C(4')	0.4820 (3)	0.7579 (4)	0.5711 (2)	0.045 (1)
C(5')	0.5671 (4)	0.5655 (4)	0.6407 (2)	0.057 (2)
C(6')	0.6499 (4)	0.4531 (4)	0.6494 (2)	0.068 (2)
C(7')	0.7325 (5)	0.4056 (5)	0.6014 (2)	0.075 (2)
C(8')	0.7329 (4)	0.4704 (4)	0.5459 (3)	0.066 (2)
C(9')	0.6485 (4)	0.5885 (4)	0.5353 (2)	0.053 (1)
C(10')	0.5631 (4)	0.6390 (4)	0.5835 (2)	0.045 (1)
O(1)	0.1391 (3)	1.0693 (2)	0.6352 (1)	0.062 (1)
C(10)	0.1559 (4)	1.1538 (4)	0.6837 (2)	0.068 (2)
O(2)	0.1723 (4)	1.1165 (3)	0.7375 (1)	0.115 (1)
C(11)	0.1518 (6)	1.2963 (4)	0.6630 (2)	0.083 (2)
O(3)	0.4665 (2)	0.9518 (2)	0.6368 (1)	0.053 (1)
C(12)	0.5811 (4)	0.9531 (4)	0.6825 (2)	0.057 (1)
O(4)	0.6230 (3)	0.8561 (2)	0.7119 (1)	0.088 (1)
C(13)	0.6494 (5)	1.0886 (4)	0.6904 (2)	0.074 (2)

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

N(1)—C(2)	1.466 (4)	C(2')—C(3')	1.402 (5)
N(1)—C(6)	1.466 (5)	C(3')—C(4')	1.368 (5)
N(1)—C(7)	1.477 (4)	C(4')—C(10')	1.408 (5)
C(2)—C(3)	1.532 (4)	C(5')—C(6')	1.352 (5)
C(2)—C(9)	1.520 (4)	C(5')—C(10')	1.416 (5)
C(3)—C(4)	1.517 (5)	C(6')—C(7')	1.394 (6)
C(3)—O(1)	1.457 (5)	C(7')—C(8')	1.345 (7)
C(4)—C(5)	1.534 (6)	C(8')—C(9')	1.412 (6)
C(4)—C(8)	1.530 (5)	C(9')—C(10')	1.424 (5)
C(5)—C(6)	1.529 (6)	O(1)—C(10)	1.331 (4)
C(7)—C(8)	1.530 (5)	C(10)—O(2)	1.195 (4)
C(9)—C(4')	1.512 (5)	C(10)—C(11)	1.500 (5)
C(9)—O(3)	1.466 (4)	O(3)—C(12)	1.333 (4)
N(1')—C(2')	1.305 (5)	C(12)—O(4)	1.199 (4)
N(1')—C(9')	1.372 (5)	C(12)—C(13)	1.495 (5)
C(2)—N(1)—C(6)	109.8 (2)	C(2')—C(3')—C(4')	120.2 (3)
C(2)—N(1)—C(7)	107.8 (2)	C(9)—C(4')—C(10')	122.6 (3)
C(6)—N(1)—C(7)	108.1 (3)	C(3')—C(4')—C(10')	117.9 (3)
N(1)—C(2)—C(3)	112.1 (3)	C(6')—C(5')—C(10')	121.5 (3)
N(1)—C(2)—C(9)	111.2 (3)	C(5')—C(6')—C(7')	120.2 (4)
C(3)—C(2)—C(9)	111.9 (3)	C(6')—C(7')—C(8')	121.2 (4)
C(2)—C(3)—C(4)	108.2 (3)	C(7')—C(8')—C(9')	120.0 (4)
C(2)—C(3)—O(1)	107.8 (3)	N(1')—C(9')—C(8')	117.1 (3)
C(4)—C(3)—O(1)	110.7 (3)	N(1')—C(9')—C(10')	123.0 (3)
C(3)—C(4)—C(5)	107.4 (3)	C(8')—C(9')—C(10')	119.9 (3)
C(3)—C(4)—C(8)	109.8 (3)	C(4')—C(10')—C(5')	125.1 (3)
C(5)—C(4)—C(8)	108.3 (3)	C(4')—C(10')—C(9')	117.9 (3)
C(4)—C(5)—C(6)	108.5 (3)	C(5')—C(10')—C(9')	117.1 (3)
N(1)—C(6)—C(5)	112.0 (3)	C(3)—O(1)—C(10)	118.9 (3)
N(1)—C(7)—C(8	112.4 (3)	O(1)—C(10)—O(2)	121.9 (3)
C(4)—C(8)—C(7)	108.0 (3)	O(1)—C(10)—C(11)	112.9 (3)
C(2)—C(9)—C(4')	114.9 (3)	O(2)—C(10)—C(11)	125.2 (3)
C(2)—C(9)—O(3)	103.8 (2)	C(9)—O(3)—C(12)	118.3 (2)
C(4')—C(9)—O(3)	108.1 (3)	C(3)—C(12)—O(4)	123.0 (3)
C(2')—N(1')—C(9')	116.7 (3)	O(3)—C(12)—C(13)	111.1 (3)
N(1')—C(2')—C(3')	124.4 (4)	O(4)—C(12)—C(13)	125.8 (3)
N(1)—C(2)—C(3)—C(4)	−9.2 (4)	C(3)—C(2)—N(1)—C(6)	−52.9 (3)
N(1)—C(6)—C(5)—C(4)	−4.8 (4)	C(3)—C(2)—N(1)—C(7)	64.6 (3)
N(1)—C(7)—C(8)—C(4)	−5.7 (4)	C(5)—C(6)—N(1)—C(2)	60.9 (3)
C(2)—C(3)—C(4)—C(5)	64.4 (4)	C(5)—C(6)—N(1)—C(7)	−56.4 (4)
C(2)—C(3)—C(4)—C(8)	−53.2 (4)	C(8)—C(7)—N(1)—C(2)	−55.5 (3)
C(6)—C(5)—C(4)—C(3)	−56.7 (4)	C(8)—C(7)—N(1)—C(6)	63.1 (4)
C(6)—C(5)—C(4)—C(8)	61.8 (4)	O(1)—C(3)—C(2)—C(9)	105.3 (3)
C(7)—C(8)—C(4)—C(3)	61.4 (4)	C(3)—C(2)—C(9)—C(4')	179.1 (3)
C(7)—C(8)—C(4)—C(5)	−55.5 (4)	C(3)—C(2—C(9)—O(3)	−63.1 (3)

