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6,6′-Dimethoxy-2,2′,3,3′,5-pentanitro-1,1′-biphenyl

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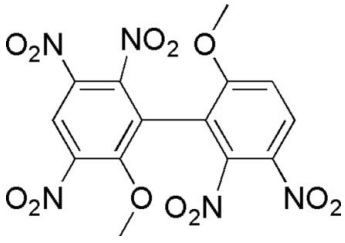
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.003 Å; R factor = 0.042; wR factor = 0.118; data-to-parameter ratio = 11.3.

In the axially chiral title compound, $C_{14}H_9N_5O_{12}$, the dihedral angle between the two benzene rings is 86.0 (8)°. In the crystal structure, the molecules display a two-dimensional framework formed by weak intermolecular C—H···O hydrogen bonds.

Related literature

For related literature, see: Chen *et al.* (2001); Fischer *et al.* (2007); Narayanan *et al.* (2005); Saito & Koizumi (2005); Xiao *et al.* (2007); Yang *et al.* (2005).



Experimental

Crystal data

$C_{14}H_9N_5O_{12}$
M_r = 439.26
Triclinic, $P\overline{1}$
a = 10.3765 (13) Å
b = 10.4423 (13) Å
c = 10.4429 (13) Å
α = 82.5650 (10)°
β = 62.2850 (10)° = 60.5200 (10)°
V = 864.73 (19) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.15 mm^{-1}
T = 291 (2) K
0.41 × 0.34 × 0.29 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.940, T_{max} = 0.958
6598 measured reflections
3194 independent reflections
2686 reflections with $I > 2\sigma(I)$
R_{int} = 0.013

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.117
S = 1.02
3194 reflections
282 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13A···O3	0.96	2.45	2.926 (3)	111
C14—H14B···O10^{i}	0.96	2.55	3.502 (3)	174
C14—H14C···O8^{ii}	0.96	2.58	3.371 (3)	140

Symmetry codes: (i) $x+1, y-1, z$; (ii) $-x+1, -y+2, -z+1$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: SI2086).

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supporting information

Acta Cryst. (2008). E**64**, o951 [doi:10.1107/S1600536808011926]

6,6′-Dimethoxy-2,2′,3,3′,5-pentanitro-1,1′-biphenyl

Yuan-Yuan Jiang, Shao-Bin Miao, Dong-Sheng Deng and Bao-Ming Ji

S1. Comment

Nitro compounds, specially aromatic nitro compounds have been widely studied owing to their potential application in, for example, pathology (Narayanan, *et al.*, 2005), materials science (Saito & Koizumi, 2005). On the other hand, in our search for chiral compounds, the title related chiral 6,6′-dimethoxy-2,3,2′,5′-tetranitro-1,1′-biphenyl compound was synthesized by Xiao *et al.*, (2007). Herein, as an extension to our previous investigation, we report the synthesis and structural characterization of the title compound.

In contrast to our highly substituted biphenyl compounds, the unsubstituted biphenyl groups in compounds synthesized by Fischer *et al.*, (2007) were found to be approximately planar. The molecular geometry in the title compound displays special behavior, the dihedral angle between the benzene rings is 94.0 (8)°, and all the nitro groups at positions 2,3,5,2′,3′ are twisted out of the corresponding rings which is 45.5 (3)°, 13.5 (5)°, 98.4 (3)°, 6.6 (4)° and 83.5 (5)°, respectively, as depicted in Fig.1. Bond lengths and angles are in good agreement with the dinitrophenyl group in the structure of 1-(2,4-dinitrophenyl)azo-1-nitrocyclohexane, reported by Yang *et al.*, (2005). One intramolecular C—H···O hydrogen bond is observed in the title molecule, and the two intermolecular C—H···O hydrogen bonding contacts (Table 1) form closed two-dimensional grid motifs (Fig. 2).

S2. Experimental

All chemicals and solvents purchased were of reagent grade and used without further purification. The precursor 6,6′-Dimethoxy-2,2′-dinitro-1,1′-biphenyl was prepared according to the reported procedure (Chen *et al.*, 2001). However, the title compound was obtained by chance when we tried to prepare the 6,6′-Dimethoxy-2,3,5,2′,3′,5′-hexanitro-1,1′-biphenyl compound. That is, the title compound was synthesized by the nitration reaction of the precursor (0.5 mmol) in 10 ml of concentrated nitric acid at room temperature for 24 h. The resulting solution was poured into 30 ml of ice water and the resulting precipitate was collected by filtration and recrystallized from ethyl acetate to obtain the title crystals, which were suitable for X-ray diffraction analysis. Cautious, the title compound has potential explosive property.

