O2	0.2782 (2)	0.1323 (3)	0.6136 (4)	0.0408 (12)
O1	0.5024 (2)	0.2281 (3)	1.1439 (4)	0.0439 (12)
N1	0.2786 (3)	0.4071 (3)	0.7943 (4)	0.0350 (13)
N2	0.3358 (2)	0.4523 (3)	0.9108 (4)	0.0351 (12)
N3	0.4500 (3)	0.4031 (3)	1.1001 (4)	0.0338 (12)
C1	0.2928 (3)	0.3000 (4)	0.7815 (4)	0.0301 (13)
C2	0.3882 (3)	0.3762 (3)	0.9786 (5)	0.0283 (14)
C3	0.5045 (3)	0.3265 (4)	1.1789 (5)	0.0344 (14)
C4	0.5666 (4)	0.3717 (5)	1.3081 (6)	0.0528 (21)
N	0.1590 (2)	0.1591 (3)	0.7169 (4)	0.0286 (12)
S2′	0.0754 (1)	0.2164 (1)	0.7460 (1)	0.0272 (3)
S1′	0.1902 (1)	0.2447 (1)	1.0456 (1)	0.0291 (3)
O3′	0.0301 (2)	0.2935 (3)	0.6415 (3)	0.0397 (11)
O2′	0.0262 (2)	0.1258 (3)	0.7845 (4)	0.0403 (12)
O1′	0.3091 (3)	0.2462 (3)	1.2901 (4)	0.0502 (14)
N1′	0.0923 (3)	0.4007 (3)	0.9096 (4)	0.0374 (12)
N2′	0.1342 (3)	0.4487 (3)	1.0364 (4)	0.0409 (13)
N3′	0.2382 (3)	0.4098 (3)	1.2443 (4)	0.0369 (13)
C1′	0.1153 (3)	0.2965 (3)	0.9014 (4)	0.0270 (13)
C2′	0.1873 (3)	0.3779 (4)	1.1151 (4)	0.0309 (14)
C3′	0.3001 (3)	0.3427 (4)	1.3245 (4)	0.0315 (13)
C4′	0.3559 (4)	0.3966 (5)	1.4531 (6)	0.0458 (18)
O1*W*	0.4700 (2)	−0.0319 (3)	0.6934 (4)	0.0469 (13)
O2*W*	0.3768 (3)	0.0355 (4)	0.4153 (4)	0.0617 (16)

Table 2. *Selected geometric parameters* (Å, °)

S2—N	1.580 (4)	N—S2′	1.593 (4)
S2—O3	1.433 (3)	S2′—O3′	1.429 (3)
S2—O2	1.446 (4)	S2′—O2′	1.440 (4)
S2—C1	1.765 (4)	S2′—C1′	1.774 (4)
S1—C1	1.721 (4)	S1′—C1′	1.722 (4)
S1—C2	1.729 (4)	S1′—C2′	1.727 (5)
O1—C3	1.216 (6)	O1′—C3′	1.213 (6)
N1—N2	1.381 (5)	N1′—N2′	1.380 (5)
N1—C1	1.303 (6)	N1′—C1′	1.299 (5)
N2—C2	1.297 (5)	N2′—C2′	1.302 (6)
N3—C2	1.382 (6)	N3′—C2′	1.377 (5)
N3—C3	1.359 (6)	N3′—C3′	1.358 (6)
C3—C4	1.500 (7)	C3′—C4′	1.494 (7)
C1—S2—N	105.6 (2)	N—S2′—C1′	104.3 (2)
O2—S2—N	115.8 (2)	N—S2′—O2′	116.2 (2)
O3—S2—N	105.1 (2)	N—S2′—O3′	105.7 (2)
O3—S2—C1	105.2 (2)	O3′—S2′—C1′	106.0 (2)
O2—S2—C1	105.8 (2)	O2′—S2′—C1′	106.4 (2)
O2—S2—O3	118.2 (2)	O2′—S2′—O3′	117.0 (2)
C1—S1—C2	84.7 (2)	C1′—S1′—C2′	85.1 (2)
N2—N1—C1	111.3 (4)	N2′—N1′—C1′	111.6 (4)
N1—N2—C2	111.3 (4)	N1′—N2′—C2′	111.4 (4)
C2—N3—C3	123.7 (4)	C2′—N3′—C3′	123.3 (4)
S1—C1—N1	116.3 (3)	S1′—C1′—N1′	116.0 (3)
S2—C1—N1	120.1 (4)	S2′—C1′—N1′	121.2 (3)
S2—C1—S1	123.4 (3)	S2′—C1′—S1′	122.7 (2)
N2—C2—N3	120.8 (4)	N2′—C2′—N3′	121.0 (4)
S1—C2—N3	122.8 (3)	S1′—C2′—N3′	123.2 (4)
S1—C2—N2	116.4 (3)	S1′—C2′—N2′	115.8 (3)
O1—C3—N3	120.9 (5)	O1′—C3′—N3′	120.9 (4)
N3—C3—C4	115.8 (4)	N3′—C3′—C4′	115.6 (4)
O1—C3—C4	123.2 (5)	O1′—C3′—C4′	123.5 (5)
S2—N—S2′	124.4 (2)		