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Hexanitrodiphenylmethane

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Abstract

An X-ray diffraction study of a crystal of 2,2',-4,4',6,6'-hexanitrodiphenylmethane showed that the two phenyl rings are essentially planar and are nearly perpendicular to each other, confirming previous conclusions drawn from ^{13}C NMR measurements.

Comment

In the course of our studies into the effect of structure upon the intrinsic reactivity of carbon acids, we have examined a number of nitro-substituted diphenylmethanes (1a)–(1g) (Fig. 1). Both kinetic data for proton abstraction/carbanion reprotonation and spectroscopic measurements (^{1}H and ^{13}C NMR,

UV/visible) on the nitrohydrocarbons and their con-
jugated diphenylmethyl anions have led to the con-
clusion that steric effects become predominant in
governing the intrinsic reactivity of the diphenyl-
methane moiety when the molecules possess at least
three *ortho*-nitro groups. Although they showed that
rotation of the two phenyl rings around the C—C
exocyclic ring bonds is rapid in all the derivatives
(1*a*)–(1*g*) at probe temperature, the NMR spectra
have suggested that the introduction of a third *ortho*-
nitro group in the diphenylmethane moiety causes a
change in the conformation of the molecules.
2,2',4,4',6,6'-Hexanitro- and 2,2',4,4',6-pentanitro-
diphenylmethanes [(1*a*) and (1*b*)] would thus exist
preferentially in a perpendicular conformation while
the less substituted derivatives (1*c*)–(1*g*) would prefer
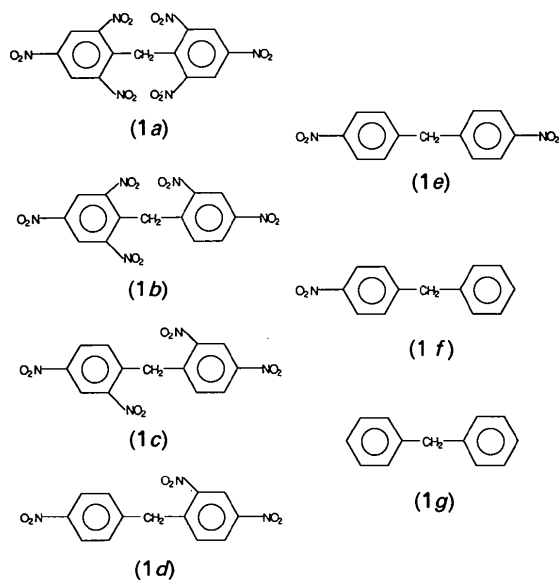a skew conformation.

