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1,2-Bis(4-nitrobenzoyl)-3,4-bis(4-nitrophenyl)cyclobutane

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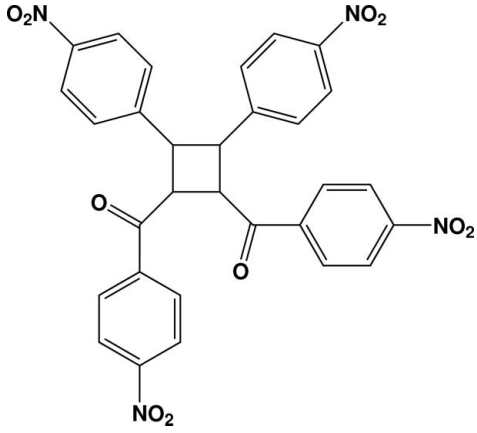
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.003 Å; R factor = 0.055; wR factor = 0.134; data-to-parameter ratio = 13.4.

In the title compound, $C_{30}H_{20}N_4O_{10}$, a typical bonding pattern is observed for the cyclobutane ring, with an average bond length of 1.560 (3) Å and bond angles of around 90°. In the crystal structure, the relatively short distances between the centroids of the benzene rings of neighbouring molecules [3.865 (3) and 3.845 (3) Å] indicate the existence of π–π interactions.

Related literature

For background and details of the 'topochemical principle' for [2 + 2] photoreactions in the solid state, see: Schmidt (1971); MacGillivray *et al.* (2000); Toh *et al.* (2005); Papaefstathiou *et al.* (2001). For crystal structures of related compounds, see: Steyl *et al.* (2005) and Toda *et al.* (1998).



Experimental

Crystal data

$C_{30}H_{20}N_4O_{10}$
M_r = 596.50
Monoclinic, $P2_1/c$
a = 17.1005 (11) Å
b = 10.6509 (6) Å
c = 15.0484 (9) Å
β = 98.1630 (11)°
V = 2713.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 291 (2) K
0.30 × 0.26 × 0.24 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.97, T_{max} = 0.97
14024 measured reflections
5326 independent reflections
3493 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.134
S = 1.04
5326 reflections
397 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2260).

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supplementary materials

Acta Cryst. (2007). E**63**, o3265 [**doi:10.1107/S1600536807028954**]

1,2-Bis(4-nitrobenzoyl)-3,4-bis(4-nitrophenyl)cyclobutane

R.-G. Xiong

Comment

Since the work of Schmidt which delineated a 'topochemical principle' for [2 + 2] photoreactions in the solid state(Schmidt, 1971) chemists have strived to design molecules that will predictably crystallize to allow such reactions to occur (MacGillivray *et al.*, 2000; Toh *et al.*, 2005; Papaefstathiou *et al.*, 2001). Such an approach to the synthesis can lead to the formation of covalent bonds 'at will' in solids to facilitate the high yield, solvent-free synthesis of molecules available either in low yields, as part of mixtures, or are not accessible in the liquid phase. Herein we present the crystal structure of the title compound, (I), accidentally synthesized through photochemical [2 + 2] cycloaddition.

The crystal data shows that in the title compound, $C_{30}H_{20}N_4O_{10}$, there is a rigid four-membered rings A (C1—C4), The C—C bond lendths of C1—C2, C2—C3, C3—C4 and C1—C4 are 1.587 (3), 1.534 (3), 1.567 (3) and 1.553 (3) Å, respectively. It's average bond lendths is 1.560 (3) Å which is longer than the typical C_{sp3}—C_{sp3} bond distance and is almost same observed in 1,2-dibenzoyl-3,4-bis(4-methoxyphenyl)cyclobutane (Steyl *et al.*, 2005), where the average C—C bond length is 1.563 (3) Å. Such an elongation has also been observed in another rigid four-membered rings derivative (Toda *et al.*, 1998) and is considered to be caused by the tensile force of rigid four-membered rings. The relatively short distances $Cg1\cdots Cg1^{i}$ of 3.865 (3) Å and $Cg2\cdots Cg3^{ii}$ of 3.845 (3) Å [*Cg*1, *Cg*2 and *Cg*3 are centroids of C18—C23, C11—C16 and C25—C30 rings, respectively] show an existence of weak π···π interactions, which contribute to the crystal packing stabilization [symmetry codes: (i) 1 − *x*, −*y*, −*z*; (ii) *x*, 1/2 − *y*, −1/2 + *z*].

