Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,3,5-Trinitro-2,4-bis(2-phenylethenyl)-benzene

Ze-Rong Guo,* Hua-Bo Li and Fang Li

State Key Laboratory of Explosion Science and Technology, Beijing Institute of Technology, Beijing 100081, People's Republic of China
Correspondence e-mail: guozr531408@sohu.com

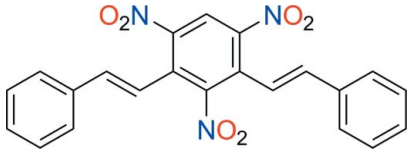
Received 25 August 2010; accepted 28 August 2010

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.082; wR factor = 0.236; data-to-parameter ratio = 12.0.

In the title compound, $C_{22}H_{15}N_3O_6$, the central benzene ring and one of the phenyl rings are essentially parallel to each other, making a dihedral angle of 1.35 (16)°. The dihedral angle between the two phenyl rings is 83.56 (19)°. Intramolecular C—H···N and C—H···O hydrogen bonds occur. In the crystal, molecules are linked through C—H···O hydrogen bonds. Furthermore, offset face-to-face π–π interactions with centroid–centroid distances of 3.644 (2) Å help to stabilize the crystal structure.

Related literature

For the preparation, see: Peng *et al.* (1995). For general background to trinitrobenzene and its derivatives, see: Ott & Benziger (1987); Kuperman *et al.* (2006). The title compound may be useful as a high energy explosive, see: Peng *et al.* (1995). For a related structure, see: Bryden (1972).



Experimental

Crystal data

$C_{22}H_{15}N_3O_6$
M_r = 417.37
Triclinic, $P\overline{1}$
a = 7.0762 (14) Å
b = 8.6625 (17) Å
c = 16.717 (3) Å
α = 101.660 (3)°
β = 92.616 (3)°
γ = 105.122 (3)°
V = 963.5 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 293 K
0.32 × 0.28 × 0.22 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
T_{min} = 0.577, T_{max} = 1.000
5265 measured reflections
3363 independent reflections
2146 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.082
$wR(F^2)$ = 0.236
S = 0.98
3363 reflections
280 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16···O2	0.93	2.60	3.398 (4)	144
C16—H16···N1	0.93	2.42	2.980 (4)	119
C18—H18···O5^{i}	0.93	2.48	3.387 (4)	166

Symmetry code: (i) $x, y+1, z$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

This work was supported by the State Key Laboratory of Explosion Science and Technology Foundation (YBKT09–10, SKLEST–ZZ–09–10), Beijing Institute of Technology.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2408).

References

Bruker (2002). *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2003). *SADABS* and *SAINT-Plus*. Bruker AXS Inc, Madison, Wisconsin, USA.
Bryden, J. H. (1972). *Acta Cryst.* B**28**, 1395–1398.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Kuperman, R. G., Checkai, R. T., Simini, M., Phillips, C. T., Kolakowski, J. E. & Kurnas, C. W. (2006). *Environ. Toxicol. Chem.* **25**, 1368–1375.
Ott, D. G. & Benziger, T. M. (1987). *J. Energ. Mater*, **5**, 343–354.
Peng, X. H., Chen, T. Y., Lu, C. X. & Sun, R. K. (1995). *Org. Prep. Proceed. Int.* **27**, 475–479.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2010). E**66**, o2486 [doi:10.1107/S1600536810034732]

1,3,5-Trinitro-2,4-bis(2-phenylethenyl)benzene

Ze-Rong Guo, Hua-Bo Li and Fang Li

S1. Comment

Trinitrobenzene and its derivatives have been extensively reported for use as energetic materials (Ott & Benziger, 1987; Kuperman *et al.*, 2006). The title compound may be useful as a high energy explosive (Peng *et al.*, 1995), and here we present its crystal structure.

In the title compound (Fig. 1), the bond distances and bond angles are similar to those in 2,4,6-trintro-*m*-xylene (Bryden, 1972). The planes of two rings (C9—C14) and (C17—C22) are approximately parallel, with a dihedral angle of 1.35 (16)°. The two phenyl rings, (C1—C6) and (C17—C22), form a dihedral angle of 83.56 (19)°. The short distance of 3.644 (2) Å (symmetry code: -*x*,-*y*,1 - *z*) between the centroids of the two parallel rings (C9—C14) and (C17—C22) indicates the existence of offset face-to-face π-π interactions. Molecules are linked through C—H···O hydrogen bonds (Table 1), which help to stabilize the crystal structure. Intramolecular C—H···N and C—H···O hydrogen bonds are also present. There is a short intermolecular contact C15···C15 (1-*x*, -*y*, 1-*z*) of 3.185 (4) Å.

