



Crystal structure of 4,4'-dinitro-[1,1'-biphenyl]-2-amine

Md. Serajul Haque Faizi,^a Ashanul Haque,^a Necmi Dege,^b Syed Imran Hasan,^a Mustafa Dege^c and Valentina A. Kalibabchuk^{d*}

^aDepartment of Chemistry, College of Science, Sultan Qaboos University, PO Box 36 Al-Khod 123, Muscat, Sultanate of , Oman, ^bOndokuz Mayıs University, Arts and Sciences Faculty, Department of Physics, 55139 Samsun, Turkey, ^cSpraying Systems Company Turkey, Esentepe Mah. Kore Şehitleri Cad. Kaya Aldoğan Sok., Serhan apt. No. 3 Daire:3 Şişli İstanbul, Turkey, and ^dDepartment of General Chemistry, O. O. Bohomolets National Medical University, Shevchenko Blvd. 13, 01601 Kiev, Ukraine. *Correspondence e-mail: kalibabchuk@ukr.net

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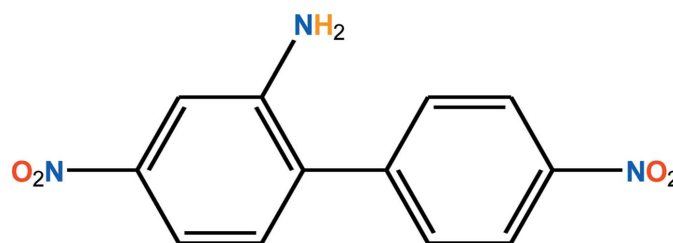
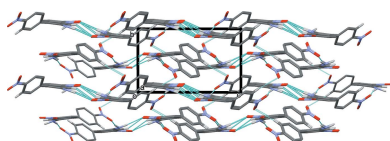
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In the title biphenyl derivative, C₁₂H₉N₃O₄, the dihedral angle between the benzene rings is 52.84 (10)°. The nitro group attached to the benzene ring is inclined to the ring by 4.03 (2)°, while the nitro group attached to the amino-substituted benzene ring is inclined to the ring by 8.84 (2)°. In the crystal, molecules are linked by two pairs of N—H...O hydrogen bonds, forming chains propagating along [101]. Within the chains, these N—H...O hydrogen bonds result in the formation of R₂²(20) and R₂²(14) ring motifs. The latter ring motif is reinforced by a pair of C—H...O hydrogen bonds, enclosing R₃¹(6) ring motifs. The chains are linked by a second C—H...O hydrogen bond, forming a three-dimensional supramolecular structure.

1. Chemical context

Biphenyl and its derivatives have been shown to play an important role in fighting cancer and arteriosclerosis in humans (Umeda *et al.*, 2005). The dihedral angle between the phenyl rings of biphenyl derivatives is associated with their affinity for cellular target molecules and, therefore, can correlate with their toxicity. The parent compound, biphenyl, adopts a planar conformation in the solid state with a dihedral angle of 0° (Trotter, 1961). The calculated dihedral angle for biphenyl derivatives without *ortho* substituents is *ca* 41° (Shaikh *et al.*, 2008). Deviations from the energetically most favourable conformation are most likely the result of crystal packing effects, which allow such compounds to adopt an energetically favorable conformation in the solid state by maximizing the lattice energy. Many research groups have calculated the inter-ring torsion angle of biphenyl in the solid state (Brock, 1980; Brock & Minton, 1989; Bastiansen & Samdal, 1985), and in the gas phase (Bastiansen & Traetteberg, 1962). We report here a detailed description of the molecular structure and supramolecular features of the title biphenyl derivative, 4,4'-dinitro-[1,1'-biphenyl]-2-amine, (I).



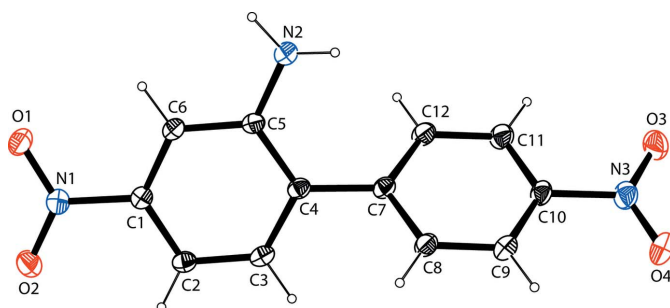


Figure 1

The molecular structure of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 40% probability level.