Experimental

1,3-Bis(4-nitrophenyl)prop-2-en-1-one (0.298 g, 2 mmol) was dissolved in ethanol (25 ml) and evaporated slowly in the air affording yellow block crystals of complex I under sunlight.

Refinement

All H atoms were geometrically positioned (C—H 0.93–0.98 Å) and included in the refinement in riding motion approximation, with $U_{iso} = 1.2U_{eq}$ of the carrier atom.

Figures

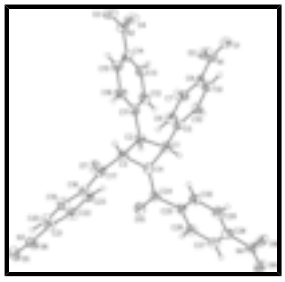


Fig. 1. The molecule structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

1,2-Bis(4-nitrobenzoyl)-3,4-bis(4-nitrophenyl)cyclobutane

Crystal data

$C_{30}H_{20}N_4O_{10}$	F_{000} = 1232
M_r = 596.50	D_x = 1.460 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 5718 reflections
a = 17.1005 (11) Å	θ = 2.1–26.1º
b = 10.6509 (6) Å	μ = 0.11 mm^{-1}
c = 15.0484 (9) Å	T = 291 (2) K
β = 98.1630 (11)º	Block, yellow
V = 2713.1 (3) Å^3	0.30 × 0.26 × 0.24 mm
Z = 4	

Data collection

Bruker SMART APEX CCD diffractometer	5326 independent reflections
Radiation source: sealed tube	3493 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.034
T = 291(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	h = −21→12
T_{min} = 0.97, T_{max} = 0.97	k = −13→13
14024 measured reflections	l = −18→18

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.055	H-atom parameters constrained
$wR(F^2)$ = 0.134	$w = 1/[\sigma^2(F_o^2) + (0.0648P)^2 + 0.0937P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
5326 reflections	$\Delta\rho_{max} = 0.22$ e Å^{-3}
397 parameters	$\Delta\rho_{min} = -0.20$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.24207 (14)	0.1731 (2)	0.27043 (15)	0.0513 (6)
H1	0.2486	0.1938	0.3345	0.062*
C2	0.27985 (14)	0.2795 (2)	0.21614 (15)	0.0478 (5)
H2	0.3139	0.3318	0.2590	0.057*
C3	0.33138 (13)	0.1800 (2)	0.17889 (15)	0.0465 (5)
H3	0.3064	0.1544	0.1190	0.056*
C4	0.30906 (14)	0.0838 (2)	0.25000 (15)	0.0465 (5)
H4	0.2886	0.0048	0.2225	0.056*
C5	0.15684 (14)	0.1418 (2)	0.23690 (16)	0.0516 (6)
C6	0.13487 (16)	0.0522 (3)	0.17200 (18)	0.0612 (7)
H6	0.1731	0.0035	0.1502	0.073*
C7	0.05493 (16)	0.0347 (3)	0.13901 (19)	0.0630 (7)
H7	0.0396	−0.0255	0.0953	0.076*
C8	0.00024 (13)	0.1065 (2)	0.17144 (16)	0.0487 (5)
C9	0.02065 (15)	0.1967 (2)	0.23477 (17)	0.0564 (6)
H9	−0.0180	0.2466	0.2546	0.068*
C10	0.09907 (15)	0.2134 (2)	0.26906 (18)	0.0578 (6)
H10	0.1133	0.2726	0.3138	0.069*
C11	0.22659 (14)	0.3643 (2)	0.15479 (17)	0.0510 (6)
C12	0.20188 (15)	0.4766 (2)	0.18928 (17)	0.0549 (6)
H12	0.2202	0.4981	0.2485	0.066*
C13	0.15098 (16)	0.5565 (2)	0.13770 (18)	0.0593 (7)
H13	0.1350	0.6313	0.1614	0.071*
C14	0.12455 (16)	0.5239 (3)	0.05148 (19)	0.0615 (7)
C15	0.14666 (15)	0.4132 (2)	0.01427 (18)	0.0588 (6)
H15	0.1271	0.3922	−0.0447	0.071*