Fig. 1. Structural formulae of compounds (1*a*)–(1*g*).

In view of the importance of precise structural
information in obtaining a better understanding of
the intrinsic reactivity of carbon acids, and notwith-
standing the occurrence of possible conformational
changes on going from the solid state to solution, we
have undertaken a structural study of the title com-
pound to check the preferred conformation inferred
from the NMR data.

The two aromatic rings are essentially planar
(deviations from the planes ≤ 0.02 Å) although the
valency angles are clearly distorted from the normal
120° around the most hindered positions (Fig. 2);
this is consistent with known substituent effects. The
steric hindrance caused by the presence of the four
ortho-nitro groups results in an inter-phenyl ring
angle of 84.65°. It thus appears that the two rings are

nearly perpendicular to each other. In the solid state,
the structure mimics very well the preferred con-
formations previously suggested for this molecule
following an NMR study carried out in dimethyl
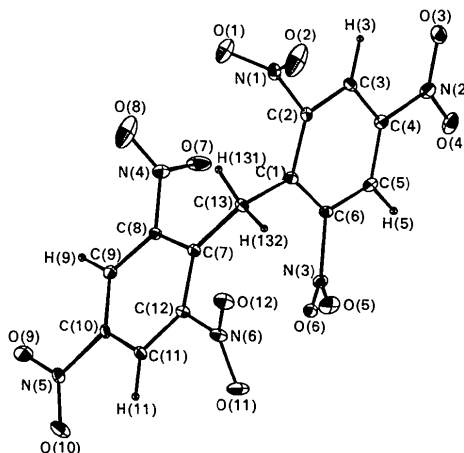sulfoxide solution (Simonnin, Xié, Terrier, Lelièvre
& Farrell, 1989).

Fig. 2. View of $C_{13}H_6N_6O_{12}$. H atoms are drawn as small circles of
arbitrary radii.

The orthogonal situation of the aromatic rings is
accompanied by an extensive rotation of the *ortho*-
nitro groups relative to these rings. The N(1)—
O(1)—O(2) and N(3)—O(5)—O(6) nitro groups are
tilted out of their aromatic planes by 83.38 and
34.57°, respectively. Similarly the N(4)—O(7)—O(8)
and N(6)—O(11)—O(12) nitro groups are twisted by
82.55 and 45.37° from the corresponding aromatic
rings. As expected the *para*-nitro groups are only
rotated slightly out of their respective aromatic
planes [6.38 and 9.47°, respectively, for the N(2)—
O(3)—O(4) and N(5)—O(9)—O(10) nitro groups].

The fact that two of the four *ortho*-nitro groups of
(1*a*) have twist angles of about 83° is remarkable as
the literature reports very few tilt angles of this order
of magnitude for nitro groups bonded to a sterically
hindered aromatic position. The twist angles of NO_2
groups are frequently in the range 35–60° when there
is only one substituent in an adjacent position. For
example, the two *ortho*-nitro groups of 2,4,6-tri-
nitrophenetole (Grammacioli, Destro & Simonetta,
1968) are twisted by 61.3 and 31.8° from the
aromatic ring while those of 2,4,6-trinitrotoluene in
its orthorhombic form are rotated by 60 and 45° out
of the attached phenyl ring in the most disfavored
structure (Carper, Davis & Extine, 1982). In fact,
larger tilt angles have only been measured for NO_2
groups located between two adjacent substituents;
examples include the 2-nitro groups of 2,4,6-trinitro-
m-xylene (Bryden 1972) and ethyl 3-methyl-
2,4,6-trinitrophenyl carbamate (Clifford & Dudis

1990) which appear to be twisted by 75 and 78.3°, respectively, from their attached aromatic planes. Another interesting example is 9-nitroanthracene in which the nitro group is tilted out of the planar carbocyclic system by 85° (Trotter, 1959) as a result of the presence of two adjacent *peri* H atoms. The twist angles (82.9 and 81.6°) found for two of the four *ortho*-nitro groups of (1a) approach this value, emphasizing the importance of the steric constraints in this tetra-*ortho*-nitro-substituted diphenylmethane.