2. Structural commentary

The molecular structure of the title compound (I), is illustrated in Fig. 1. The dihedral angle between the two rings of the biphenyl unit is $52.84(10)^\circ$. The nitro group (N3/O3/O4) is inclined to the benzene ring (C7–C12) to which it is attached by $4.03(2)^\circ$. The nitro group (N1/O1/O2) is inclined to the amino-substituted benzene ring (C1–C6), to which it is attached, by $8.84(2)^\circ$. The amino N atom, N2, lies in the plane of the C1–C6 benzene ring, and the N2–C5 bond length of $1.375(3)$ Å clearly indicates a single bond. The C1–N1 distance of $1.466(3)$ Å is slightly less than the C10–N3 bond distance of $1.477(3)$ Å, which indicates that the 2-amino group containing a benzene ring (C1–C6) is more conjugated with the nitro group (N1/O1/O2) than is the other nitro group (N3/O3/O4) with respect to the C7–C12 benzene ring. The bond length of the C4–C7 bridge is $1.482(3)$ Å, which indicates a single bond, and is similar to the same bond length of $1.494(2)$ Å reported for dimethyl 2,2'-dinitrophenyl-4,4'-dicarboxylate (Lehane *et al.*, 2014), and *ca* 1.493 Å observed in 2,2'-dinitrophenyl (Sekine *et al.*, 1994).

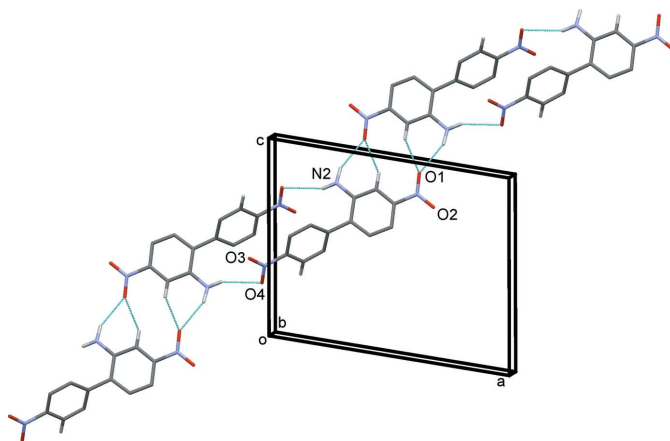


Figure 2

A view of the N–H...O and C–H...O hydrogen bonds (dashed lines; see Table 1), in the crystal of (I), forming chains that propagate along [101].

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2–H2B...O1 ⁱ	0.92 (2)	2.36 (2)	3.229 (3)	157 (2)
N2–H2A...O4 ⁱⁱ	0.89 (2)	2.50 (2)	3.345 (3)	157 (2)
C6–H6...O1 ⁱ	0.93	2.54	3.308 (3)	140
C9–H9...O3 ⁱⁱⁱ	0.93	2.57	3.496 (3)	174

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

3. Supramolecular features

In the crystal, molecules are linked by two pairs of N–H...O hydrogen bonds, forming chains propagating along the [101] direction. Within the chains, these N–H...O hydrogen bonds result in the formation of $R_2^2(20)$ and $R_2^2(14)$ ring motifs (Table 1 and Fig. 2). The latter ring motif is reinforced by a pair of C–H...O hydrogen bonds, enclosing $R_2^1(6)$ ring motifs (Table 1 and Fig. 2). The chains are linked by a second C–H...O hydrogen bond (Table 1), forming a three-dimensional supramolecular structure, as illustrated in Figs. 3 and 4.