C16	0.19831 (16)	0.3346 (2)	0.06639 (17)	0.0601 (7)
H16	0.2144	0.2605	0.0418	0.072*
C17	0.41546 (15)	0.2195 (2)	0.17426 (15)	0.0497 (5)
C18	0.47535 (14)	0.1283 (2)	0.15019 (15)	0.0466 (5)
C19	0.54917 (15)	0.1712 (3)	0.14035 (18)	0.0584 (6)
H19	0.5615	0.2554	0.1513	0.070*
C20	0.60527 (15)	0.0923 (2)	0.11459 (17)	0.0560 (6)
H20	0.6556	0.1220	0.1098	0.067*
C21	0.58645 (14)	−0.0291 (2)	0.09623 (15)	0.0493 (6)
C22	0.51468 (15)	−0.0784 (2)	0.10701 (16)	0.0535 (6)
H22	0.5037	−0.1631	0.0964	0.064*
C23	0.45837 (14)	0.0018 (2)	0.13435 (16)	0.0515 (6)
H23	0.4090	−0.0295	0.1421	0.062*
C24	0.36941 (14)	0.0631 (2)	0.33040 (15)	0.0453 (5)
C25	0.34748 (13)	−0.0183 (2)	0.40435 (15)	0.0451 (5)
C26	0.39091 (14)	−0.0081 (2)	0.48922 (16)	0.0523 (6)
H26	0.4313	0.0509	0.4992	0.063*
C27	0.37552 (16)	−0.0831 (2)	0.55852 (18)	0.0587 (6)
H27	0.4052	−0.0766	0.6151	0.070*
C28	0.31505 (15)	−0.1683 (2)	0.54202 (17)	0.0539 (6)
C29	0.27006 (15)	−0.1799 (2)	0.46023 (17)	0.0552 (6)
H29	0.2297	−0.2391	0.4510	0.066*
C30	0.28551 (14)	−0.1019 (2)	0.39095 (17)	0.0529 (6)
H30	0.2539	−0.1061	0.3354	0.063*
N1	−0.08286 (14)	0.0903 (2)	0.13593 (15)	0.0591 (5)
N2	0.07123 (13)	0.6107 (2)	−0.00524 (16)	0.0608 (6)
N3	0.64516 (13)	−0.1109 (2)	0.06240 (13)	0.0562 (5)
N4	0.30011 (13)	−0.2532 (2)	0.61511 (15)	0.0561 (5)
O1	−0.13121 (11)	0.16035 (19)	0.16093 (12)	0.0681 (5)
O2	−0.10009 (11)	0.00350 (18)	0.08137 (13)	0.0669 (5)
O3	0.04865 (12)	0.57942 (18)	−0.08239 (15)	0.0708 (5)
O4	0.05367 (11)	0.70834 (19)	0.02810 (13)	0.0674 (5)
O5	0.71007 (11)	−0.06971 (17)	0.06117 (12)	0.0618 (5)
O6	0.62652 (10)	−0.21424 (16)	0.03760 (11)	0.0532 (4)
O7	0.43348 (10)	0.32942 (16)	0.18512 (12)	0.0588 (4)
O8	0.33738 (11)	−0.24460 (17)	0.68674 (12)	0.0636 (5)
O9	0.25094 (11)	−0.33148 (18)	0.59804 (12)	0.0681 (5)
O10	0.43402 (10)	0.11166 (17)	0.33775 (12)	0.0590 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0532 (14)	0.0555 (14)	0.0430 (12)	0.0094 (11)	−0.0011 (10)	−0.0029 (10)
C2	0.0485 (13)	0.0510 (13)	0.0429 (11)	0.0063 (10)	0.0031 (10)	−0.0036 (10)
C3	0.0492 (12)	0.0489 (13)	0.0397 (11)	0.0089 (10)	0.0003 (9)	−0.0022 (9)
C4	0.0480 (13)	0.0484 (13)	0.0437 (12)	0.0042 (10)	0.0086 (10)	−0.0044 (10)
C5	0.0528 (14)	0.0532 (14)	0.0492 (13)	0.0076 (11)	0.0080 (11)	0.0114 (11)
C6	0.0532 (15)	0.0659 (16)	0.0620 (15)	0.0087 (12)	−0.0003 (12)	−0.0079 (13)