S3. Refinement

H atoms were positioned geometrically and treated as riding, with C—H bonding lengths constrained to 0.93 (aromatic H), 0.96 Å (methyl H), and with *U*ĩso~(H) = 1.2Ueq (aromatic H) or *U*ĩso~(H) = 1.5Ueq (methyl H).

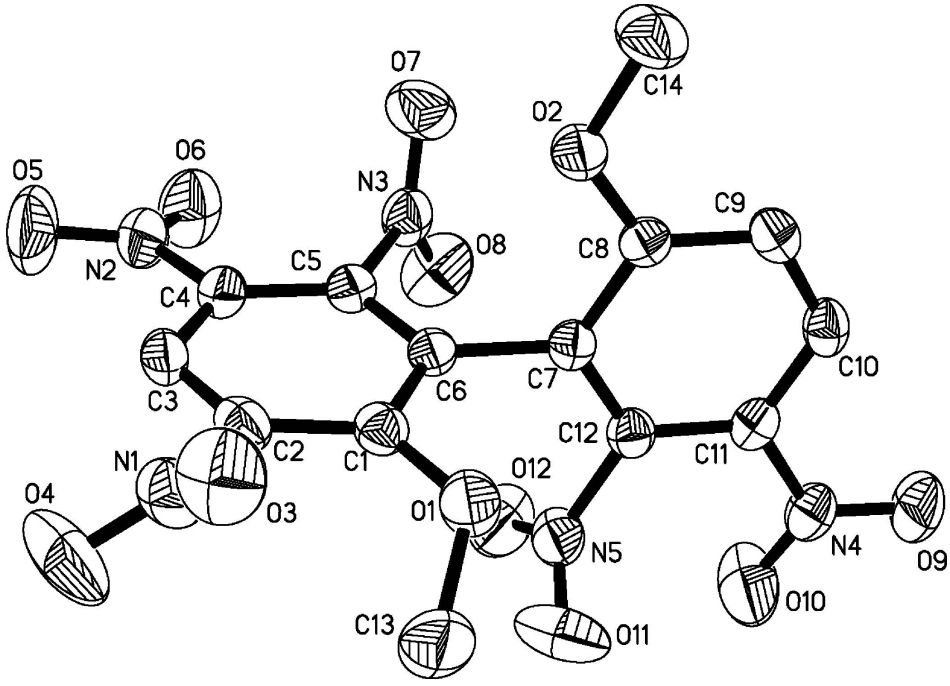

Figure 1

Atom numbering scheme for the title compound with 30% probability displacement ellipsoids.

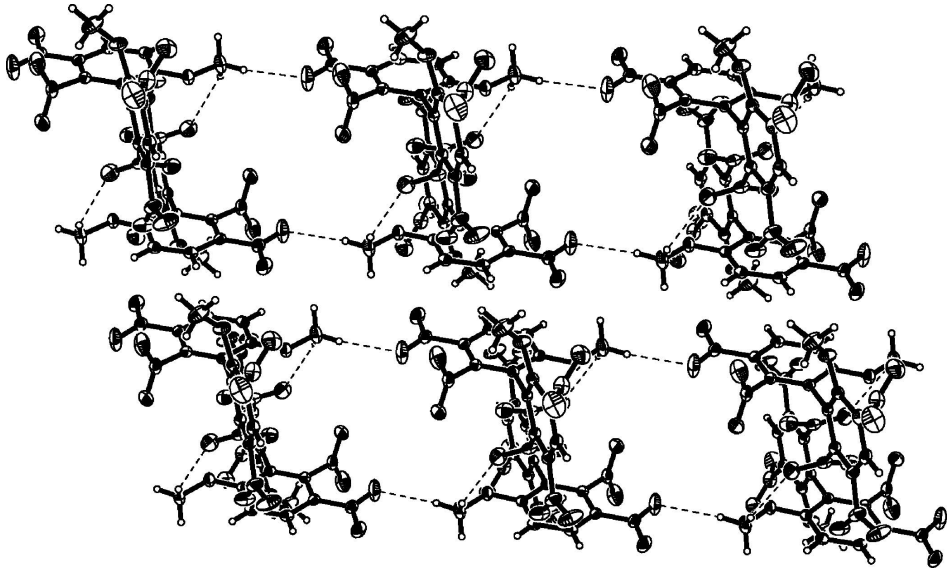

Figure 2

View of the two-dimensional sheet structure. (C—H···O interactions are represented as broken lines).