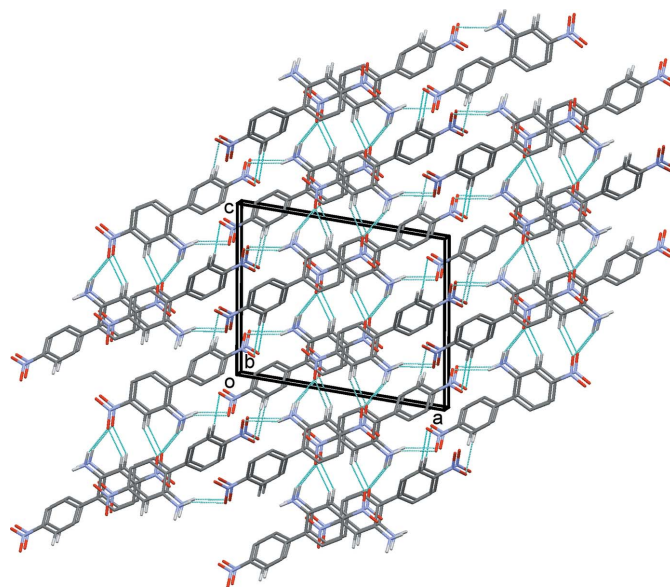


Figure 3

A view along the *b* axis of the crystal packing of (I). Hydrogen bonds are shown as dashed lines (see Table 1) and, for clarity, only H atoms H2A, H2B, H6 and H9 have been included.

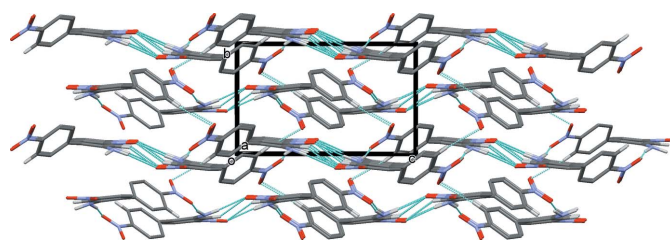


Figure 4

A view along the *a* axis of the crystal packing of (I). Hydrogen bonds are shown as dashed lines (see Table 1) and, for clarity, only H atoms H2A, H2B, H6 and H9 have been included.

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₁₂ H ₉ N ₃ O ₄
<i>M_r</i>	259.22
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	14.2940 (11), 7.0352 (6), 11.6043 (9)
β (°)	99.437 (6)
<i>V</i> (Å ³)	1151.15 (16)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ^{−1})	0.12
Crystal size (mm)	0.34 × 0.20 × 0.07
Data collection	
Diffractometer	Stoe IPDS 2
Absorption correction	Integration (<i>X-RED32</i> ; Stoe & Cie, 2002)
<i>T</i> _{min} , <i>T</i> _{max}	0.980, 0.993
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	6476, 2566, 1052
<i>R</i> _{int}	0.044
(sin θ/λ) _{max} (Å ^{−1})	0.646
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.040, 0.092, 0.81
No. of reflections	2566
No. of parameters	180
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
Δρ _{max} , Δρ _{min} (e Å ^{−3})	0.10, −0.12

Computer programs: *X-AREA* and *X-RED32* (Stoe & Cie, 2002), *SHELXT* (Sheldrick 2015a), *SHELXL2016* (Sheldrick, 2015b), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.38, update February 2017; Groom *et al.*, 2016) revealed the structure of two similar compounds *viz* 4'-nitro-2-biphenylamine (II) (CSD refcode DIWFEU; Sutherland & Ali-Adib, 1986) and 4,4'-dinitrobiphenyl (III) (DNTDPH; Boonstra, 1963). In (II), the benzene rings are inclined to one another by 54.64 (6)°, compared to *ca* 32.91° in (III), and to 52.84 (2)° in the title compound (I). In (II), the nitro group is inclined to the benzene ring to which it is attached by 7.08 (6)°, compared to *ca* 3.55 and 10.14° in (III) and 8.3 (2)° in the title compound (I).

5. Synthesis and crystallization

The title compound (I), was prepared by a literature procedure (Ol'khovik *et al.*, 2008). Orange prismatic crystals,

suitable for single-crystal X-ray analysis, were grown by slow evaporation of a solution in ethanol.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The N-bound H atoms were located in a difference Fourier map and refined with *U*_{iso}(H) = 1.2*U*_{eq}(N). The C-bound H atoms were included in calculated positions and refined as riding: C–H = 0.93–0.96 Å with *U*_{iso}(H) = 1.2*U*_{eq}(C).