Table 3. *Contact distances* (Å)

S1···O1	2.667 (4)	O1*W*···O1^{ii}	2.795 (5)
S1′···O1′	2.661 (4)	O1*W*···O3′^{iii}	3.073 (5)
S1···S2	3.070 (2)	O1*W*···N1′^{iii}	2.944 (5)
S2···S2′	2.807 (3)	O1*W*···O2*W*	2.875 (5)
S1···S1′	3.552 (3)	O1*W*···O2*W*^{iv}	2.919 (6)
S1′···S2′	3.069 (2)	O2*W*···O1′^{v}	2.875 (6)
N3′···O2^{i}	3.030 (5)	O2*W*···O3^{vi}	3.051 (6)
N3···O2′^{i}	2.863 (5)	O2*W*···N1^{vi}	3.189 (6)

Symmetry codes: (i) $\frac{1}{2} - x, \frac{1}{2} + y, 2 - z$; (ii) $1 - x, -y, 2 - z$; (iii) $\frac{1}{2} + x, \frac{1}{2} - y, z$; (iv) $1 - x, -y, 1 - z$; (v) $x, y, z - 1$; (vi) $\frac{1}{2} - x, y - \frac{1}{2}, 1 - z$.

Data collection: Philips PW1100/10 software. Cell refinement: Philips PW1100/10 software. Data reduction: *STRUFA* (*ZOAK7*; Vicković, 1975). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELX*76 (Sheldrick, 1976). Molecular graphics: *PLUTON* (Spek, 1982), *ORTEP*II (Johnson, 1976).

This work was supported by the Ministry of Science, Technology and Informatics of the Republic of Croatia.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: KA1039). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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2-Nitrobiphenyl and 2,2′-Dinitrobiphenyl

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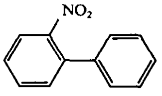
Abstract

2-Nitrobiphenyl, $C_{12}H_9NO_2$, and 2,2′-dinitrobiphenyl, $C_{12}H_8N_2O_4$, are not planar. The molecule of 2,2′-dinitrobiphenyl is located on a crystallographic twofold

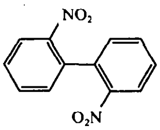
rotation axis and has C_2 symmetry. The dihedral angle between the two phenyl rings [(C1-C6)^(C7-C12)] and that between the phenyl ring and the nitro group [(C1-C6)^(N1,O2,O3)] are 63.1 (3) and 44.7 (4)°, respectively, for 2-nitrobiphenyl, and 62.6 (3) and 39.0 (4)°, respectively, for 2,2′-dinitrobiphenyl.