S2. Experimental

The title compound was synthesized using 2,4,6-trinitro-*m*-xylene and benzaldehyde as the starting materials, according to the literature method (Peng *et al.*, 1995). Single crystals suitable for *X*–ray diffraction were prepared by slow evaporation of a solution of the title compound in acetone at room temperature.

S3. Refinement

All H atoms were placed in calculated positions, with C—H = 0.93 Å; U_{iso}(H) = 1.2U_{eq}(C).

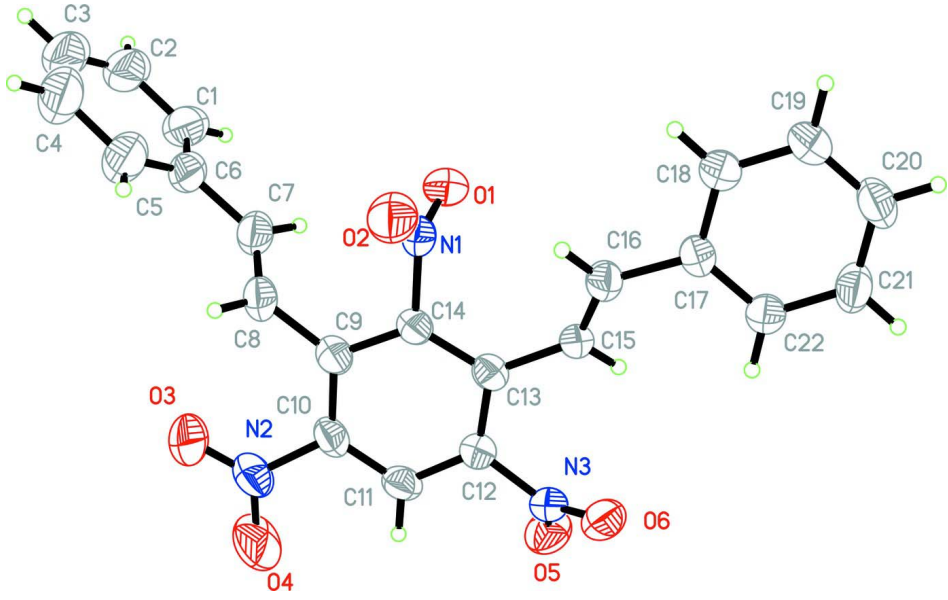


Figure 1

The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as a small spheres of arbitrary radius.