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Crystal structure of 4,4'-dinitro-[1,1'-biphenyl]-2-amine

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Valentina A. Kalibabchuk

Computing details

Data collection: *X-Area* (Stoe & Cie, 2002); cell refinement: *X-Area* (Stoe & Cie, 2002); data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXT* (Sheldrick 2015a); program(s) used to refine structure: *SHELXL2016* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

4,4'-Dinitro-[1,1'-biphenyl]-2-amine

Crystal data

$C_{12}H_9N_3O_4$
 $M_r = 259.22$
Monoclinic, $P2_1/c$
 $a = 14.2940$ (11) Å
 $b = 7.0352$ (6) Å
 $c = 11.6043$ (9) Å
 $\beta = 99.437$ (6)°
 $V = 1151.15$ (16) Å³
 $Z = 4$

$F(000) = 536$
 $D_x = 1.496$ Mg m⁻³
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3570 reflections
 $\theta = 2.1\text{--}27.8^\circ$
 $\mu = 0.12$ mm⁻¹
 $T = 296$ K
Prism, orange
 $0.34 \times 0.20 \times 0.07$ mm

Data collection

Stoe IPDS 2
diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4
mm long-fine focus
Plane graphite monochromator
Detector resolution: 6.67 pixels mm⁻¹
rotation method scans
Absorption correction: integration
(*X-RED32*; Stoe & Cie, 2002)

$T_{\min} = 0.980$, $T_{\max} = 0.993$
6476 measured reflections
2566 independent reflections
1052 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.044$
 $\theta_{\max} = 27.4^\circ$, $\theta_{\min} = 2.9^\circ$
 $h = -18 \rightarrow 18$
 $k = -8 \rightarrow 9$
 $l = -14 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.092$
 $S = 0.81$
2566 reflections
180 parameters
2 restraints
Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map
Hydrogen site location: mixed
H atoms treated by a mixture of independent
and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0353P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.10$ e Å⁻³
 $\Delta\rho_{\min} = -0.12$ e Å⁻³

Special details

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

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.61664 (11)	0.3867 (2)	0.93876 (16)	0.0867 (5)
N1	0.60769 (13)	0.3912 (3)	0.8317 (2)	0.0701 (5)
O3	−0.08732 (12)	0.2401 (3)	0.36959 (17)	0.1108 (7)
O2	0.67457 (11)	0.3941 (3)	0.77943 (16)	0.1004 (6)
N2	0.26998 (16)	0.4451 (3)	0.8191 (2)	0.0831 (6)
N3	−0.02768 (15)	0.3445 (4)	0.3418 (2)	0.0899 (7)
O4	−0.04065 (12)	0.4408 (3)	0.25269 (19)	0.1165 (7)
C5	0.34478 (14)	0.4181 (3)	0.76003 (19)	0.0575 (5)
C6	0.43668 (14)	0.4150 (3)	0.82181 (19)	0.0597 (5)
H6	0.447162	0.429120	0.902589	0.072*
C4	0.33093 (14)	0.3924 (3)	0.63808 (18)	0.0578 (5)
C2	0.50098 (15)	0.3718 (3)	0.64471 (19)	0.0630 (6)
H2	0.553081	0.358487	0.606754	0.076*
C8	0.21562 (15)	0.4992 (3)	0.4654 (2)	0.0704 (6)
H8	0.260703	0.585579	0.448436	0.084*
C7	0.23591 (14)	0.3858 (3)	0.56438 (18)	0.0604 (5)
C1	0.51178 (14)	0.3912 (3)	0.76354 (19)	0.0565 (5)
C12	0.16757 (15)	0.2578 (3)	0.5889 (2)	0.0737 (6)
H12	0.180146	0.181271	0.655006	0.088*
C3	0.41015 (15)	0.3728 (3)	0.58389 (19)	0.0642 (6)
H3	0.401257	0.359785	0.503076	0.077*
C11	0.08146 (16)	0.2435 (3)	0.5161 (2)	0.0787 (7)
H11	0.035605	0.158226	0.532243	0.094*
C10	0.06496 (16)	0.3583 (4)	0.4192 (2)	0.0709 (6)
C9	0.13043 (16)	0.4857 (3)	0.3926 (2)	0.0754 (6)
H9	0.117272	0.561654	0.326283	0.090*
H2B	0.2854 (15)	0.490 (3)	0.8945 (17)	0.106 (9)*
H2A	0.2140 (13)	0.484 (4)	0.780 (2)	0.114 (10)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0876 (11)	0.1025 (13)	0.0647 (12)	0.0106 (9)	−0.0035 (9)	−0.0071 (11)
N1	0.0702 (12)	0.0638 (12)	0.0744 (15)	0.0050 (10)	0.0068 (12)	−0.0060 (12)
O3	0.0786 (11)	0.1494 (18)	0.1005 (16)	−0.0237 (12)	0.0033 (10)	−0.0310 (13)
O2	0.0715 (10)	0.1330 (15)	0.0988 (14)	−0.0058 (11)	0.0202 (10)	−0.0176 (12)
N2	0.0719 (13)	0.1179 (18)	0.0591 (14)	−0.0019 (12)	0.0092 (11)	−0.0076 (13)
N3	0.0814 (16)	0.1079 (19)	0.0760 (18)	0.0001 (13)	0.0000 (14)	−0.0284 (14)
O4	0.1077 (14)	0.1460 (18)	0.0828 (15)	0.0023 (12)	−0.0234 (11)	0.0033 (14)

