Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$$B_{eq} = \frac{8\pi^2}{3}\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
P(1)	0.41670 (5)	0.00680 (6)	0.25607 (5)	2.39 (2)
N(1)	0.4287 (1)	−0.1424 (2)	0.2603 (1)	2.58 (8)
N(2)	0.5000	0.0847 (3)	0.2500	2.5 (1)
C(1)	0.5000	−0.1944 (3)	0.2500	2.3 (1)
C(2)	0.5000	−0.3332 (3)	0.2500	2.4 (1)
C(3)	0.5576 (2)	−0.3985 (3)	0.2222 (2)	3.2 (1)
C(4)	0.5567 (2)	−0.5252 (3)	0.2213 (2)	3.8 (1)
C(5)	0.5000	−0.5903 (4)	0.2500	3.6 (2)
C(6)	0.4009 (2)	0.0591 (2)	0.3512 (2)	2.6 (1)
C(7)	0.4700 (2)	0.1276 (3)	0.4189 (2)	3.2 (1)
C(8)	0.4576 (2)	0.1638 (3)	0.4927 (2)	3.9 (1)
C(9)	0.3758 (3)	0.1353 (3)	0.4987 (2)	4.1 (1)
C(10)	0.3063 (2)	0.0686 (4)	0.4315 (2)	4.9 (2)
C(11)	0.3185 (2)	0.0304 (3)	0.3580 (2)	4.1 (1)
C(12)	0.3050 (2)	0.0401 (2)	0.1617 (2)	2.5 (1)
C(13)	0.2821 (2)	0.1608 (3)	0.1334 (2)	3.9 (1)
C(14)	0.1962 (2)	0.1889 (3)	0.0622 (2)	4.6 (1)
C(15)	0.1324 (2)	0.0981 (3)	0.0183 (2)	4.2 (1)
C(16)	0.1532 (2)	−0.0209 (3)	0.0459 (2)	4.1 (1)
C(17)	0.2390 (2)	−0.0514 (3)	0.1177 (2)	3.4 (1)

Table 2. *Geometric parameters* (Å, °)

P(1)—N(1)	1.626 (2)	C(7)—C(8)	1.382 (4)
P(1)—N(2)	1.601 (2)	C(8)—C(9)	1.371 (4)
P(1)—C(6)	1.798 (3)	C(9)—C(10)	1.372 (4)
P(1)—C(12)	1.799 (3)	C(10)—C(11)	1.382 (4)
N(1)—C(1)	1.334 (2)	C(12)—C(13)	1.382 (4)
C(1)—C(2)	1.504 (5)	C(12)—C(17)	1.387 (4)
C(2)—C(3)	1.382 (3)	C(13)—C(14)	1.379 (4)
C(3)—C(4)	1.372 (4)	C(14)—C(15)	1.363 (4)
C(4)—C(5)	1.378 (4)	C(15)—C(16)	1.358 (4)
C(6)—C(7)	1.383 (4)	C(16)—C(17)	1.390 (4)
C(6)—C(11)	1.387 (4)		

N(1)—P(1)—N(2)	116.4 (1)	P(1)—C(6)—C(11)	120.0 (2)
N(1)—P(1)—C(6)	109.5 (1)	C(7)—C(6)—C(11)	118.9 (3)
N(1)—P(1)—C(12)	106.7 (1)	C(6)—C(7)—C(8)	120.2 (3)
N(2)—P(1)—C(6)	109.1 (1)	C(7)—C(8)—C(9)	120.6 (3)
N(2)—P(1)—C(12)	110.6 (1)	C(8)—C(9)—C(10)	119.7 (3)
C(6)—P(1)—C(12)	103.8 (1)	C(9)—C(10)—C(11)	120.2 (3)
P(1)—N(1)—C(1)	120.1 (2)	C(6)—C(11)—C(10)	120.4 (3)
P(1)—N(2)—P(1′)	116.4 (2)	P(1)—C(12)—C(13)	119.5 (2)
N(1)—C(1)—N(1′)	130.1 (3)	P(1)—C(12)—C(17)	122.1 (2)
N(1)—C(1)—C(2)	114.9 (2)	C(13)—C(12)—C(17)	118.4 (3)
C(1)—C(2)—C(3)	120.8 (2)	C(12)—C(13)—C(14)	120.6 (3)
C(3)—C(2)—C(3′)	118.4 (3)	C(13)—C(14)—C(15)	120.6 (3)
C(2)—C(3)—C(4)	120.7 (3)	C(14)—C(15)—C(16)	119.6 (3)
C(3)—C(4)—C(5)	120.9 (3)	C(15)—C(16)—C(17)	120.8 (3)
C(4)—C(5)—C(4′)	118.4 (4)	C(12)—C(17)—C(16)	120.0 (3)
P(1)—C(6)—C(7)	121.1 (2)		