6,6′-Dimethoxy-2,2′,3,3′,5-pentanitro-1,1′-biphenyl

Crystal data

$C_{14}H_9N_5O_{12}$
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Triclinic, $P\overline{1}$
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$b = 10.4423\ (13)$ Å
$c = 10.4429\ (13)$ Å
$\alpha = 82.565\ (1)°$

β = 62.285 (1)°
γ = 60.520 (1)°
V = 864.73 (19) Å^3
Z = 2
F(000) = 448
D_x = 1.687 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 2971 reflections
θ = 2.4–25.5°
μ = 0.15 mm^{-1}
T = 291 K
Block, yellow
0.41 × 0.34 × 0.29 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.940, T_{max} = 0.958

6598 measured reflections
3194 independent reflections
2686 reflections with $I > 2\sigma(I)$
R_{int} = 0.013
θ_{max} = 25.5°, θ_{min} = 2.4°
h = −12→12
k = −12→12
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.117
S = 1.02
3194 reflections
282 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
$w = 1/[\sigma^2(F_o^2) + (0.059P)^2 + 0.3851P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 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	0.36354 (18)	0.70656 (16)	0.19497 (14)	0.0448 (3)
O2	0.69388 (15)	0.72440 (14)	0.24022 (14)	0.0382 (3)
O3	0.4217 (2)	0.40331 (19)	0.2500 (2)	0.0678 (5)
O4	0.1905 (2)	0.4489 (2)	0.4428 (3)	0.0852 (6)
O5	0.2186 (3)	0.6187 (2)	0.84423 (19)	0.0803 (6)
O6	0.2172 (2)	0.8273 (2)	0.83302 (16)	0.0648 (5)
O7	0.5003 (2)	0.8533 (2)	0.57692 (17)	0.0582 (4)
O8	0.2549 (2)	1.03379 (17)	0.61824 (19)	0.0640 (5)
O9	0.2989 (2)	1.33902 (17)	0.06894 (18)	0.0571 (4)
O10	0.0962 (2)	1.3106 (2)	0.2303 (2)	0.0846 (7)