C5	0.0680 (13)	0.0557 (13)	0.0501 (13)	−0.0050 (10)	0.0135 (11)	−0.0001 (10)
C6	0.0709 (13)	0.0582 (13)	0.0481 (12)	−0.0029 (10)	0.0045 (11)	0.0007 (10)
C4	0.0708 (13)	0.0515 (12)	0.0512 (13)	−0.0050 (10)	0.0102 (11)	0.0016 (11)
C2	0.0746 (14)	0.0591 (14)	0.0573 (15)	−0.0005 (11)	0.0171 (12)	−0.0026 (11)
C8	0.0774 (14)	0.0767 (15)	0.0542 (14)	−0.0036 (12)	0.0025 (12)	0.0066 (12)
C7	0.0715 (13)	0.0594 (13)	0.0490 (13)	−0.0049 (11)	0.0063 (11)	−0.0043 (11)
C1	0.0645 (12)	0.0457 (12)	0.0580 (15)	0.0001 (10)	0.0063 (11)	−0.0007 (11)
C12	0.0873 (15)	0.0735 (15)	0.0578 (15)	−0.0149 (13)	0.0047 (13)	0.0043 (13)
C3	0.0862 (15)	0.0601 (13)	0.0468 (13)	−0.0011 (11)	0.0123 (12)	0.0004 (11)
C11	0.0838 (16)	0.0794 (16)	0.0702 (18)	−0.0193 (13)	0.0045 (13)	−0.0057 (15)
C10	0.0702 (14)	0.0817 (17)	0.0562 (16)	0.0010 (12)	−0.0033 (12)	−0.0183 (13)
C9	0.0838 (15)	0.0808 (17)	0.0577 (15)	0.0032 (13)	0.0001 (13)	0.0054 (13)

Geometric parameters (Å, °)