Symmetry code: (′) $1 - x, y, 0.5 - z$.

Space groups *C*2/*c* and *Cc* were indicated from systematic absences (hkl, $h + k = 2n + 1$ and $h0l$, $h = 2n + 1$ and $l = 2n + 1$); the former was chosen and confirmed by successful analysis. Data were corrected for Lorentz, polarization and absorption effects. The structure was solved by direct methods using *SAPI*91 (Fan, 1991). Refinement of the structure was by full-matrix least-squares calculations, initially with isotropic and finally with anistropic temperature factors for the non-H atoms. At an intermediate stage in the refinement a difference map revealed maxima consistent with the positions of the H atoms, which were incuded in the subsequent cycles of refinement with fixed isotropic temperature factors. All computer programs used in this study were part of the *TEXSAN* package (Molecular Structure Corporation, 1992) installed on a Silicon Graphics Personal Iris 4D/35 computer.

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Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55551 (21 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: BR1015]

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Structures of (*E*,*E*)-*o*-Nitroacetophenone Azine (I), (*E*,*Z*)-*o*-Nitroacetophenone Azine (II) and (*E*,*E*)-*o*-Nitrobenzaldehyde Azine (III)

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Abstract

In compounds (I) and (II) the *o*-nitro group is *anti* to the methyl group where as in (III), which lacks the methyl, it is *syn* to the H atom. Distortions from planarity indicate that the nitro group experiences

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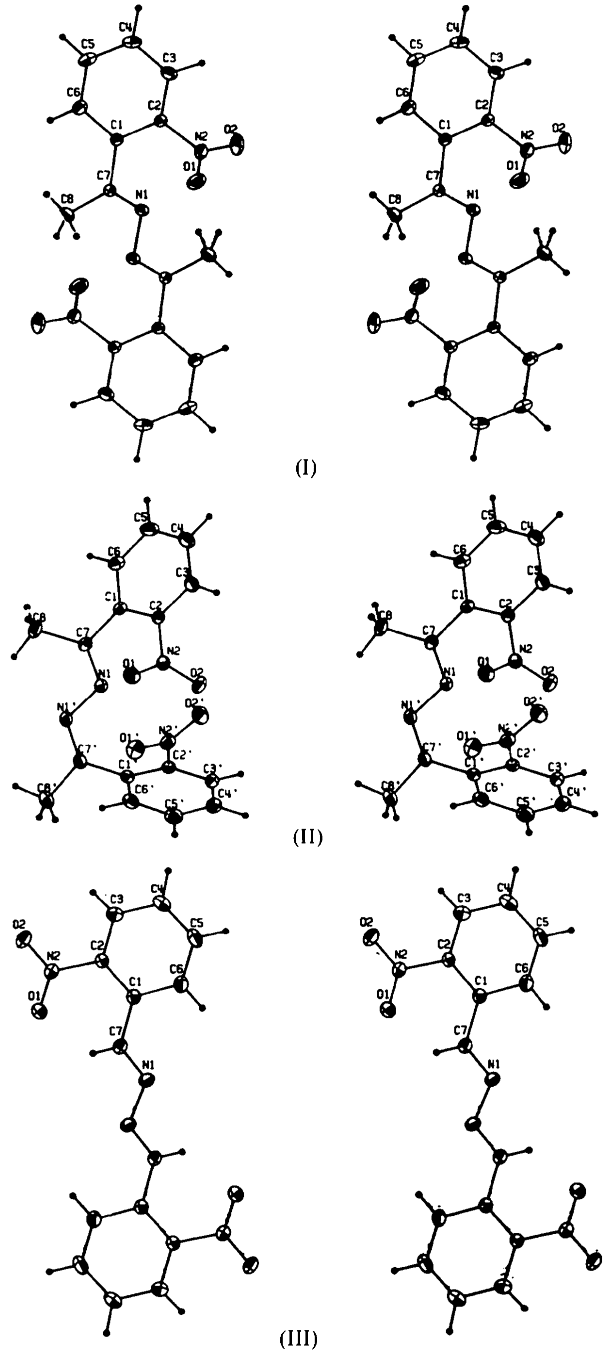
stronger repulsion from the lone pair on N than from CH.