C7	0.0588 (16)	0.0633 (16)	0.0618 (15)	0.0047 (13)	−0.0088 (13)	−0.0081 (13)
C8	0.0433 (12)	0.0533 (13)	0.0515 (13)	−0.0105 (11)	0.0140 (10)	0.0147 (11)
C9	0.0597 (15)	0.0497 (14)	0.0598 (15)	0.0166 (12)	0.0081 (12)	0.0136 (12)
C10	0.0609 (15)	0.0561 (15)	0.0599 (14)	0.0143 (12)	0.0203 (12)	0.0095 (12)
C11	0.0510 (13)	0.0500 (13)	0.0541 (13)	0.0116 (11)	0.0147 (11)	0.0058 (11)
C12	0.0545 (14)	0.0590 (15)	0.0528 (14)	0.0183 (12)	0.0132 (11)	0.0002 (11)
C13	0.0663 (16)	0.0515 (14)	0.0651 (16)	0.0170 (12)	0.0266 (13)	0.0165 (12)
C14	0.0620 (16)	0.0591 (16)	0.0653 (16)	0.0108 (12)	0.0157 (13)	0.0305 (13)
C15	0.0600 (16)	0.0597 (16)	0.0541 (14)	0.0070 (12)	−0.0007 (12)	0.0139 (12)
C16	0.0673 (16)	0.0534 (14)	0.0576 (15)	0.0265 (12)	0.0015 (12)	0.0058 (12)
C17	0.0582 (14)	0.0444 (13)	0.0459 (12)	0.0028 (11)	0.0053 (10)	0.0024 (10)
C18	0.0480 (12)	0.0505 (13)	0.0407 (11)	0.0028 (10)	0.0041 (9)	0.0051 (10)
C19	0.0562 (15)	0.0601 (15)	0.0586 (14)	−0.0125 (12)	0.0074 (12)	−0.0097 (12)
C20	0.0557 (15)	0.0589 (16)	0.0564 (14)	−0.0107 (12)	0.0184 (12)	−0.0023 (12)
C21	0.0466 (13)	0.0590 (15)	0.0420 (12)	0.0068 (11)	0.0052 (10)	0.0048 (10)
C22	0.0615 (15)	0.0461 (13)	0.0534 (14)	0.0022 (11)	0.0097 (11)	0.0044 (11)
C23	0.0477 (13)	0.0531 (14)	0.0559 (14)	0.0010 (11)	0.0142 (11)	0.0080 (11)
C24	0.0455 (13)	0.0430 (12)	0.0478 (12)	0.0076 (10)	0.0077 (10)	−0.0049 (10)
C25	0.0466 (12)	0.0420 (12)	0.0460 (12)	0.0087 (10)	0.0039 (10)	−0.0006 (9)
C26	0.0492 (13)	0.0545 (14)	0.0501 (13)	−0.0020 (11)	−0.0031 (10)	0.0060 (11)
C27	0.0560 (15)	0.0634 (16)	0.0532 (14)	0.0083 (13)	−0.0045 (11)	0.0092 (12)
C28	0.0593 (15)	0.0425 (13)	0.0602 (15)	0.0093 (11)	0.0090 (12)	0.0130 (11)
C29	0.0551 (14)	0.0508 (14)	0.0586 (14)	−0.0033 (11)	0.0047 (11)	0.0039 (11)
C30	0.0450 (13)	0.0599 (15)	0.0524 (13)	−0.0018 (11)	0.0026 (10)	−0.0015 (11)
N1	0.0540 (12)	0.0598 (13)	0.0608 (13)	0.0059 (11)	−0.0017 (10)	0.0126 (11)
N2	0.0618 (13)	0.0553 (13)	0.0653 (14)	0.0142 (11)	0.0088 (11)	0.0298 (11)
N3	0.0546 (13)	0.0653 (15)	0.0479 (11)	0.0064 (11)	0.0049 (9)	0.0010 (10)
N4	0.0564 (13)	0.0480 (12)	0.0615 (13)	−0.0013 (10)	0.0005 (11)	0.0181 (9)
O1	0.0551 (11)	0.0851 (14)	0.0651 (11)	0.0209 (10)	0.0122 (9)	0.0273 (10)
O2	0.0621 (11)	0.0652 (12)	0.0650 (11)	−0.0193 (9)	−0.0194 (9)	0.0111 (10)
O3	0.0671 (12)	0.0650 (12)	0.0735 (13)	0.0146 (9)	−0.0133 (10)	0.0153 (10)
O4	0.0670 (12)	0.0633 (12)	0.0662 (11)	0.0141 (10)	−0.0104 (9)	0.0162 (10)
O5	0.0615 (12)	0.0660 (11)	0.0625 (11)	0.0013 (9)	0.0247 (9)	−0.0231 (9)
O6	0.0545 (10)	0.0524 (10)	0.0579 (10)	0.0135 (8)	0.0260 (8)	−0.0019 (8)
O7	0.0618 (10)	0.0510 (10)	0.0661 (11)	−0.0042 (8)	0.0177 (9)	−0.0080 (8)
O8	0.0646 (11)	0.0615 (11)	0.0602 (11)	−0.0165 (9)	−0.0063 (9)	0.0229 (8)
O9	0.0729 (12)	0.0657 (11)	0.0595 (10)	−0.0248 (10)	−0.0116 (9)	0.0278 (9)
O10	0.0528 (10)	0.0618 (11)	0.0622 (11)	−0.0123 (9)	0.0076 (8)	0.0047 (8)