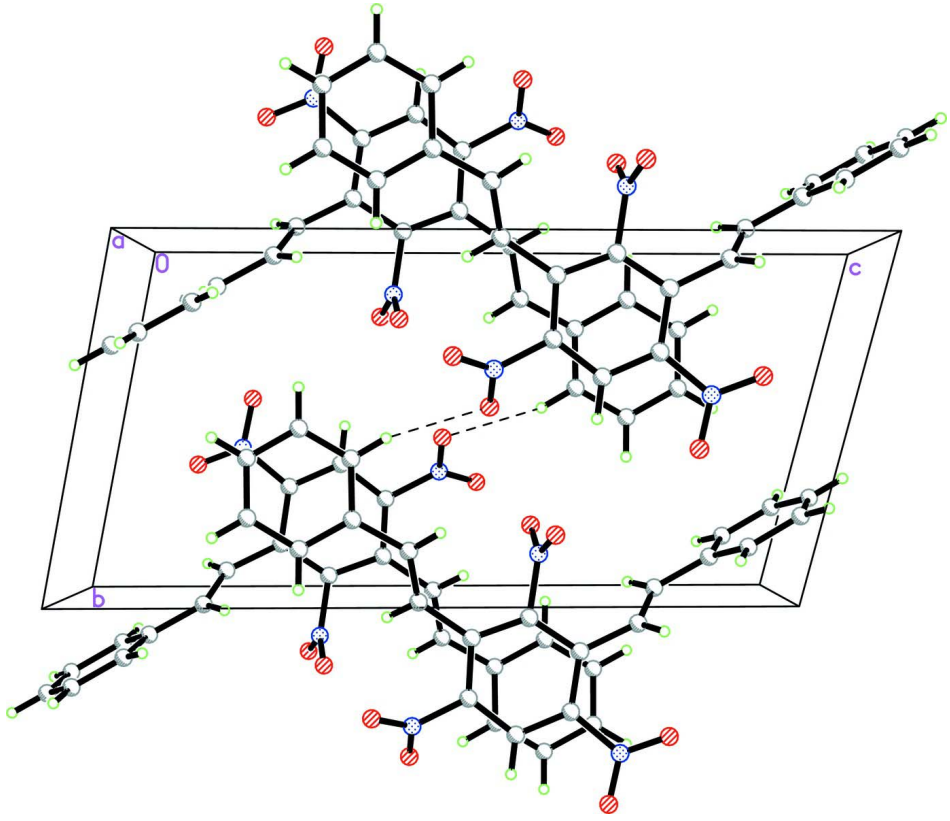


Figure 2

The packing of the title compound, viewed along the *a*-axis. Intermolecular hydrogen bonds are shown as dashed lines.

1,3,5-Trinitro-2,4-bis(2-phenylethenyl)benzene

Crystal data

$C_{22}H_{15}N_3O_6$
$M_r = 417.37$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.0762$ (14) Å
$b = 8.6625$ (17) Å
$c = 16.717$ (3) Å
$\alpha = 101.660$ (3)°
$\beta = 92.616$ (3)°
$\gamma = 105.122$ (3)°
$V = 963.5$ (3) Å^3
$Z = 2$
$F(000) = 432$
$D_x = 1.439$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1118 reflections
$\theta = 2.5$–22.8°
$\mu = 0.11$ mm^{-1}
$T = 293$ K
Block, colorless
0.32 × 0.28 × 0.22 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
$T_{min} = 0.577$, $T_{max} = 1.000$
5265 measured reflections
3363 independent reflections
2146 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.5°$
$h = -8 \rightarrow 8$
$k = -10 \rightarrow 9$
$l = -18 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.082$
$wR(F^2) = 0.236$
$S = 0.98$
3363 reflections
280 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1716P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.66$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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}
O1	0.4557 (4)	0.2087 (3)	0.37673 (15)	0.0606 (7)
O2	0.1502 (4)	0.1919 (3)	0.34477 (15)	0.0629 (7)
O3	0.0777 (6)	−0.3754 (4)	0.12446 (17)	0.1042 (13)

O4	0.0663 (6)	−0.5709 (4)	0.18422 (17)	0.0944 (11)
O5	0.2954 (4)	−0.4565 (3)	0.47219 (15)	0.0599 (7)
O6	0.1092 (4)	−0.3227 (3)	0.53578 (14)	0.0558 (7)
N1	0.2829 (5)	0.1337 (3)	0.35892 (14)	0.0450 (7)
N2	0.0966 (4)	−0.4259 (4)	0.18514 (18)	0.0576 (8)
N3	0.2018 (4)	−0.3561 (3)	0.47819 (16)	0.0413 (6)
C1	0.5959 (7)	0.1705 (4)	0.0976 (2)	0.0659 (11)
H1	0.6973	0.1494	0.1272	0.079*
C2	0.6401 (8)	0.2529 (5)	0.0357 (2)	0.0796 (13)
H2	0.7691	0.2860	0.0230	0.096*
C3	0.4936 (11)	0.2845 (6)	−0.0061 (3)	0.0892 (16)
H3	0.5228	0.3398	−0.0482	0.107*
C4	0.3043 (10)	0.2385 (6)	0.0110 (3)	0.0914 (16)
H4	0.2057	0.2629	−0.0187	0.110*
C5	0.2581 (7)	0.1525 (5)	0.0745 (2)	0.0739 (12)
H5	0.1289	0.1199	0.0869	0.089*
C6	0.4058 (6)	0.1181 (4)	0.11752 (19)	0.0533 (9)
C7	0.3715 (6)	0.0306 (4)	0.18496 (19)	0.0502 (9)
H7	0.4820	0.0413	0.2202	0.060*
C8	0.2044 (5)	−0.0607 (4)	0.20150 (18)	0.0479 (8)
H8	0.0901	−0.0756	0.1677	0.057*
C9	0.1924 (4)	−0.1401 (4)	0.27196 (18)	0.0403 (7)
C10	0.1482 (5)	−0.3101 (4)	0.26559 (18)	0.0417 (8)
C11	0.1561 (4)	−0.3773 (4)	0.33316 (18)	0.0413 (8)
H11	0.1338	−0.4899	0.3271	0.050*
C12	0.1978 (4)	−0.2745 (3)	0.40967 (17)	0.0369 (7)
C13	0.2335 (4)	−0.1039 (3)	0.42426 (17)	0.0352 (7)
C14	0.2324 (4)	−0.0458 (3)	0.35209 (17)	0.0358 (7)
C15	0.2759 (4)	−0.0028 (3)	0.50832 (17)	0.0351 (7)
H15	0.3253	−0.0496	0.5470	0.042*
C16	0.2545 (4)	0.1434 (4)	0.53706 (17)	0.0390 (7)
H16	0.2098	0.1960	0.4999	0.047*
C17	0.2962 (4)	0.2302 (3)	0.62389 (17)	0.0367 (7)
C18	0.3403 (5)	0.3997 (4)	0.6440 (2)	0.0480 (8)
H18	0.3405	0.4570	0.6026	0.058*
C19	0.3838 (6)	0.4843 (4)	0.7246 (2)	0.0557 (9)
H19	0.4147	0.5982	0.7372	0.067*
C20	0.3820 (5)	0.4014 (4)	0.7870 (2)	0.0559 (9)
H20	0.4124	0.4589	0.8414	0.067*
C21	0.3350 (5)	0.2343 (4)	0.76815 (19)	0.0519 (9)
H21	0.3313	0.1781	0.8102	0.062*
C22	0.2930 (5)	0.1474 (4)	0.68758 (18)	0.0433 (8)
H22	0.2624	0.0335	0.6757	0.052*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0682 (18)	0.0454 (14)	0.0558 (15)	−0.0073 (13)	−0.0013 (12)	0.0152 (11)