Comment

The four pairs of C=N and N—N bond lengths determined here agree with each other within experimental error. They also agree with other accurately determined C=N and N—N distances in compounds containing the grouping Ph—C(*R*)=N—N=C(*R*)—Ph, where *R* = H or CH_3 (Mom & de With, 1978; García-Mina, Arrese, Martínez-Ripoll, García-Blanco & Serrano, 1982; Sereda, Antipin, Timofeeva & Struchkov, 1988). The torsion angle

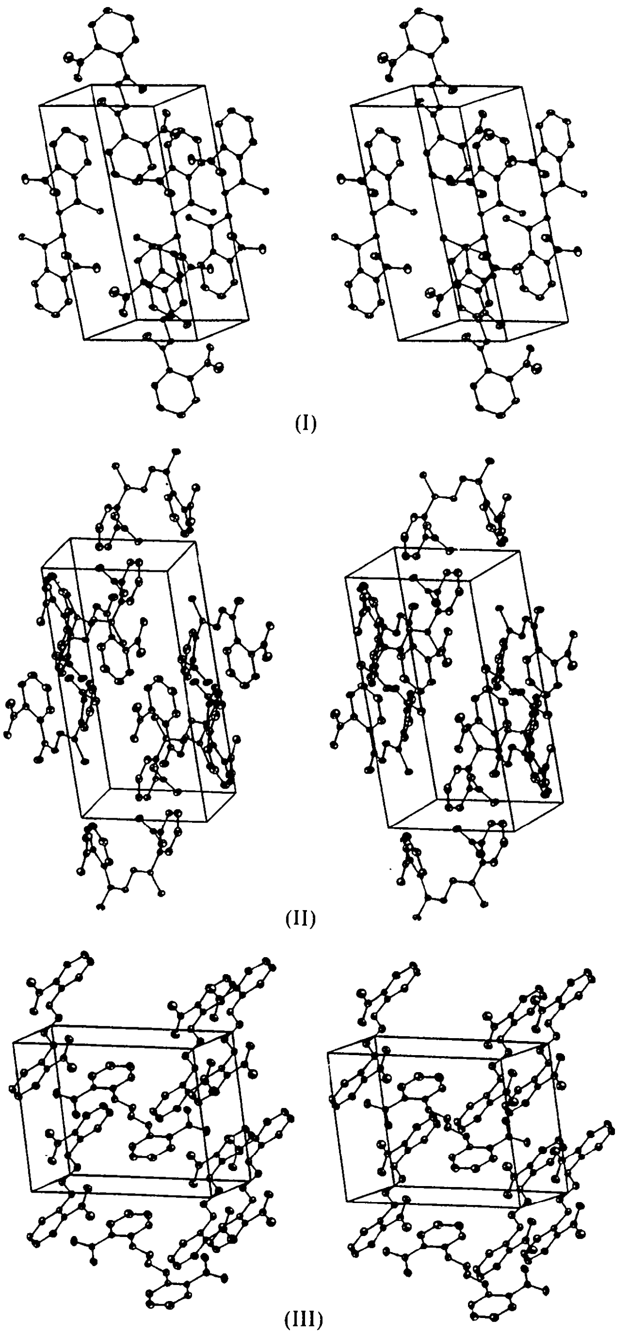


(I)