The aromatic C—C distances are in the expected range (1.36–1.40 Å) with the benzene ring angles generally markedly greater than 120° at the positions of nitro substitution, as commonly found in nitro-aromatics. The two exocyclic C—C bonds [C(1)—C(13) 1.515 (7), C(7)—C(13) 1.529 (7) Å] compare well with available data for such systems, as do the C—NO_2 bonds which average 1.478 Å [C—NO_2 bonds average 1.478 and 1.468 Å in 2,4,6-tri-nitrotoluene (Carper, Davis & Extine, 1982) and 2,2′,4,4′,6,6′-hexanitrostilbene (Gérard & Hardy 1988), respectively]. In contrast to these results, the N—O bonds are not all in the usual range (1.19–1.22 Å) for aromatic NO_2 groups; although they are attached to their corresponding rings *via* normal C—N single bonds, the two *ortho*-nitro groups which are subject to the most extensive twistings show rather short N—O distances [N(1)—O(2) 1.116 (7), N(4)—O(8) 1.153 (8) Å]. Similar unusual N—O bond lengths have been reported, however; *e.g.* an N—O distance of 1.137 (8) Å has recently been quoted in a X-ray study of 2,4-dinitroanisole (Nyburg, Faerman, Prasad, Palleros & Nudelman, 1987) as well as a value of 1.13 Å in an old study of 4,4′-dinitrobiphenyl (Boonstra, 1963) and they probably arise from packing effects. A number of short intermolecular distances are observed [O(1)—O(12) ($\frac{1}{2}$ + x, $\frac{1}{2}$ − y, $\frac{1}{2}$ + z) 2.975 (9), C(10)—O(4)(2 − x, − y, 1 − z) 2.968 (7), C(5)—O(5)(2 − x, − y, 1 − z) 3.028 (7), O(10)—O(11)(1 − x, − y, − z) 2.951 (7) and O(9)—O(12)($\frac{1}{2}$ + x, $\frac{1}{2}$ − y, − $\frac{1}{2}$ + z) 3.065 (7) Å] and O(2) and O(8) are less involved in interactions

between molecules than other O atoms [O(2)—O(4) ($\frac{3}{2}$ − x, $\frac{1}{2}$ + y, $\frac{3}{2}$ − z) 3.134 (8) and O(3)—O(8)($\frac{1}{2}$ + x, $\frac{1}{2}$ − y, $\frac{1}{2}$ + z) 3.252 (9) Å]. This probably explains the short N—O distances observed.

Experimental

Crystal data

$C_{13}H_6N_6O_{12}$	Cu $K\alpha$ radiation
M_r = 438.221	λ = 1.5418 Å
Monoclinic	Cell parameters from 25
$P2_1/n$	reflections
a = 10.671 (3) Å	θ = 16–24°
b = 12.840 (2) Å	μ = 0.15 mm^{-1}
c = 12.303 (4) Å	T = 293 K
β = 97.74 (3)°	Prism
V = 1670 (6) Å^3	0.12 × 0.07 × 0.05 mm
Z = 4	Orange
D_x = 1.742 Mg m^{-3}	

Data collection

Philips PW 1100 diffrac-tometer	1635 observed reflections [$I > 3\sigma(I)$]
Flying step scan	θ_{max} = 70°
Absorption correction: empirical	h = −12 → 12
T_{min} = 0.827, T_{max} = 1.174	k = 0 → 15
	l = 0 → 14
3027 measured reflections	3 standard reflections
3027 independent reflections	frequency: 60 min intensity variation: <0.01%

Refinement

Refinement on F	$\Delta\rho_{max}$ = 0.05 e Å^{-3}
Final R = 0.068	$\Delta\rho_{min}$ = −0.36 e Å^{-3}
wR = 0.059	Extinction correction: Larson
S = 1.5	(1969)
1635 reflections	Extinction coefficient: 17 (2)
282 parameters	Atomic scattering factors
Only H-atom U's refined	from *International Tables*
w = 1.0	*for X-ray Crystallography*
$(\Delta/\sigma)_{max}$ = 0.07	(1974, Vol. IV)

Fig. 3. Stereoview of $C_{13}H_6N_6O_{12}$.