O2	0.0861 (19)	0.0507 (15)	0.0599 (16)	0.0323 (14)	0.0044 (13)	0.0132 (12)
O3	0.180 (4)	0.072 (2)	0.0320 (16)	−0.007 (2)	−0.0013 (17)	0.0030 (14)
O4	0.155 (3)	0.0493 (18)	0.0638 (19)	0.0272 (18)	−0.0128 (18)	−0.0140 (14)
O5	0.0746 (17)	0.0522 (15)	0.0633 (16)	0.0263 (13)	0.0098 (12)	0.0245 (12)
O6	0.0698 (16)	0.0471 (14)	0.0498 (15)	0.0096 (12)	0.0190 (12)	0.0151 (11)
N1	0.0638 (19)	0.0409 (15)	0.0280 (14)	0.0108 (15)	0.0040 (12)	0.0074 (11)
N2	0.068 (2)	0.0486 (19)	0.0429 (18)	0.0054 (15)	0.0006 (14)	−0.0056 (14)
N3	0.0465 (16)	0.0338 (14)	0.0398 (15)	0.0042 (12)	0.0049 (12)	0.0084 (11)
C1	0.096 (3)	0.047 (2)	0.053 (2)	0.015 (2)	0.020 (2)	0.0127 (17)
C2	0.125 (4)	0.057 (3)	0.051 (2)	0.011 (3)	0.022 (3)	0.015 (2)
C3	0.159 (5)	0.058 (3)	0.046 (2)	0.019 (3)	0.017 (3)	0.014 (2)
C4	0.147 (5)	0.075 (3)	0.057 (3)	0.041 (3)	−0.009 (3)	0.017 (2)
C5	0.110 (3)	0.065 (3)	0.053 (2)	0.030 (2)	0.006 (2)	0.020 (2)
C6	0.086 (3)	0.0400 (18)	0.0337 (18)	0.0197 (18)	0.0083 (17)	0.0050 (14)
C7	0.069 (2)	0.048 (2)	0.0352 (18)	0.0197 (18)	0.0029 (15)	0.0086 (14)
C8	0.059 (2)	0.051 (2)	0.0295 (17)	0.0140 (17)	−0.0004 (14)	0.0042 (14)
C9	0.0413 (17)	0.0392 (17)	0.0362 (17)	0.0080 (13)	0.0004 (13)	0.0038 (13)
C10	0.0440 (18)	0.0400 (17)	0.0330 (16)	0.0072 (14)	0.0008 (13)	−0.0035 (13)
C11	0.0452 (18)	0.0293 (16)	0.0442 (18)	0.0058 (13)	0.0052 (14)	0.0019 (13)
C12	0.0367 (16)	0.0353 (16)	0.0368 (17)	0.0074 (12)	0.0032 (12)	0.0074 (13)
C13	0.0317 (16)	0.0353 (16)	0.0356 (16)	0.0074 (12)	0.0013 (12)	0.0042 (12)
C14	0.0377 (17)	0.0320 (15)	0.0344 (16)	0.0067 (12)	0.0027 (12)	0.0039 (12)
C15	0.0393 (17)	0.0313 (16)	0.0318 (15)	0.0043 (12)	−0.0002 (12)	0.0083 (12)
C16	0.0436 (18)	0.0398 (17)	0.0335 (16)	0.0118 (13)	0.0001 (13)	0.0083 (13)
C17	0.0361 (16)	0.0396 (17)	0.0317 (16)	0.0097 (13)	0.0021 (12)	0.0031 (13)
C18	0.065 (2)	0.0358 (17)	0.0421 (18)	0.0130 (15)	0.0056 (15)	0.0073 (14)
C19	0.078 (2)	0.0366 (18)	0.046 (2)	0.0108 (17)	0.0036 (17)	0.0008 (15)
C20	0.072 (2)	0.050 (2)	0.0381 (19)	0.0164 (18)	−0.0009 (16)	−0.0058 (16)
C21	0.070 (2)	0.057 (2)	0.0328 (17)	0.0241 (18)	0.0047 (15)	0.0125 (15)
C22	0.055 (2)	0.0367 (16)	0.0390 (17)	0.0126 (14)	0.0058 (14)	0.0087 (13)