(II)

(III)

Fig. 1. *ORTEP*II (Johnson, 1976) stereodrawings of molecules (I), (II) and (III). Non-H atoms are represented as 20% probability thermal ellipsoids.



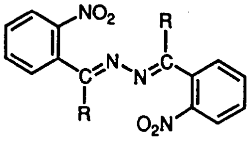
(I)

(II)

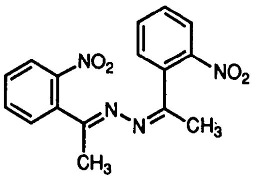
(III)

Fig. 2. The molecular packing in compounds (I), (II) and (III). In each diagram the *x* axis is horizontal and the *z* axis directed upward.

C—N—N—C is 166.1 (3)° in (II), the only molecule in which the planarity of this group is not demanded. The tendency of the phenyl group to be coplanar with the adjacent C=N is well established (Burke-Laing & Laing, 1976; García-Mina *et al.*, 1982; Ciajolo, Sirigu & Tuzi, 1985). In these compounds crowding between the *o*-nitro group and the adjacent CH (III) or N1 [(I) and (II), *E* isomer] causes the angle between the phenyl plane and C7=N1 to be 31.1, 38.5 and 37.0°, respectively; the NO_2 group deviates from the phenyl by 22.0, 52.0 and 59.2°. It appears that the lone pair on N1 causes a greater distortion than CH. Relevant non-bonded intramolecular contacts are C8···N1′ = 2.718 Å in (I), C8···N1′ = 2.731, O1···N1 = 2.953 and C6′···C8′ = 3.133 Å in (II), and C7···O1 = 2.672 Å in (III).



R = CH_3 (I), H (III)



(II)

Stereodrawings of the molecules are shown in Fig. 1 and packing diagrams (*ORTEP*II; Johnson, 1976) in Fig. 2. No C, N, O intermolecular contacts less than 3.4 Å are found in (I). In compound (II) there is a close contact N2···O2 = 3.204 Å between molecules related by the center of symmetry at $(0, 0, \frac{1}{2})$, and N2′···O1 = 3.217, C2···O2′ = 3.251 Å between molecules related by the **a** translation. In (III) the closest contacts are between molecules related by 2_1 at $x, z = \frac{1}{4}, \frac{1}{4}$, namely N2···O2 = 2.982, O1···O2 = 3.198 and C7···O2 = 3.247 Å.

Experimental

Compound (I)

Crystal data

$C_{16}H_{14}N_4O_4$
$M_r = 326.3$
Monoclinic
$P2_1/n$
$a = 7.815\ (2)$ Å
$b = 7.070\ (1)$ Å
$c = 14.475\ (3)$ Å
$\beta = 97.07\ (3)^\circ$
$V = 793.8\ (3)$ Å^3
$Z = 2$
$D_x = 1.365$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 15 reflections
$\theta = 10.4$–12.3°
$\mu = 0.109$ mm^{-1}
$T = 293$ K
Plate
0.4 × 0.35 × 0.1 mm
Pale yellow
Crystal source: from ethanol

Data collection

Syntex $P\bar{1}$ diffractometer
$\theta/2\theta$ scans
Absorption correction: none
2638 measured reflections
2325 independent reflections
1119 observed reflections $[I > 2.3\sigma(I)]$
$R_{\rm int} = 0.035$

$\theta_{\max} = 30^\circ$
$h = 0 \rightarrow 11$
$k = 0 \rightarrow 9$
$l = -20 \rightarrow 20$
3 standard reflections monitored every 100 reflections
intensity variation: none