O11	0.0882 (2)	1.0384 (2)	0.2635 (2)	0.0761 (6)
O12	0.04620 (19)	1.1239 (2)	0.46358 (18)	0.0702 (5)
N1	0.3036 (2)	0.4748 (2)	0.3675 (2)	0.0507 (5)
N2	0.2378 (2)	0.7181 (2)	0.77767 (18)	0.0484 (4)
N3	0.3645 (2)	0.90493 (19)	0.58132 (16)	0.0404 (4)
N4	0.2444 (2)	1.26902 (17)	0.15879 (17)	0.0391 (4)
N5	0.1327 (2)	1.06936 (18)	0.3386 (2)	0.0433 (4)
C1	0.3442 (2)	0.69672 (19)	0.33107 (19)	0.0316 (4)
C2	0.3056 (2)	0.59612 (19)	0.4225 (2)	0.0351 (4)
C3	0.2736 (2)	0.6019 (2)	0.5661 (2)	0.0371 (4)
H3	0.2441	0.5362	0.6249	0.045*
C4	0.2859 (2)	0.7060 (2)	0.62141 (19)	0.0351 (4)
C5	0.3359 (2)	0.80022 (19)	0.52985 (19)	0.0314 (4)
C6	0.3661 (2)	0.79704 (18)	0.38642 (18)	0.0283 (4)
C7	0.4211 (2)	0.89880 (18)	0.28967 (17)	0.0280 (4)
C8	0.5928 (2)	0.85656 (18)	0.21610 (18)	0.0287 (4)
C9	0.6454 (2)	0.9505 (2)	0.12600 (18)	0.0330 (4)
H9	0.7584	0.9224	0.0769	0.040*
C10	0.5303 (2)	1.08464 (19)	0.10979 (18)	0.0331 (4)
H10	0.5660	1.1471	0.0507	0.040*
C11	0.3623 (2)	1.12714 (18)	0.18047 (18)	0.0308 (4)
C12	0.3096 (2)	1.03275 (19)	0.26904 (18)	0.0302 (4)
C13	0.2548 (4)	0.6888 (3)	0.1570 (3)	0.0651 (7)
H13A	0.3124	0.5908	0.1070	0.098*
H13B	0.2243	0.7609	0.0946	0.098*
H13C	0.1559	0.7028	0.2442	0.098*
C14	0.8715 (2)	0.6715 (2)	0.1654 (3)	0.0536 (6)
H14A	0.9102	0.6645	0.0619	0.080*
H14B	0.9285	0.5755	0.1910	0.080*
H14C	0.8939	0.7394	0.1934	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0591 (9)	0.0572 (9)	0.0359 (7)	−0.0397 (8)	−0.0238 (7)	0.0089 (6)
O2	0.0289 (6)	0.0334 (7)	0.0451 (7)	−0.0130 (5)	−0.0157 (6)	0.0099 (5)
O3	0.0824 (13)	0.0479 (9)	0.0718 (12)	−0.0313 (9)	−0.0322 (10)	−0.0061 (8)
O4	0.0745 (13)	0.0756 (13)	0.1234 (17)	−0.0582 (11)	−0.0347 (12)	0.0068 (12)
O5	0.1272 (17)	0.1048 (15)	0.0559 (10)	−0.0899 (15)	−0.0508 (11)	0.0482 (10)
O6	0.0882 (13)	0.0741 (12)	0.0384 (8)	−0.0475 (10)	−0.0264 (8)	0.0091 (8)
O7	0.0600 (10)	0.0829 (12)	0.0526 (9)	−0.0446 (9)	−0.0309 (8)	0.0070 (8)
O8	0.0900 (13)	0.0396 (9)	0.0696 (11)	−0.0276 (9)	−0.0460 (10)	0.0029 (7)
O9	0.0681 (10)	0.0444 (8)	0.0624 (10)	−0.0317 (8)	−0.0342 (8)	0.0286 (7)
O10	0.0399 (9)	0.0592 (11)	0.1113 (16)	−0.0129 (8)	−0.0246 (10)	0.0458 (11)
O11	0.0482 (10)	0.0769 (12)	0.1132 (16)	−0.0263 (9)	−0.0453 (10)	−0.0055 (11)
O12	0.0383 (8)	0.0812 (12)	0.0476 (10)	−0.0124 (8)	−0.0077 (7)	0.0123 (9)
N1	0.0541 (11)	0.0396 (9)	0.0703 (13)	−0.0277 (9)	−0.0332 (10)	0.0094 (9)
N2	0.0543 (11)	0.0646 (12)	0.0385 (9)	−0.0381 (10)	−0.0243 (8)	0.0213 (9)

N3	0.0540 (10)	0.0481 (10)	0.0313 (8)	−0.0321 (9)	−0.0224 (7)	0.0098 (7)
N4	0.0467 (10)	0.0305 (8)	0.0402 (9)	−0.0181 (7)	−0.0226 (8)	0.0103 (7)
N5	0.0327 (8)	0.0344 (9)	0.0536 (11)	−0.0137 (7)	−0.0189 (8)	0.0149 (7)
C1	0.0280 (8)	0.0314 (9)	0.0333 (9)	−0.0139 (7)	−0.0132 (7)	0.0033 (7)
C2	0.0309 (9)	0.0296 (9)	0.0464 (10)	−0.0163 (7)	−0.0173 (8)	0.0042 (8)
C3	0.0335 (9)	0.0347 (10)	0.0450 (11)	−0.0203 (8)	−0.0185 (8)	0.0158 (8)
C4	0.0338 (9)	0.0400 (10)	0.0328 (9)	−0.0198 (8)	−0.0162 (8)	0.0116 (8)
C5	0.0305 (9)	0.0312 (9)	0.0340 (9)	−0.0153 (7)	−0.0166 (7)	0.0064 (7)
C6	0.0247 (8)	0.0257 (8)	0.0322 (9)	−0.0112 (7)	−0.0132 (7)	0.0055 (7)
C7	0.0317 (9)	0.0279 (8)	0.0263 (8)	−0.0158 (7)	−0.0136 (7)	0.0036 (6)
C8	0.0308 (9)	0.0288 (8)	0.0281 (8)	−0.0143 (7)	−0.0147 (7)	0.0022 (7)
C9	0.0314 (9)	0.0375 (9)	0.0306 (9)	−0.0202 (8)	−0.0109 (7)	0.0026 (7)
C10	0.0427 (10)	0.0336 (9)	0.0288 (9)	−0.0250 (8)	−0.0146 (8)	0.0060 (7)
C11	0.0383 (9)	0.0271 (8)	0.0288 (8)	−0.0156 (7)	−0.0177 (7)	0.0048 (7)
C12	0.0303 (9)	0.0311 (9)	0.0281 (8)	−0.0153 (7)	−0.0127 (7)	0.0037 (7)
C13	0.098 (2)	0.0792 (18)	0.0680 (15)	−0.0620 (16)	−0.0593 (15)	0.0260 (13)
C14	0.0295 (10)	0.0445 (12)	0.0705 (15)	−0.0120 (9)	−0.0182 (10)	0.0085 (10)