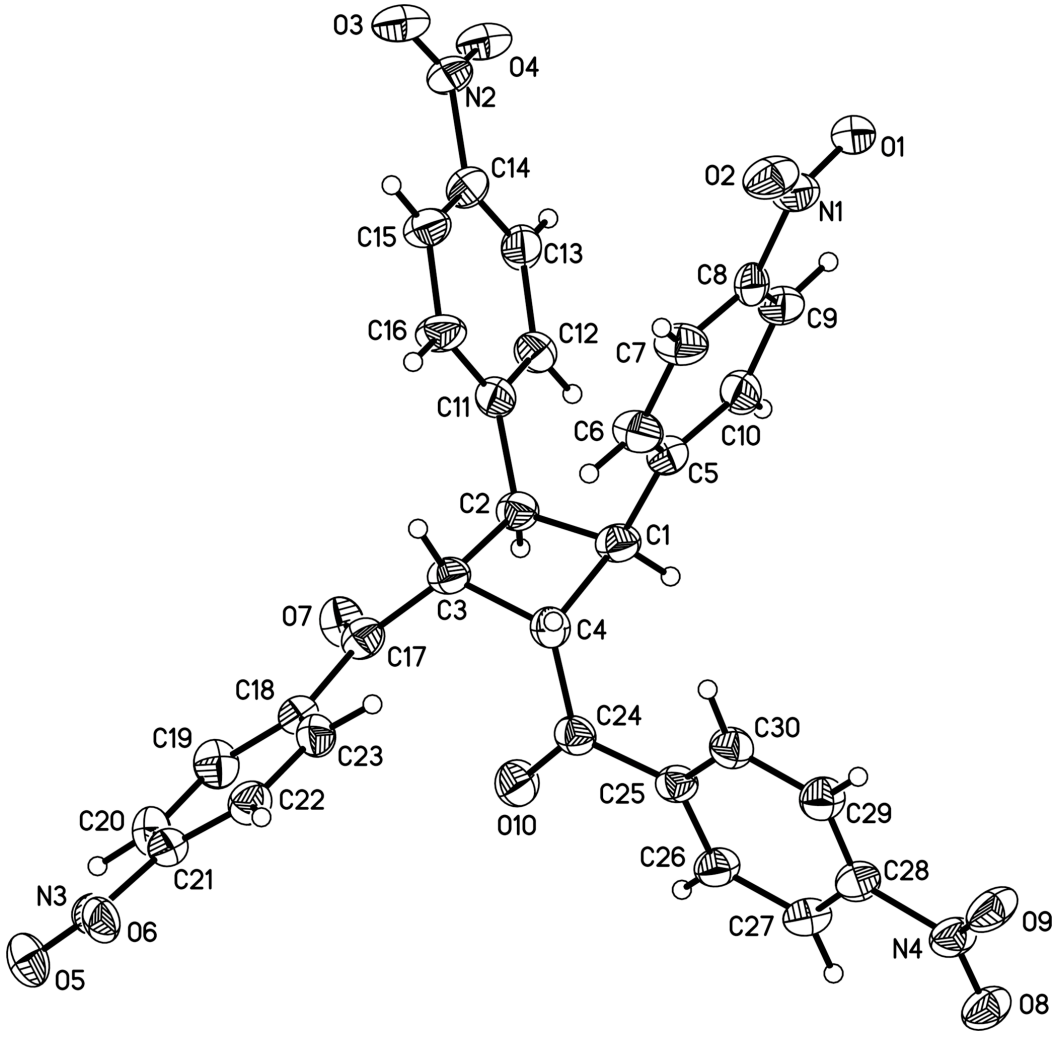
Geometric parameters (Å, °)