Comment

New triplet species for the title compounds (I) and (II) were detected by EPR after UV irradiation in ethanol glasses with an Xe-Hg lamp at 77 K (Tanigaki, Yagi & Higuchi, 1988). This work was undertaken to establish a relationship between the molecular structure and the triplet species.



(I)



(II)

Corresponding bond distances and angles are in good agreement with those of 4-nitrobiphenyl (III) (Casalone, Gavezzotti & Simonetta, 1973) and 4,4′-dinitrobiphenyl (IV) (Boonstra, 1963; Brock & Haller, 1984), whereas the torsion angles around the central C—C bond of the biphenyl group and the C—N bond are significantly different from those of the aforementioned *para*-substituted biphenyl molecules [33 and 2° about C—C in (III) and (IV), respectively, and 37.2 (3) and 6.6 (6)° about C—N in (III) and (IV), respectively]. The short intramolecular interatomic distances are 3.242 (4) and 3.239 (4) Å for N1···C8 and O1···C8, respectively, in 2-nitrobiphenyl, and 3.213 (3) and 3.116 (3) Å for N1···C5′ and O1···C5′, respectively, in 2,2′-dinitrobiphenyl. The relationship between the molecular structure and EPR spectra will be discussed elsewhere.

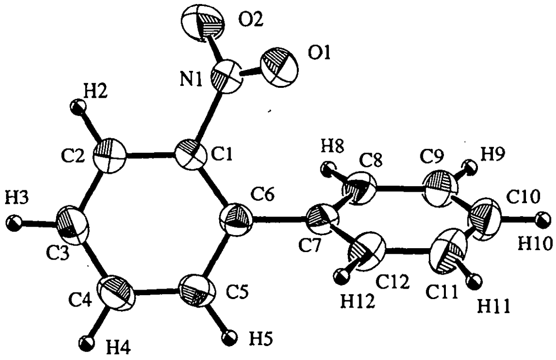


Fig. 1. Molecular structure of 2-nitrobiphenyl showing the labelling of the atoms. Displacement ellipsoids are shown at 30% probability.

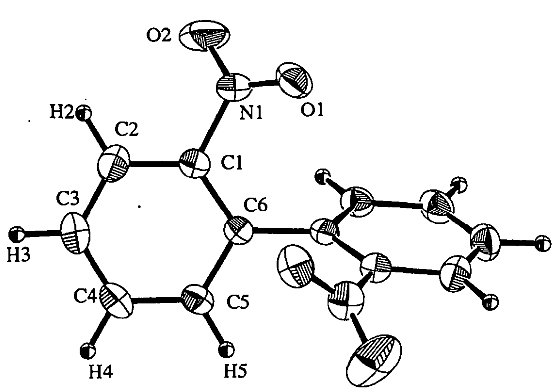


Fig. 2. Molecular structure of 2,2′-dinitrobiphenyl showing the labelling of the atoms. Displacement ellipsoids are shown at 30% probability.

Experimental

Compound (I)

Crystal data

$C_{12}H_9NO_2$
M_r = 199.21
Monoclinic
$P2_1/n$
a = 17.462 (1) Å
b = 7.5531 (4) Å
c = 7.8964 (5) Å
β = 98.937 (5)°
V = 1028.8 (1) Å^3
Z = 4
D_x = 1.29 Mg m^{-3}

Cu $K\alpha$ radiation
λ = 1.54184 Å
Cell parameters from 18 reflections
θ = 20-27.5°
μ = 0.641 mm^{-1}
T = 296.15 K
0.3 × 0.3 × 0.3 mm
Light yellow

Data collection

Rigaku AFC-4 diffractometer
ω-2θ scans
Absorption correction: none
1789 measured reflections
1789 independent reflections
1510 observed reflections [$F_o > 3.0\sigma(F_o)$]

θ_{max} = 62.5°
h = −20 → 20
k = 0 → 8
l = 0 → 8
3 standard reflections monitored every 50 reflections intensity variation: 3.9%