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

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

	x	y	z	U_{eq}
C(1)	0.7251 (5)	0.1309 (4)	0.5632 (4)	0.0476
C(2)	0.7514 (5)	0.1851 (4)	0.6614 (4)	0.0481
C(3)	0.8413 (5)	0.1571 (5)	0.7465 (4)	0.0525
C(4)	0.9131 (5)	0.0704 (4)	0.7329 (5)	0.0529
C(5)	0.8925 (5)	0.0109 (4)	0.6397 (5)	0.0519
C(6)	0.7969 (5)	0.0417 (4)	0.5578 (4)	0.0465
C(7)	0.6510 (5)	0.1693 (4)	0.3564 (4)	0.0465
C(8)	0.7519 (5)	0.2249 (4)	0.3233 (4)	0.0468
C(9)	0.7780 (5)	0.2315 (4)	0.2169 (4)	0.0551
C(10)	0.7027 (5)	0.1758 (4)	0.1394 (4)	0.0478
C(11)	0.6012 (5)	0.1185 (4)	0.1626 (4)	0.0522
C(12)	0.5775 (5)	0.1184 (4)	0.2692 (4)	0.0513
C(13)	0.6221 (5)	0.1681 (5)	0.4747 (4)	0.0542
N(1)	0.6789 (5)	0.2795 (4)	0.6805 (4)	0.0690
N(2)	1.0140 (5)	0.0406 (4)	0.8219 (5)	0.0692

N(3)	0.7726 (5)	−0.0308 (4)	0.4638 (4)	0.0616
N(4)	0.8378 (5)	0.2834 (4)	0.4044 (4)	0.0685
N(5)	0.7331 (6)	0.1763 (4)	0.0245 (4)	0.0678
N(6)	0.4645 (5)	0.0590 (4)	0.2900 (4)	0.0681
O(1)	0.7095 (6)	0.3597 (5)	0.6440 (6)	0.1292
O(2)	0.5962 (7)	0.2744 (5)	0.7269 (8)	0.1392
O(3)	1.0231 (5)	0.0914 (4)	0.9055 (4)	0.0969
O(4)	1.0818 (5)	−0.0307 (4)	0.8041 (5)	0.0917
O(5)	0.8627 (5)	−0.0785 (4)	0.4381 (4)	0.0896
O(6)	0.6632 (4)	−0.0419 (3)	0.4215 (3)	0.0721
O(7)	0.9231 (6)	0.2386 (5)	0.4553 (5)	0.1115
O(8)	0.8257 (7)	0.3721 (6)	0.4130 (8)	0.1401
O(9)	0.8153 (6)	0.2349 (4)	0.0047 (4)	0.0945
O(10)	0.6763 (5)	0.1166 (5)	−0.0391 (4)	0.0937
O(11)	0.4480 (5)	−0.0251 (4)	0.2460 (4)	0.0949
O(12)	0.3906 (4)	0.1001 (4)	0.3454 (4)	0.0865