Refinement

Refinement on F
Final $R = 0.055$
$wR = 0.040$
$S = 2.375$
1119 reflections
136 parameters

Only coordinates of H atoms refined
$w = \sigma^{-2}$
$(\Delta/\sigma)_{\max} = 0.142$
$\Delta\rho_{\max} = 0.24$ e Å^{-3}
$\Delta\rho_{\min} = -0.26$ e Å^{-3}

Compound (II)

Crystal data

$C_{16}H_{14}N_4O_4$
$M_r = 326.3$
Monoclinic
$P2_1/c$
$a = 7.713\ (1)$ Å
$b = 13.359\ (2)$ Å
$c = 15.557\ (2)$ Å
$\beta = 99.85\ (1)^\circ$
$V = 1579.3\ (4)$ Å^3
$Z = 4$
$D_x = 1.372$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 15 reflections
$\theta = 10.1$–11.8°
$\mu = 0.110$ mm^{-1}
$T = 293$ K
Plate
0.5 × 0.4 × 0.2 mm
Pale yellow
Crystal source: from ethanol

Data collection

Syntex $P\bar{1}$ diffractometer
$\theta/2\theta$ scans
Absorption correction: none
4059 measured reflections
3640 independent reflections
2393 observed reflections $[I > 2.3\sigma(I)]$
$R_{\rm int} = 0.037$

$\theta_{\max} = 27.5^\circ$
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 17$
$l = -19 \rightarrow 19$
3 standard reflections monitored every 100 reflections
intensity variation: none

Refinement

Refinement on F
Final $R = 0.044$
$wR = 0.033$
$S = 2.661$
2393 reflections
272 parameters

Only coordinates of H atoms refined
$w = \sigma^{-2}$
$(\Delta/\sigma)_{\max} = 0.054$
$\Delta\rho_{\max} = 0.21$ e Å^{-3}
$\Delta\rho_{\min} = -0.22$ e Å^{-3}

Compound (III)

Crystal data

$C_{14}H_{10}N_4O_4$
$M_r = 298.3$
Monoclinic
$P2_1/n$
$a = 11.905\ (3)$ Å
$b = 6.274\ (1)$ Å
$c = 9.176\ (1)$ Å
$\beta = 94.97\ (1)^\circ$

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 15 reflections
$\theta = 10.1$–12.0°
$\mu = 0.110$ mm^{-1}
$T = 293$ K
Prism

$V = 682.8$ (2) Å^3
$Z = 2$
$D_x = 1.451$ Mg m^{-3}

0.18 × 0.37 × 0.38 mm
Pale yellow
Crystal source: from ethanol

Data collection

Syntex $P\bar{1}$ diffractometer
$\theta/2\theta$ scans
Absorption correction: none
2248 measured reflections
2006 independent reflections
1102 observed reflections [$I > 2.3\sigma(I)$]
$R_{\text{int}} = 0.029$

$\theta_{\max} = 30°$
$h = 0 \rightarrow 16$
$k = 0 \rightarrow 8$
$l = -12 \rightarrow 12$
3 standard reflections monitored every 100 reflections intensity variation: none

Refinement

Refinement on F
Final $R = 0.051$
$wR = 0.038$
$S = 2.575$
1102 reflections
119 parameters

Only coordinates of H atoms refined
$w = \sigma^{-2}$
$(\Delta/\sigma)_{\max} = 0.039$
$\Delta\rho_{\max} = 0.26$ e Å^{-3}
$\Delta\rho_{\min} = -0.24$ e Å^{-3}