Refinement

Refinement on F
R = 0.089
wR = 0.107
S = 1.9
1510 reflections
172 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F) + 0.004F_o]$

$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for compound* (I)

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
C1	0.05984 (14)	0.1578 (3)	0.2775 (3)	0.0568
C2	0.00242 (17)	0.2811 (4)	0.2202 (4)	0.0671
C3	0.0145 (2)	0.4542 (4)	0.2693 (5)	0.0762

C4	0.0824 (2)	0.5020 (4)	0.3730 (5)	0.0797
C5	0.13815 (19)	0.3760 (4)	0.4307 (4)	0.0701
C6	0.12774 (15)	0.1986 (3)	0.3848 (3)	0.0562
C7	0.18730 (15)	0.0659 (3)	0.4556 (3)	0.0563
C8	0.16850 (17)	−0.0670 (4)	0.5643 (4)	0.0652
C9	0.2236 (2)	−0.1896 (5)	0.6334 (4)	0.0800
C10	0.2977 (2)	−0.1832 (5)	0.5950 (4)	0.0844
C11	0.31699 (19)	−0.0506 (6)	0.4893 (5)	0.0884
C12	0.26182 (17)	0.0745 (5)	0.4186 (4)	0.0720
N1	0.04658 (15)	−0.0237 (3)	0.2126 (4)	0.0705
O1	0.09879 (15)	−0.1006 (3)	0.1608 (4)	0.0923
O2	−0.01639 (15)	−0.0896 (3)	0.2099 (5)	0.1182

Table 2. *Geometric parameters* (Å, °) *for compound* (I)

C1—C2	1.391 (4)	C7—C8	1.392 (4)
C1—C6	1.381 (3)	C7—C12	1.379 (4)
C1—N1	1.469 (4)	C8—C9	1.385 (4)
C2—C3	1.371 (5)	C9—C10	1.374 (5)
C3—C4	1.380 (5)	C10—C11	1.378 (6)
C4—C5	1.387 (5)	C11—C12	1.402 (5)
C5—C6	1.392 (4)	N1—O1	1.205 (4)
C6—C7	1.489 (4)	N1—O2	1.204 (4)
C2—C1—C6	123.8 (2)	C6—C7—C8	119.9 (2)
C2—C1—N1	116.4 (2)	C6—C7—C12	121.1 (3)
C6—C1—N1	119.7 (2)	C8—C7—C12	119.0 (3)
C1—C6—C5	116.1 (2)	C1—N1—O1	118.8 (3)
C1—C6—C7	124.3 (2)	C1—N1—O2	119.1 (3)
C5—C6—C7	119.6 (2)	O1—N1—O2	122.1 (3)
N1—C1—C6—C7	−6.2 (4)	C1—C6—C7—C8	−62.9 (4)
C6—C1—N1—O1	−44.2 (4)		

Compound (II)

Crystal data

$C_{12}H_8N_2O_4$
M_r = 244.206
Monoclinic
$C2/c$
a = 13.067 (3) Å
b = 8.271 (2) Å
c = 10.634 (2) Å
β = 102.73 (2)°
V = 1121.1 (4) Å^3
Z = 4
D_x = 1.447 Mg m^{-3}

Mo $K\alpha$ radiation
λ = 0.71069 Å
Cell parameters from 25 reflections
θ = 14.4-15.0°
μ = 0.104 mm^{-1}
T = 296.15 K
Prism
0.5 × 0.45 × 0.3 mm
Light yellow

Data collection

Rigaku AFC-5*R* diffractometer
ω-2θ scans
Absorption correction: none
1445 measured reflections
1384 independent reflections
952 observed reflections [$I > 3.0\sigma(I)$]

$\theta_{\max}$ = 27.5°
h = 0 → 16
k = 0 → 10
l = −13 → 13
3 standard reflections monitored every 100 reflections intensity variation: 3.3%

