34**, 2381–2384.
- Keumi, U., Umeda, T., Inoue, Y. & Kitajima, H. (1989). *Bull. Chem. Soc. Jpn.* **62**, 89–95.
- Keumi, T., Yamada, H., Takahashi, H. & Kitajima, H. (1982). *Bull. Chem. Soc. Jpn.* **55**, 629–630.
- Reppart, W. J., Gallucci, J. C., Lundstedt, A. P. & Gerkin, G. E. (1984). *Acta Cryst.* **C40**, 1572–1576.
- Sheldrick, G. M. (1985). *SHELXS86. Program for the Solution of Crystal Structures*. Univ. of Göttingen, Germany.
- Wagner, A. & Malmros, G. (1979). *Acta Cryst.* **B35**, 2220–2222.
- Walker, N. & Stuart, D. (1983). *Acta Cryst.* **A39**, 158–166.

Acta Cryst. (1995). **C51**, 2683–2685

Hexyltris(2,4,6-trimethoxyphenyl)-phosphonium Iodide

PENNY A. CHALONER, R. M. HARRISON AND
PETER B. HITCHCOCK

*School of Chemistry and Molecular Sciences,
University of Sussex, Falmer, Brighton, England*

(Received 18 January 1994; accepted 21 November 1994)

Abstract

The structure of hexyltris(2,4,6-trimethoxyphenyl)-phosphonium iodide, $[(C_6H_13)(C_9H_{11}O_3)_3P]^+ \cdot I^-$, [HexylTMPP]I, shows slightly distorted tetrahedral geometry at the P atom. The alkyl chains are extended in parallel pairs.

Comment

We have been interested for some time in the use of phosphonium salts as materials for second harmonic generation (SHG) and in their solid-state ^{31}P NMR spectra. There has been considerable interest in the use of the basic hindered phosphine tris(2,4,6-trimethoxyphenyl)phosphine (TMPP) as a ligand in organometallic chemistry (Chen & Dunbar, 1991), and the structures of $[CH_3TMPP][Co_2Cl_6]$ (Dunbar, Quilleveré & Haefner, 1991) and $[CH_3TMPP]I$ (Chaloner, Harrison & Hitchcock, 1993) have been determined.

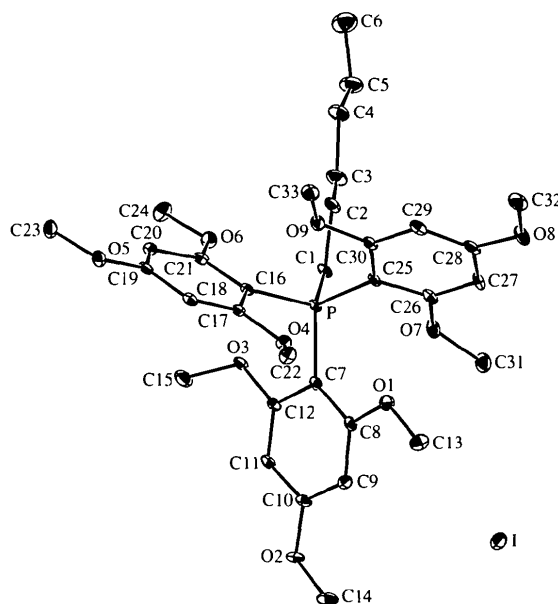
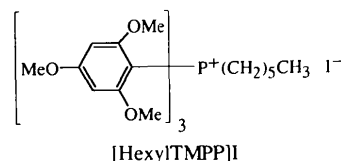


Fig. 1. Molecular structure and numbering scheme for [HexylTMPP]I.

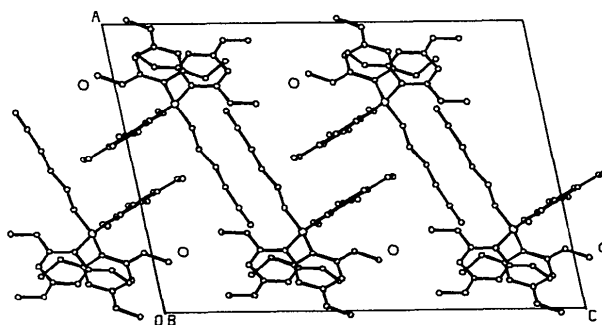


Fig. 2. Packing diagram for [HexylTMPP]I.