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$$B_{\text{eq}} = (8\pi^2/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
(I)				
C1	0.6230 (3)	0.3485 (4)	0.1868 (2)	2.7 (1)
C2	0.4719 (4)	0.3054 (4)	0.2246 (2)	3.1 (1)
C3	0.4606 (4)	0.2927 (5)	0.3118 (2)	4.0 (2)
C4	0.6099 (5)	0.3190 (5)	0.3797 (2)	4.5 (2)
C5	0.7644 (5)	0.3555 (5)	0.3458 (2)	4.1 (2)
C6	0.7714 (4)	0.3708 (5)	0.2503 (2)	3.4 (1)
C7	0.6253 (3)	0.3868 (4)	0.0862 (2)	2.6 (1)
C8	0.7770 (5)	0.3227 (6)	0.0399 (2)	4.4 (2)
N1	0.4952 (3)	0.4823 (4)	0.0479 (1)	3.1 (1)
N2	0.3123 (4)	0.2563 (5)	0.1625 (2)	4.6 (2)
O1	0.3226 (3)	0.1346 (4)	0.1038 (2)	5.8 (1)
O2	0.1803 (3)	0.3392 (5)	0.1765 (2)	8.4 (2)
(II)				
C1	0.0954 (3)	0.1940 (2)	0.7111 (1)	2.9 (1)
C2	0.0567 (3)	0.1538 (2)	0.6274 (1)	2.9 (1)
C3	−0.0223 (3)	0.2077 (2)	0.5553 (2)	3.9 (1)
C4	−0.0661 (4)	0.3063 (2)	0.5670 (2)	4.7 (1)
C5	−0.0303 (4)	0.3494 (2)	0.6484 (2)	4.8 (1)
C6	0.0502 (3)	0.2940 (2)	0.7201 (2)	4.1 (1)
C7	0.1843 (3)	0.1363 (2)	0.7880 (1)	2.9 (1)
C8	0.1262 (4)	0.1538 (2)	0.8744 (2)	4.3 (1)
N1	0.3040 (2)	0.0753 (1)	0.7738 (1)	3.3 (1)
N2	0.0862 (3)	0.0465 (1)	0.6121 (1)	3.4 (1)
O1	0.0108 (2)	−0.0146 (1)	0.6513 (1)	4.5 (1)
O2	0.1785 (2)	0.0251 (1)	0.5584 (1)	5.1 (1)
C1′	0.4916 (3)	−0.0862 (2)	0.7405 (1)	3.0 (1)
C2′	0.5732 (3)	−0.0313 (2)	0.6826 (1)	3.0 (1)
C3′	0.5846 (3)	−0.0634 (2)	0.5992 (2)	3.8 (1)
C4′	0.5137 (4)	−0.1558 (2)	0.5726 (2)	4.6 (2)
C5′	0.4332 (4)	−0.2127 (2)	0.6278 (2)	4.8 (2)
C6′	0.4214 (4)	−0.1784 (2)	0.7111 (2)	4.1 (2)
C7′	0.4739 (3)	−0.0528 (2)	0.8309 (1)	3.4 (1)
C8′	0.5628 (4)	−0.1164 (3)	0.9047 (2)	5.3 (2)
N1′	0.3830 (2)	0.0216 (2)	0.8491 (1)	3.6 (1)
N2′	0.6548 (3)	0.0651 (2)	0.7097 (1)	3.9 (2)
O1′	0.7262 (2)	0.0748 (1)	0.7859 (1)	5.0 (2)
O2′	0.6496 (3)	0.1310 (1)	0.6542 (1)	5.6 (2)
(III)				
C1	0.5021 (2)	−0.1274 (4)	0.2996 (3)	3.0 (1)
C2	0.5671 (2)	0.0529 (4)	0.2755 (3)	2.9 (1)
C3	0.5314 (2)	0.2154 (5)	0.1811 (3)	4.0 (1)
C4	0.4289 (3)	0.2024 (5)	0.1103 (3)	4.9 (2)
C5	0.3570 (3)	0.0285 (6)	0.1318 (3)	5.1 (2)
C6	0.3950 (2)	−0.1358 (5)	0.2238 (3)	4.2 (1)
C7	0.5420 (2)	−0.3078 (4)	0.3925 (3)	3.3 (1)
N1	0.4725 (2)	−0.4136 (3)	0.4612 (2)	3.7 (1)
N2	0.6788 (2)	0.0796 (4)	0.3562 (2)	3.6 (1)
O1	0.7004 (2)	−0.0174 (3)	0.4705 (2)	4.5 (1)
O2	0.7453 (2)	0.2019 (3)	0.3055 (2)	5.6 (1)