Refinement

R = 0.046
wR = 0.065
S = 2.76
952 reflections
86 parameters
Only H-atom U's refined
Calculated weights $w = 1/\sigma^2(F)$

$(\Delta/\sigma)_{\max}$ = 0.03
$\Delta\rho_{\max}$ = 0.23 e Å^{-3}
$\Delta\rho_{\min}$ = −0.23 e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 3. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for compound* (II)

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
O1	−0.14274 (12)	0.4689 (2)	0.74630 (14)	0.0717
O2	−0.22097 (16)	0.3650 (4)	0.8822 (2)	0.1308
N1	−0.14456 (14)	0.3824 (2)	0.83736 (19)	0.0631
C1	−0.04927 (14)	0.2928 (2)	0.89809 (17)	0.0460
C2	−0.02598 (17)	0.2803 (3)	1.03117 (19)	0.0608
C3	0.06394 (19)	0.2012 (3)	1.09100 (19)	0.0645
C4	0.12841 (15)	0.1332 (3)	1.0191 (2)	0.0597
C5	0.10336 (13)	0.1457 (2)	0.88598 (18)	0.0506
C6	0.01398 (12)	0.2270 (2)	0.82195 (16)	0.0403

Table 4. *Geometric parameters* (Å, °) *for compound* (II)

O1—N1	1.208 (3)	C2—C3	1.373 (3)
O2—N1	1.206 (3)	C3—C4	1.376 (3)
N1—C1	1.470 (2)	C4—C5	1.385 (3)
C1—C2	1.384 (3)	C5—C6	1.389 (2)
C1—C6	1.389 (3)	C6—C6$^{\rm i}$	1.493 (2)
O1—N1—O2	123.5 (2)	C2—C1—C6	122.8 (2)
O1—N1—C1	119.1 (2)	C1—C6—C5	116.6 (2)
O2—N1—C1	117.4 (2)	C1—C6—C6$^{\rm i}$	123.7 (1)
N1—C1—C2	117.4 (2)	C5—C6—C6$^{\rm i}$	119.5 (2)
N1—C1—C6	119.8 (2)		
O1—N1—C1—C6	−38.3 (3)	N1—C1—C6—C6$^{\rm i}$	−6.3 (3)

Symmetry code: (i) $-x, y, \frac{3}{2} - z$.

The somewhat large *R* value for 2-nitrobiphenyl may be the result of bad crystallinity. For compound (I), data were collected using *AFC*-4 *Diffractometer Control Software* (Rigaku Corporation, 1974). The structure of (I) was solved using *MULTAN*78 (Main *et al.*, 1978) and refined with *SHELX*76 (Sheldrick, 1976). For compound (II), data were collected using *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1988). The structure of (II) was solved using *TEXSAN* (Molecular Structure Corporation, 1989). The figures were prepared using *ORTEP*II (Johnson, 1976).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: AS1085). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1994). C**50**, 1104–1106

Ein gesättigter anorganischer Phosphor(V)-Hydrazin-Schwefel(IV)-Sechsring mit Twist-Boot-Konformation

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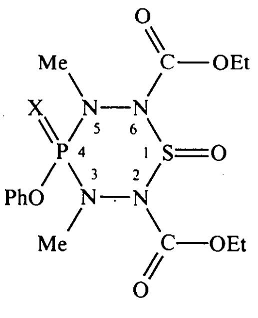
(*Eingegangen am* 3. *November* 1993; *angenommen am* 8. *Dezember* 1993)

Abstract

Diethyl 3,5-dimethyl-1-oxo-4-phenoxy-4-thioxo-1-thia-2,3,5,6-tetraaza-4λ^5-phosphacyclohexane-2,6-dicarboxylate, $C_{14}H_{21}N_4O_6PS_2$, was synthesized as a second example of an inorganic heterocycle containing sulfur(IV), phosphorus(V) and two substituted hydrazine units. The molecular structure is very similar to that of the corresponding P=O compound. It is the *E* isomer. The ring adopts a conformation between the boat and twist forms with large P—N—N—S torsion angles [75.4 (4) and 66.2 (6)°]. The mean N—N bond distance of 1.381 (7) Å is at the lower end of the expected range and there are, as in the P=O compound, two different S—N distances in the ring [1.713 (5) and 1.758 (6) Å].