C1—C5	1.510 (3)	C17—O7	1.215 (3)
C1—C4	1.553 (3)	C17—C18	1.493 (3)
C1—C2	1.587 (3)	C18—C19	1.370 (3)
C1—H1	0.9800	C18—C23	1.392 (3)
C2—C11	1.503 (3)	C19—C20	1.372 (4)
C2—C3	1.534 (3)	C19—H19	0.9300
C2—H2	0.9800	C20—C21	1.352 (3)
C3—C17	1.509 (3)	C20—H20	0.9300

C3—C4	1.567 (3)	C21—C22	1.366 (3)
C3—H3	0.9800	C21—N3	1.474 (3)
C4—C24	1.491 (3)	C22—C23	1.392 (3)
C4—H4	0.9800	C22—H22	0.9300
C5—C6	1.379 (4)	C23—H23	0.9300
C5—C10	1.388 (3)	C24—O10	1.211 (3)
C6—C7	1.399 (4)	C24—C25	1.500 (3)
C6—H6	0.9300	C25—C30	1.377 (3)
C7—C8	1.351 (4)	C25—C26	1.387 (3)
C7—H7	0.9300	C26—C27	1.369 (3)
C8—C9	1.364 (4)	C26—H26	0.9300
C8—N1	1.456 (3)	C27—C28	1.371 (4)
C9—C10	1.378 (4)	C27—H27	0.9300
C9—H9	0.9300	C28—C29	1.361 (4)
C10—H10	0.9300	C28—N4	1.474 (3)
C11—C16	1.386 (4)	C29—C30	1.388 (3)
C11—C12	1.394 (3)	C29—H29	0.9300
C12—C13	1.375 (3)	C30—H30	0.9300
C12—H12	0.9300	N1—O1	1.212 (3)
C13—C14	1.357 (4)	N1—O2	1.244 (3)
C13—H13	0.9300	N2—O4	1.211 (3)
C14—C15	1.381 (4)	N2—O3	1.217 (3)
C14—N2	1.481 (3)	N3—O6	1.191 (3)
C15—C16	1.378 (3)	N3—O5	1.196 (3)
C15—H15	0.9300	N4—O8	1.175 (3)
C16—H16	0.9300	N4—O9	1.186 (3)
C5—C1—C4	120.2 (2)	C15—C16—C11	121.0 (2)
C5—C1—C2	115.44 (18)	C15—C16—H16	119.5
C4—C1—C2	88.26 (17)	C11—C16—H16	119.5
C5—C1—H1	110.4	O7—C17—C18	119.3 (2)
C4—C1—H1	110.4	O7—C17—C3	119.2 (2)
C2—C1—H1	110.4	C18—C17—C3	121.3 (2)
C11—C2—C3	121.33 (19)	C19—C18—C23	118.5 (2)
C11—C2—C1	119.33 (19)	C19—C18—C17	118.9 (2)
C3—C2—C1	89.53 (17)	C23—C18—C17	122.6 (2)
C11—C2—H2	108.3	C18—C19—C20	121.2 (2)
C3—C2—H2	108.3	C18—C19—H19	119.4
C1—C2—H2	108.3	C20—C19—H19	119.4
C17—C3—C2	115.09 (19)	C21—C20—C19	119.2 (2)
C17—C3—C4	122.68 (18)	C21—C20—H20	120.4
C2—C3—C4	89.65 (17)	C19—C20—H20	120.4
C17—C3—H3	109.2	C20—C21—C22	122.4 (2)
C2—C3—H3	109.2	C20—C21—N3	118.8 (2)
C4—C3—H3	109.2	C22—C21—N3	118.8 (2)
C24—C4—C1	112.03 (18)	C21—C22—C23	118.0 (2)
C24—C4—C3	116.30 (19)	C21—C22—H22	121.0
C1—C4—C3	89.60 (17)	C23—C22—H22	121.0
C24—C4—H4	112.3	C18—C23—C22	120.6 (2)
C1—C4—H4	112.3	C18—C23—H23	119.7