Geometric parameters (Å, º)

O1—N1	1.217 (3)	C8—H8	0.9300
O2—N1	1.211 (3)	C9—C14	1.394 (4)
O3—N2	1.199 (4)	C9—C10	1.404 (4)
O4—N2	1.214 (4)	C10—C11	1.376 (4)
O5—N3	1.216 (3)	C11—C12	1.372 (4)
O6—N3	1.218 (3)	C11—H11	0.9300
N1—C14	1.481 (4)	C12—C13	1.401 (4)
N2—C10	1.472 (4)	C13—C14	1.398 (4)
N3—C12	1.465 (4)	C13—C15	1.469 (4)
C1—C2	1.376 (5)	C15—C16	1.311 (4)
C1—C6	1.382 (5)	C15—H15	0.9300
C1—H1	0.9300	C16—C17	1.471 (4)
C2—C3	1.341 (7)	C16—H16	0.9300
C2—H2	0.9300	C17—C18	1.385 (4)
C3—C4	1.356 (7)	C17—C22	1.397 (4)

C3—H3	0.9300	C18—C19	1.376 (4)
C4—C5	1.420 (6)	C18—H18	0.9300
C4—H4	0.9300	C19—C20	1.379 (5)
C5—C6	1.370 (5)	C19—H19	0.9300
C5—H5	0.9300	C20—C21	1.364 (5)
C6—C7	1.476 (5)	C20—H20	0.9300
C7—C8	1.315 (5)	C21—C22	1.381 (4)
C7—H7	0.9300	C21—H21	0.9300
C8—C9	1.475 (4)	C22—H22	0.9300

O2—N1—O1	126.0 (3)	C9—C10—N2	121.2 (3)
O2—N1—C14	117.4 (3)	C12—C11—C10	118.6 (3)
O1—N1—C14	116.5 (3)	C12—C11—H11	120.7
O3—N2—O4	122.9 (3)	C10—C11—H11	120.7
O3—N2—C10	119.5 (3)	C11—C12—C13	124.4 (3)
O4—N2—C10	117.5 (3)	C11—C12—N3	115.1 (3)
O5—N3—O6	124.5 (3)	C13—C12—N3	120.5 (2)
O5—N3—C12	116.7 (3)	C14—C13—C12	113.1 (3)
O6—N3—C12	118.8 (2)	C14—C13—C15	126.0 (3)
C2—C1—C6	122.2 (4)	C12—C13—C15	120.9 (3)
C2—C1—H1	118.9	C9—C14—C13	126.6 (3)
C6—C1—H1	118.9	C9—C14—N1	114.9 (3)
C3—C2—C1	118.7 (5)	C13—C14—N1	118.4 (2)
C3—C2—H2	120.7	C16—C15—C13	129.8 (3)
C1—C2—H2	120.7	C16—C15—H15	115.1
C2—C3—C4	122.1 (5)	C13—C15—H15	115.1
C2—C3—H3	118.9	C15—C16—C17	124.7 (3)
C4—C3—H3	118.9	C15—C16—H16	117.7
C3—C4—C5	119.3 (5)	C17—C16—H16	117.7
C3—C4—H4	120.3	C18—C17—C22	118.3 (3)
C5—C4—H4	120.3	C18—C17—C16	119.5 (3)
C6—C5—C4	119.4 (5)	C22—C17—C16	122.2 (3)
C6—C5—H5	120.3	C19—C18—C17	120.8 (3)
C4—C5—H5	120.3	C19—C18—H18	119.6
C5—C6—C1	118.3 (4)	C17—C18—H18	119.6
C5—C6—C7	123.0 (4)	C18—C19—C20	120.4 (3)
C1—C6—C7	118.6 (3)	C18—C19—H19	119.8
C8—C7—C6	128.2 (3)	C20—C19—H19	119.8
C8—C7—H7	115.9	C21—C20—C19	119.4 (3)
C6—C7—H7	115.9	C21—C20—H20	120.3
C7—C8—C9	122.1 (3)	C19—C20—H20	120.3
C7—C8—H8	118.9	C20—C21—C22	120.9 (3)
C9—C8—H8	118.9	C20—C21—H21	119.5
C14—C9—C10	114.8 (3)	C22—C21—H21	119.5
C14—C9—C8	120.5 (3)	C21—C22—C17	120.1 (3)
C10—C9—C8	124.7 (3)	C21—C22—H22	120.0
C11—C10—C9	122.3 (3)	C17—C22—H22	120.0
C11—C10—N2	116.5 (3)		