Table 2. *Geometric parameters* (Å, °)

	(I)	(II)	(II′)	(III)
C1—C2	1.394 (3)	1.392 (3)	1.393 (3)	1.399 (3)
C2—C3	1.381 (3)	1.384 (3)	1.382 (3)	1.380 (3)
C3—C4	1.385 (4)	1.379 (4)	1.384 (3)	1.376 (4)
C4—C5	1.382 (5)	1.374 (4)	1.372 (4)	1.382 (4)
C5—C6	1.393 (4)	1.393 (3)	1.391 (4)	1.383 (4)
C1—C6	1.397 (3)	1.394 (3)	1.390 (3)	1.399 (3)
C1—C7	1.483 (3)	1.489 (3)	1.503 (3)	1.471 (3)
C7—C8	1.501 (4)	1.505 (3)	1.497 (3)	
C2—N2	1.485 (3)	1.476 (3)	1.463 (3)	1.475 (3)
C7—N1	1.288 (3)	1.278 (3)	1.276 (3)	1.270 (3)
N1—N1′	1.420 (3)	1.418 (2)		1.424 (3)
N2—O1	1.218 (4)	1.223 (2)	1.225 (2)	1.221 (2)
N2—O2	1.225 (4)	1.220 (3)	1.229 (3)	1.222 (3)
C1—C2—C3	124.2 (2)	123.4 (2)	123.4 (3)	123.5 (2)
C2—C3—C4	118.0 (3)	118.3 (2)	118.2 (2)	118.3 (2)
C3—C4—C5	120.2 (3)	120.4 (2)	120.3 (2)	120.3 (3)
C4—C5—C6	120.6 (3)	120.5 (2)	120.6 (2)	120.7 (2)
C5—C6—C1	120.8 (2)	120.8 (2)	120.9 (2)	120.7 (2)
C2—C1—C6	116.2 (2)	116.6 (2)	116.6 (2)	116.4 (2)
C2—C1—C7	122.5 (2)	123.2 (2)	124.9 (2)	123.9 (2)
C6—C1—C7	121.1 (2)	120.3 (2)	118.5 (2)	119.6 (2)
C1—C7—C8	119.3 (2)	118.1 (2)	116.5 (2)	
C1—C7—N1	114.5 (2)	116.0 (2)	125.5 (2)	119.9 (2)
C8—C7—N1	126.2 (2)	126.0 (2)	117.9 (2)	
C7—N1—N1′	112.3 (2)	113.6 (2)	112.7 (2)	110.8 (2)
C3—C2—N2	115.5 (2)	115.7 (2)	116.8 (2)	116.5 (2)
C1—C2—N2	120.2 (2)	120.7 (2)	119.8 (2)	120.0 (2)
C2—N2—O1	117.6 (3)	117.9 (2)	118.1 (2)	119.2 (2)
C2—N2—O2	116.7 (3)	117.5 (2)	117.8 (2)	117.8 (2)
O1—N2—O2	125.6 (3)	124.5 (2)	124.0 (2)	123.0 (2)

For compounds (I)–(II) the atomic scattering factors for C, N, O were from Cromer & Liberman (1970) and for H from Stewart, Davidson & Simpson (1965). All structures were solved with *MULTAN* (Main, Woolfson, Lessinger, Germain & Declercq, 1974) and refined by full-matrix methods.