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

C(1)—C(2)	1.390 (7)	C(1)—C(6)	1.384 (7)
C(1)—C(13)	1.515 (7)	C(2)—C(3)	1.370 (7)
C(2)—N(1)	1.473 (7)	C(3)—C(4)	1.374 (7)
C(4)—C(5)	1.371 (7)	C(4)—N(2)	1.479 (7)
C(5)—C(6)	1.391 (7)	C(6)—N(3)	1.480 (7)
C(7)—C(8)	1.397 (7)	C(7)—C(12)	1.402 (7)
C(7)—C(13)	1.529 (7)	C(8)—C(9)	1.377 (7)
C(8)—N(4)	1.467 (7)	C(9)—C(10)	1.364 (8)
C(10)—C(11)	1.370 (7)	C(10)—N(5)	1.493 (6)
C(11)—C(12)	1.368 (7)	C(12)—N(6)	1.478 (7)
N(1)—O(1)	1.187 (7)	N(1)—O(2)	1.116 (7)
N(2)—O(3)	1.211 (6)	N(2)—O(4)	1.205 (6)
N(3)—O(5)	1.217 (6)	N(3)—O(6)	1.220 (6)
N(4)—O(7)	1.182 (7)	N(4)—O(8)	1.153 (8)
N(5)—O(9)	1.205 (7)	N(5)—O(10)	1.200 (7)
N(6)—O(11)	1.211 (6)	N(6)—O(12)	1.229 (6)
C(6)—C(1)—C(2)	114.1 (5)	C(13)—C(1)—C(2)	120.5 (5)
C(13)—C(1)—C(6)	125.4 (5)	C(3)—C(2)—C(1)	124.8 (5)
N(1)—C(2)—C(1)	120.2 (5)	N(1)—C(2)—C(3)	115.0 (5)
C(4)—C(3)—C(2)	117.7 (5)	C(5)—C(4)—C(3)	121.6 (5)
N(2)—C(4)—C(3)	118.8 (5)	N(2)—C(4)—C(5)	119.6 (5)
C(6)—C(5)—C(4)	117.8 (5)	C(5)—C(6)—C(1)	123.9 (5)
N(3)—C(6)—C(1)	121.2 (5)	N(3)—C(6)—C(5)	114.9 (5)
C(12)—C(7)—C(8)	112.9 (5)	C(13)—C(7)—C(8)	123.0 (5)
C(13)—C(7)—C(12)	124.1 (5)	C(9)—C(8)—C(7)	124.8 (5)
N(4)—C(8)—C(7)	120.0 (5)	N(4)—C(8)—C(9)	115.2 (5)
C(10)—C(9)—C(8)	117.1 (5)	C(11)—C(10)—C(9)	123.0 (5)
N(5)—C(10)—C(9)	118.5 (5)	N(5)—C(10)—C(11)	118.6 (5)
C(12)—C(11)—C(10)	117.0 (5)	C(11)—C(12)—C(7)	125.1 (5)
N(6)—C(12)—C(7)	119.5 (5)	N(6)—C(12)—C(11)	115.3 (5)
C(7)—C(13)—C(1)	117.9 (5)	O(1)—N(1)—C(2)	118.5 (6)
O(2)—N(1)—C(2)	120.1 (6)	O(2)—N(1)—O(1)	121.4 (7)
O(3)—N(2)—C(4)	117.2 (5)	O(4)—N(2)—C(4)	117.2 (6)
O(4)—N(2)—O(3)	125.6 (6)	O(5)—N(3)—C(6)	117.2 (5)
O(6)—N(3)—C(6)	117.7 (5)	O(6)—N(3)—O(5)	125.0 (5)
O(7)—N(4)—C(8)	118.5 (6)	O(8)—N(4)—C(8)	120.0 (6)
O(8)—N(4)—O(7)	121.3 (7)	O(9)—N(5)—C(10)	116.8 (6)
O(10)—N(5)—C(10)	117.4 (6)	O(10)—N(5)—O(9)	125.7 (5)
O(11)—N(6)—C(12)	117.1 (5)	O(12)—N(6)—C(12)	118.3 (5)
O(12)—N(6)—O(11)	124.4 (6)		

An orange crystal of the title compound was obtained according to the procedure of Shipp, Kaplan & Sitzmann (1972). The structure was solved using direct methods (*SHELXS*86; Sheldrick, 1986) and successive Fourier maps. H-atom positions were calculated. All calculations were performed using *CRYSTALS* (Watkin, Carruthers & Betteridge, 1985) on a VAX 6310 computer. Final atomic coordinates are given in Table 1, intramolecular bond distances and angles in Table 2. Fig. 2 shows the molecule with the numbering system and Fig. 3 is a stereoscopic view of the packing; both were drawn using *ORTEP* (Johnson, 1965).

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4-[2-Benzoyl-1-(benzoylmethyl)ethyl][2.2]-paracyclophane

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Abstract

The unsymmetrically substituted [2.2]paracyclophane moiety of the title compound, 1,5-diphenyl-3-(tricyclo-[8.2.2.2^{4,7}]hexadeca-4,6,10,12,13,15-hexaen-5-yl)-1,5-pentanedione, exhibits geometrical features typical of known paracyclophane derivatives; the benzene rings are non-planar and have a shallow boat conformation with folding angles of 11.8–14.0°. The dimethylene-bridge