Geometric parameters (Å, º)

O1—C1	1.337 (2)	C2—C3	1.380 (3)
O1—C13	1.451 (3)	C3—C4	1.379 (3)
O2—C8	1.341 (2)	C3—H3	0.9300
O2—C14	1.443 (2)	C4—C5	1.396 (2)
O3—N1	1.225 (3)	C5—C6	1.382 (2)
O4—N1	1.211 (2)	C6—C7	1.503 (2)
O5—N2	1.220 (2)	C7—C12	1.379 (2)
O6—N2	1.223 (2)	C7—C8	1.414 (2)
O7—N3	1.215 (2)	C8—C9	1.399 (2)
O8—N3	1.214 (2)	C9—C10	1.377 (3)
O9—N4	1.212 (2)	C9—H9	0.9300
O10—N4	1.212 (2)	C10—C11	1.381 (3)
O11—N5	1.218 (2)	C10—H10	0.9300
O12—N5	1.197 (2)	C11—C12	1.396 (2)
N1—C2	1.470 (2)	C13—H13A	0.9600
N2—C4	1.470 (2)	C13—H13B	0.9600
N3—C5	1.481 (2)	C13—H13C	0.9600
N4—C11	1.459 (2)	C14—H14A	0.9600
N5—C12	1.478 (2)	C14—H14B	0.9600
C1—C2	1.405 (2)	C14—H14C	0.9600
C1—C6	1.413 (2)		
C1—O1—C13	120.36 (16)	C5—C6—C7	120.87 (15)
C8—O2—C14	118.30 (14)	C1—C6—C7	119.98 (15)
O4—N1—O3	124.87 (19)	C12—C7—C8	118.36 (15)
O4—N1—C2	118.4 (2)	C12—C7—C6	122.25 (15)
O3—N1—C2	116.66 (17)	C8—C7—C6	119.39 (14)
O5—N2—O6	124.23 (18)	O2—C8—C9	125.08 (15)

O5—N2—C4	117.39 (18)	O2—C8—C7	115.04 (14)
O6—N2—C4	118.38 (16)	C9—C8—C7	119.88 (15)
O8—N3—O7	126.09 (18)	C10—C9—C8	120.20 (16)
O8—N3—C5	117.95 (16)	C10—C9—H9	119.9
O7—N3—C5	115.89 (17)	C8—C9—H9	119.9
O9—N4—O10	122.95 (17)	C9—C10—C11	120.58 (16)
O9—N4—C11	118.70 (16)	C9—C10—H10	119.7
O10—N4—C11	118.34 (15)	C11—C10—H10	119.7
O12—N5—O11	125.41 (19)	C10—C11—C12	119.36 (16)
O12—N5—C12	118.04 (18)	C10—C11—N4	118.98 (15)
O11—N5—C12	116.54 (17)	C12—C11—N4	121.66 (16)
O1—C1—C2	126.17 (16)	C7—C12—C11	121.61 (16)
O1—C1—C6	116.23 (15)	C7—C12—N5	117.27 (15)
C2—C1—C6	117.61 (16)	C11—C12—N5	121.06 (15)
C3—C2—C1	122.38 (16)	O1—C13—H13A	109.5
C3—C2—N1	116.34 (16)	O1—C13—H13B	109.5
C1—C2—N1	121.24 (17)	H13A—C13—H13B	109.5
C2—C3—C4	119.28 (16)	O1—C13—H13C	109.5
C2—C3—H3	120.4	H13A—C13—H13C	109.5
C4—C3—H3	120.4	H13B—C13—H13C	109.5
C3—C4—C5	119.40 (16)	O2—C14—H14A	109.5
C3—C4—N2	118.23 (16)	O2—C14—H14B	109.5
C5—C4—N2	122.31 (17)	H14A—C14—H14B	109.5
C6—C5—C4	121.87 (16)	O2—C14—H14C	109.5
C6—C5—N3	116.95 (15)	H14A—C14—H14C	109.5
C4—C5—N3	121.15 (15)	H14B—C14—H14C	109.5
C5—C6—C1	119.15 (15)		