C3—C4—H4	112.3	C22—C23—H23	119.7
C6—C5—C10	119.4 (2)	O10—C24—C4	121.9 (2)
C6—C5—C1	122.8 (2)	O10—C24—C25	120.0 (2)
C10—C5—C1	117.6 (2)	C4—C24—C25	118.1 (2)
C5—C6—C7	119.8 (3)	C30—C25—C26	119.0 (2)
C5—C6—H6	120.1	C30—C25—C24	122.2 (2)
C7—C6—H6	120.1	C26—C25—C24	118.7 (2)
C8—C7—C6	119.2 (2)	C27—C26—C25	121.3 (2)
C8—C7—H7	120.4	C27—C26—H26	119.3
C6—C7—H7	120.4	C25—C26—H26	119.3
C7—C8—C9	122.0 (2)	C26—C27—C28	118.0 (2)
C7—C8—N1	119.4 (2)	C26—C27—H27	121.0
C9—C8—N1	118.7 (2)	C28—C27—H27	121.0
C8—C9—C10	119.4 (2)	C29—C28—C27	122.6 (2)
C8—C9—H9	120.3	C29—C28—N4	118.9 (2)
C10—C9—H9	120.3	C27—C28—N4	118.5 (2)
C9—C10—C5	120.1 (3)	C28—C29—C30	118.8 (2)
C9—C10—H10	119.9	C28—C29—H29	120.6
C5—C10—H10	119.9	C30—C29—H29	120.6
C16—C11—C12	118.1 (2)	C25—C30—C29	120.1 (2)
C16—C11—C2	123.4 (2)	C25—C30—H30	119.9
C12—C11—C2	118.5 (2)	C29—C30—H30	119.9
C13—C12—C11	121.5 (3)	O1—N1—O2	123.6 (2)
C13—C12—H12	119.3	O1—N1—C8	119.1 (2)
C11—C12—H12	119.3	O2—N1—C8	117.2 (2)
C14—C13—C12	118.7 (2)	O4—N2—O3	124.5 (2)
C14—C13—H13	120.7	O4—N2—C14	117.8 (2)
C12—C13—H13	120.7	O3—N2—C14	117.7 (2)
C13—C14—C15	122.2 (2)	O6—N3—O5	122.8 (2)
C13—C14—N2	119.1 (3)	O6—N3—C21	119.3 (2)
C15—C14—N2	118.7 (3)	O5—N3—C21	117.9 (2)
C16—C15—C14	118.6 (3)	O8—N4—O9	121.9 (2)
C16—C15—H15	120.7	O8—N4—C28	120.5 (2)
C14—C15—H15	120.7	O9—N4—C28	117.5 (2)

Fig. 1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