O1—N1	1.228 (2)	C2—C1	1.369 (3)
N1—O2	1.214 (2)	C2—C3	1.372 (3)
N1—C1	1.466 (3)	C2—H2	0.9300
O3—N3	1.209 (2)	C8—C9	1.367 (3)
N2—C5	1.375 (3)	C8—C7	1.389 (3)
N2—H2B	0.922 (17)	C8—H8	0.9300
N2—H2A	0.894 (17)	C7—C12	1.392 (3)
N3—O4	1.224 (3)	C12—C11	1.378 (3)
N3—C10	1.477 (3)	C12—H12	0.9300
C5—C6	1.390 (3)	C3—H3	0.9300
C5—C4	1.408 (3)	C11—C10	1.373 (3)
C6—C1	1.370 (3)	C11—H11	0.9300
C6—H6	0.9300	C10—C9	1.368 (3)
C4—C3	1.389 (3)	C9—H9	0.9300
C4—C7	1.482 (3)		
O2—N1—O1	123.1 (2)	C7—C8—H8	119.5
O2—N1—C1	118.3 (2)	C8—C7—C12	118.8 (2)
O1—N1—C1	118.63 (19)	C8—C7—C4	120.41 (19)
C5—N2—H2B	115.9 (14)	C12—C7—C4	120.6 (2)
C5—N2—H2A	119.6 (17)	C2—C1—C6	122.8 (2)
H2B—N2—H2A	116 (2)	C2—C1—N1	119.0 (2)
O3—N3—O4	123.1 (2)	C6—C1—N1	118.2 (2)
O3—N3—C10	118.6 (3)	C11—C12—C7	120.5 (2)
O4—N3—C10	118.3 (3)	C11—C12—H12	119.7
N2—C5—C6	119.4 (2)	C7—C12—H12	119.7
N2—C5—C4	121.8 (2)	C2—C3—C4	122.7 (2)
C6—C5—C4	118.80 (19)	C2—C3—H3	118.6
C1—C6—C5	119.9 (2)	C4—C3—H3	118.6
C1—C6—H6	120.1	C10—C11—C12	118.4 (2)
C5—C6—H6	120.1	C10—C11—H11	120.8
C3—C4—C5	118.49 (19)	C12—C11—H11	120.8
C3—C4—C7	118.3 (2)	C9—C10—C11	122.6 (2)

C5—C4—C7	123.25 (18)	C9—C10—N3	119.0 (3)
C1—C2—C3	117.28 (19)	C11—C10—N3	118.4 (2)
C1—C2—H2	121.4	C8—C9—C10	118.6 (2)
C3—C2—H2	121.4	C8—C9—H9	120.7
C9—C8—C7	121.0 (2)	C10—C9—H9	120.7
C9—C8—H8	119.5		
N2—C5—C6—C1	−179.0 (2)	O2—N1—C1—C6	−170.96 (19)
C4—C5—C6—C1	1.3 (3)	O1—N1—C1—C6	9.7 (3)
N2—C5—C4—C3	177.7 (2)	C8—C7—C12—C11	0.2 (3)
C6—C5—C4—C3	−2.6 (3)	C4—C7—C12—C11	−175.9 (2)
N2—C5—C4—C7	−2.1 (3)	C1—C2—C3—C4	0.0 (3)
C6—C5—C4—C7	177.60 (19)	C5—C4—C3—C2	2.0 (3)
C9—C8—C7—C12	−0.3 (3)	C7—C4—C3—C2	−178.2 (2)
C9—C8—C7—C4	175.8 (2)	C7—C12—C11—C10	0.0 (3)
C3—C4—C7—C8	−50.6 (3)	C12—C11—C10—C9	−0.1 (3)
C5—C4—C7—C8	129.1 (2)	C12—C11—C10—N3	−179.4 (2)
C3—C4—C7—C12	125.4 (2)	O3—N3—C10—C9	−175.5 (2)
C5—C4—C7—C12	−54.9 (3)	O4—N3—C10—C9	3.9 (3)
C3—C2—C1—C6	−1.4 (3)	O3—N3—C10—C11	3.8 (3)
C3—C2—C1—N1	−179.90 (18)	O4—N3—C10—C11	−176.8 (2)
C5—C6—C1—C2	0.7 (3)	C7—C8—C9—C10	0.2 (3)
C5—C6—C1—N1	179.24 (19)	C11—C10—C9—C8	0.0 (3)
O2—N1—C1—C2	7.6 (3)	N3—C10—C9—C8	179.3 (2)
O1—N1—C1—C2	−171.76 (19)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N2—H2B \cdots O1 ⁱ	0.92 (2)	2.36 (2)	3.229 (3)	157 (2)
N2—H2A \cdots O4 ⁱⁱ	0.89 (2)	2.50 (2)	3.345 (3)	157 (2)
C6—H6 \cdots O1 ⁱ	0.93	2.54	3.308 (3)	140
C9—H9 \cdots O3 ⁱⁱⁱ	0.93	2.57	3.496 (3)	174

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