Kommentar

Wir haben kürzlich über die Darstellung von schwefelhaltigen Phosphor(V)-Hydrazin-Sechsringen aus Dihydrazido-Derivaten der Phosphorsäure und Schwefel dichlorid bzw. Thionylchlorid und die Röntgenstruktur eines der Zielmoleküle (1) berichtet (Engelhardt & Simon, 1992, 1993). Jetzt gelang uns auch die Kristallisation der Verbindung (2), die ein entsprechendes Thiophosphorsäure-Derivat darstellt. Die Struktur wurde zum Vergleich der interessanten konformativen Eigenschaften dieser Ringe und ihrer Bindungsverhältnisse untersucht.



(1) $X = O$
(2) $X = S$

Die asymmetrische Einheit wird durch ein Molekül der Verbindung gebildet (Fig. 1). Es handelt sich um das Isomer mit *E*-Konfiguration: S am Phosphor und O am Schwefel befinden sich auf entgegengesetzten Seiten der gewellten 'Ringebene'. Dies ist die gleiche Konfiguration, wie sie für (1) gefunden wurde, obwohl (1) nach den Cahn-Ingold-Prelog'schen Prioritätsregeln als *Z*-Isomeres bezeichnet werden muß. Dort hat die Phenoxy-Gruppe am Phosphor Vorrang vor dem endständigen Sauerstoff, da letzterer an Elementen der 3. Periode nicht als 'doppelt'-gebunden gerechnet wird (Cahn, Ingold & Prelog, 1966). Bezüglich der Ringkonformation besteht ebenfalls eine sehr grosse Ähnlichkeit zwischen (1) und (2), wie aus einem Vergleich der endocyclischen Torsionswinkel um die Bindungen im Ring hervorgeht (Fig. 2). Der Ring in (2) ist etwas stärker gewellt. Dies geht ausser aus den meist größeren Torsionswinkeln auch aus dem Ringfaltungsparameter Q = 0,744 (5) gegenüber Q = 0,739 (5) Å für (1) hervor (Cremer & Pople, 1975). Q ist ein Mass für die mittlere Abweichung der Ringatome von einer Bezugsebene. Die Ringfaltung läßt sich nach den gleichen Autoren durch einen weiteren Parameter q (°) beschreiben: Werte für (2) und [(1)] q = 87,6 (4) [85,2 (3)]°. q = 0° entspricht einer reinen Sessel-, q = 90° einer reinen Twist- bzw. Boot-Konformation. Ein dritter Parameter Φ beschreibt schliesslich die Lage auf dem sogenannten Pseudorotationscyclus zwischen Boot- und Twist-Konformationen: Φ = 291,2 (3) [296,1 (3)]°. Φ = 270° entspricht einer reinen Twist-, Φ = 300° einer reinen Boot-Konformation. Bei (2) ist die Boot-Konformation demnach deutlich stärker in Richtung auf eine Twist-Konformation verdrillt.

In beiden Verbindungen nehmen die Phenoxy-Gruppe am P und der Sauerstoff am S 'axiale' Positionen ein, während S bzw. [O] am Phosphor mehr in äquatorialer Richtung stehen. Auffällig ist auch die unterschiedliche Stellung der beiden Ethoxycarbonyl-Substituenten. Während der an N(4) äquatorial ausgerichtet ist, besitzt der an N(2) eine quasi-axiale Stellung. Auch dieses Phänomen findet sich ganz analog in der Verbindung (1). Beide Verbindungen zeigen auch zwei auffällig ver-