C6—C1—C2—C3	0.7 (6)	C11—C12—C13—C14	−3.0 (4)
C1—C2—C3—C4	0.2 (7)	N3—C12—C13—C14	177.4 (2)
C2—C3—C4—C5	−0.6 (7)	C11—C12—C13—C15	179.6 (3)
C3—C4—C5—C6	0.1 (6)	N3—C12—C13—C15	0.0 (4)
C4—C5—C6—C1	0.7 (5)	C10—C9—C14—C13	0.4 (5)
C4—C5—C6—C7	179.5 (4)	C8—C9—C14—C13	−177.6 (3)
C2—C1—C6—C5	−1.1 (5)	C10—C9—C14—N1	178.9 (3)
C2—C1—C6—C7	−180.0 (3)	C8—C9—C14—N1	0.8 (4)
C5—C6—C7—C8	18.2 (5)	C12—C13—C14—C9	2.8 (4)
C1—C6—C7—C8	−163.0 (4)	C15—C13—C14—C9	−179.9 (3)
C6—C7—C8—C9	−179.5 (3)	C12—C13—C14—N1	−175.6 (2)
C7—C8—C9—C14	65.4 (4)	C15—C13—C14—N1	1.7 (4)
C7—C8—C9—C10	−112.4 (4)	O2—N1—C14—C9	74.1 (3)
C14—C9—C10—C11	−3.9 (4)	O1—N1—C14—C9	−104.5 (3)
C8—C9—C10—C11	174.0 (3)	O2—N1—C14—C13	−107.4 (3)
C14—C9—C10—N2	178.0 (3)	O1—N1—C14—C13	74.1 (3)
C8—C9—C10—N2	−4.0 (5)	C14—C13—C15—C16	26.2 (5)
O3—N2—C10—C11	176.3 (3)	C12—C13—C15—C16	−156.8 (3)
O4—N2—C10—C11	−0.5 (5)	C13—C15—C16—C17	177.8 (3)
O3—N2—C10—C9	−5.6 (5)	C15—C16—C17—C18	156.0 (3)
O4—N2—C10—C9	177.7 (3)	C15—C16—C17—C22	−24.0 (5)
C9—C10—C11—C12	3.8 (5)	C22—C17—C18—C19	1.4 (5)
N2—C10—C11—C12	−178.1 (3)	C16—C17—C18—C19	−178.7 (3)
C10—C11—C12—C13	−0.1 (5)	C17—C18—C19—C20	−0.8 (5)
C10—C11—C12—N3	179.5 (3)	C18—C19—C20—C21	−0.5 (6)
O5—N3—C12—C11	47.8 (4)	C19—C20—C21—C22	1.2 (5)
O6—N3—C12—C11	−130.5 (3)	C20—C21—C22—C17	−0.6 (5)
O5—N3—C12—C13	−132.5 (3)	C18—C17—C22—C21	−0.7 (5)
O6—N3—C12—C13	49.1 (4)	C16—C17—C22—C21	179.4 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16···O2	0.93	2.60	3.398 (4)	144
C16—H16···N1	0.93	2.42	2.980 (4)	119
C18—H18···O5^{i}	0.93	2.48	3.387 (4)	166

Symmetry code: (i) *x*, *y*+1, *z*.