C13—O1—C1—C2	39.2 (3)	C2—C1—C6—C7	175.07 (15)
C13—O1—C1—C6	−141.22 (19)	C5—C6—C7—C12	−95.4 (2)
O1—C1—C2—C3	−174.24 (17)	C1—C6—C7—C12	84.4 (2)
C6—C1—C2—C3	6.2 (3)	C5—C6—C7—C8	84.9 (2)
O1—C1—C2—N1	8.1 (3)	C1—C6—C7—C8	−95.26 (19)
C6—C1—C2—N1	−171.47 (16)	C14—O2—C8—C9	−1.7 (3)
O4—N1—C2—C3	45.1 (3)	C14—O2—C8—C7	178.11 (16)
O3—N1—C2—C3	−132.0 (2)	C12—C7—C8—O2	−179.37 (14)
O4—N1—C2—C1	−137.1 (2)	C6—C7—C8—O2	0.3 (2)
O3—N1—C2—C1	45.8 (3)	C12—C7—C8—C9	0.4 (2)
C1—C2—C3—C4	−2.5 (3)	C6—C7—C8—C9	−179.88 (15)
N1—C2—C3—C4	175.21 (16)	O2—C8—C9—C10	−179.60 (15)
C2—C3—C4—C5	−2.2 (3)	C7—C8—C9—C10	0.6 (2)
C2—C3—C4—N2	175.03 (16)	C8—C9—C10—C11	−0.9 (3)
O5—N2—C4—C3	12.9 (3)	C9—C10—C11—C12	0.0 (2)
O6—N2—C4—C3	−166.04 (19)	C9—C10—C11—N4	−179.06 (15)
O5—N2—C4—C5	−170.01 (19)	O9—N4—C11—C10	6.8 (2)
O6—N2—C4—C5	11.1 (3)	O10—N4—C11—C10	−174.16 (19)
C3—C4—C5—C6	3.1 (3)	O9—N4—C11—C12	−172.27 (17)
N2—C4—C5—C6	−173.96 (16)	O10—N4—C11—C12	6.8 (3)

C3—C4—C5—N3	−174.78 (16)	C8—C7—C12—C11	−1.3 (2)
N2—C4—C5—N3	8.2 (3)	C6—C7—C12—C11	179.06 (15)
O8—N3—C5—C6	81.7 (2)	C8—C7—C12—N5	175.72 (15)
O7—N3—C5—C6	−95.50 (19)	C6—C7—C12—N5	−3.9 (2)
O8—N3—C5—C4	−100.3 (2)	C10—C11—C12—C7	1.0 (2)
O7—N3—C5—C4	82.5 (2)	N4—C11—C12—C7	−179.88 (15)
C4—C5—C6—C1	0.6 (3)	C10—C11—C12—N5	−175.84 (16)
N3—C5—C6—C1	178.61 (15)	N4—C11—C12—N5	3.2 (2)
C4—C5—C6—C7	−179.53 (15)	O12—N5—C12—C7	84.0 (2)
N3—C5—C6—C7	−1.6 (2)	O11—N5—C12—C7	−94.7 (2)
O1—C1—C6—C5	175.27 (15)	O12—N5—C12—C11	−99.0 (2)
C2—C1—C6—C5	−5.1 (2)	O11—N5—C12—C11	82.3 (2)
O1—C1—C6—C7	−4.6 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13*A*···O3	0.96	2.45	2.926 (3)	111
C14—H14*B*···O10^{i}	0.96	2.55	3.502 (3)	174
C14—H14*C*···O8^{ii}	0.96	2.58	3.371 (3)	140

Symmetry codes: (i) *x*+1, *y*−1, *z*; (ii) −*x*+1, −*y*+2, −*z*+1.