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55554 (20 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: SP1003]

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Structure of Dibenzofuran-d_8, $C_{12}D_8O$, at 173 K

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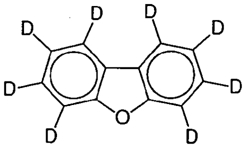
Abstract

Crystalline dibenzofuran-d_8 has been found to exhibit disorder of the type described previously for dibenzofuran. The disordered molecules are related to the ordered molecules by a 180° rotation about an axis passing through the molecular center of mass and perpendicular to the furan ring. In the present structure 11(2)% of the molecules were found to adopt this alternate orientation. The molecules are bisected by a mirror plane normal to the furan ring and containing the O atom. The average bond length in the benzenoid ring is 1.392 (10) Å. The furan ring and the benzenoid ring are separately planar, but form a dihedral angle of 1.45 (9)° with each other.

Comment

The crystal structure of dibenzofuran, $C_{12}H_8O$, as determined by Reppart, Gallucci, Lundstedt & Gerkin (1984), was found to manifest a type of disorder such that 9(2)% of the molecules are related to the ordered molecules by a 180° rotation about an axis passing through the molecular center of mass and perpendicular to the furan ring. The present study of the crystal structure of dibenzofuran-d_8, $C_{12}D_8O$ (I), was undertaken to determine to what extent such disorder might be present in this close analog of dibenzofuran.



(I)

Dibenzofuran-d_8 with a stated isotopic purity of 98.8 at. % was used as received from MSD Isotopes. The experimental sample was obtained by sublimation at low pressure. Analysis of the crystal structure showed that the type of disorder present in dibenzofuran is present also in dibenzofuran-d_8, and to a very similar extent: the refined population of the disordered molecule in the present study is 11(2)%.

Most bond lengths and angles for the ordered and disordered molecules of dibenzofuran-d_8 agree with the values for dibenzofuran within the combined e.s.d.'s; the three bond lengths which do not are found to agree within twice the combined e.s.d.'s. The average bond length for the benzenoid ring of dibenzofuran-d_8 is 1.392 (10) Å. The molecules are bisected by a mirror plane normal to the furan ring and containing O. The furan ring and benzene ring are separately planar, but form a dihedral angle of 1.45 (9)° with each other.

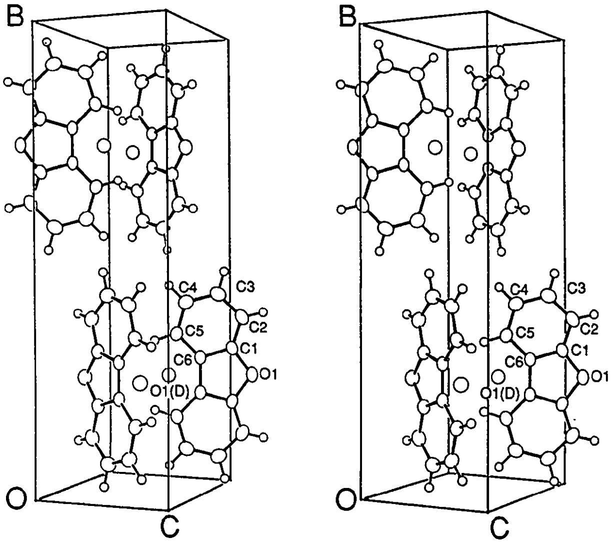


Fig. 1. A stereoview of the unit cell for dibenzofuran-d_8 drawn using *ORTEP*II (Johnson, 1976). One asymmetric unit is labeled using our numbering scheme. The position of the O atom of a disordered molecule is also shown.

Experimental

Crystal data

$C_{12}D_8O$
$M_r = 176.20$
Orthorhombic
Pnma
$a = 7.526$ (2) Å
$b = 19.107$ (2) Å
$c = 5.785$ (2) Å
$V = 831.9$ (4) Å^3
$Z = 4$
$D_x = 1.41$ Mg m^{-3}
Mo $K\bar{\alpha}$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 25 reflections
$\theta = 13.5–15.0°$
$\mu = 0.0786$ mm^{-1}
$T = 173$ (2) K
Plate
0.50 × 0.46 × 0.23 mm
Colorless
Crystal source: sublimation [temperature $\simeq$ 348(5) K; pressure $\simeq$ 13.33 Pa]

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