Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Ethyl 4-nitrophenylacetate

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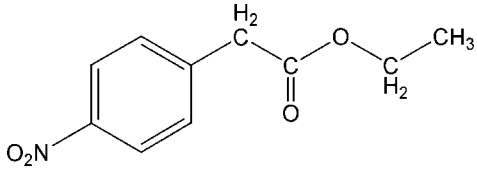
Received 19 November 2007; accepted 8 December 2007

Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.006 Å; R factor = 0.050; wR factor = 0.122; data-to-parameter ratio = 8.5.

In the asymmetric unit of the title compound, $C_{10}H_{11}NO_4$, there are two crystallographically independent molecules, which are connected *via* a C—H···O hydrogen bond. The crystal structure is stabilized by this hydrogen bond together with an N—O···π contact [O···*Cg* 3.297 (5) Å; *Cg* is the centroid of one of the benzene rings].

Related literature

For related literature, see: Brown *et al.* (2006); Shokat *et al.* (1991); Sagamihara (1988).



Experimental

Crystal data

$C_{10}H_{11}NO_4$
M_r = 209.20
Orthorhombic, $Pca2_1$
a = 15.9132 (13) Å
b = 5.2298 (4) Å
c = 24.878 (2) Å
V = 2070.4 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 292 (2) K
0.40 × 0.04 × 0.02 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.959, T_{max} = 0.998
13522 measured reflections
2318 independent reflections
1422 reflections with $I > 2\sigma(I)$
R_{int} = 0.065

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.122
S = 1.01
2318 reflections
273 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O5	0.93	2.47	3.186 (6)	134

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

The authors acknowledge the teachers of the College of Chemistry of Central China Normal University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2259).

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 doi:10.1107/S1600536807066184

supporting information

Acta Cryst. (2008). E**64**, o443 [doi:10.1107/S1600536807066184]

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S1. Comment

Ethyl 4-nitrophenylacetate, (I), has been widely used as an intermediator of the anti-rheumatoid drugs (Kevan *et al.*, 1991; Sagamihara, 1988). The similar compound, cyclodecyl 4-nitrophenylacetate, has been reported by Brown *et al.* (2006). Here we present the molecular structure of (I), as shown in Fig. 1. In the asymmetric unit of (I), there is a dimer *via* a C—H···O interaction (Table 1). The angles involving the acetate groups in the dimer are 126.7 (4), 124.0 (4), 126.1 (4) and 123.1 (4)°, and the average distances of C=O and C—O are 1.202 (5) and 2.792 (5) Å, respectively. The C—N bond lengths on the benzene ring range from 1.202 (5) to 1.219 (4) Å. The benzene ring planes of the two independent molecules are nearly directional parallel with the dihedral angle of 19.2 (2)°, but no significant π-π interaction. The molecular packing diagram of (I) is stabilized by N1—O2···π contact [O2···Cg^{i} 3.297 (5) Å, N1—O2···Cg^{i} 156.3 (3)°; *Cg* is the centroid of the benzene C11—C16 ring; symmetry code: (i) 1/2 + *x*, 1 - *y*, *z*] together with hydrogen bond, as shown in Fig. 2.

S2. Experimental

Ethyl 4-nitrophenylacetate was obtained from the Jiachen Chemical Company Inc, ShangHai. The crystals were grown by vapour diffusion of 95% ethanol.

S3. Refinement

After their location in a difference map, all H atoms were fixed geometrically at ideal positions (C–H = 0.93–0.96 Å) and allowed to ride on the parent C atoms, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). In the absence of significant anomalous scattering effects, Friedel pairs have been merged.

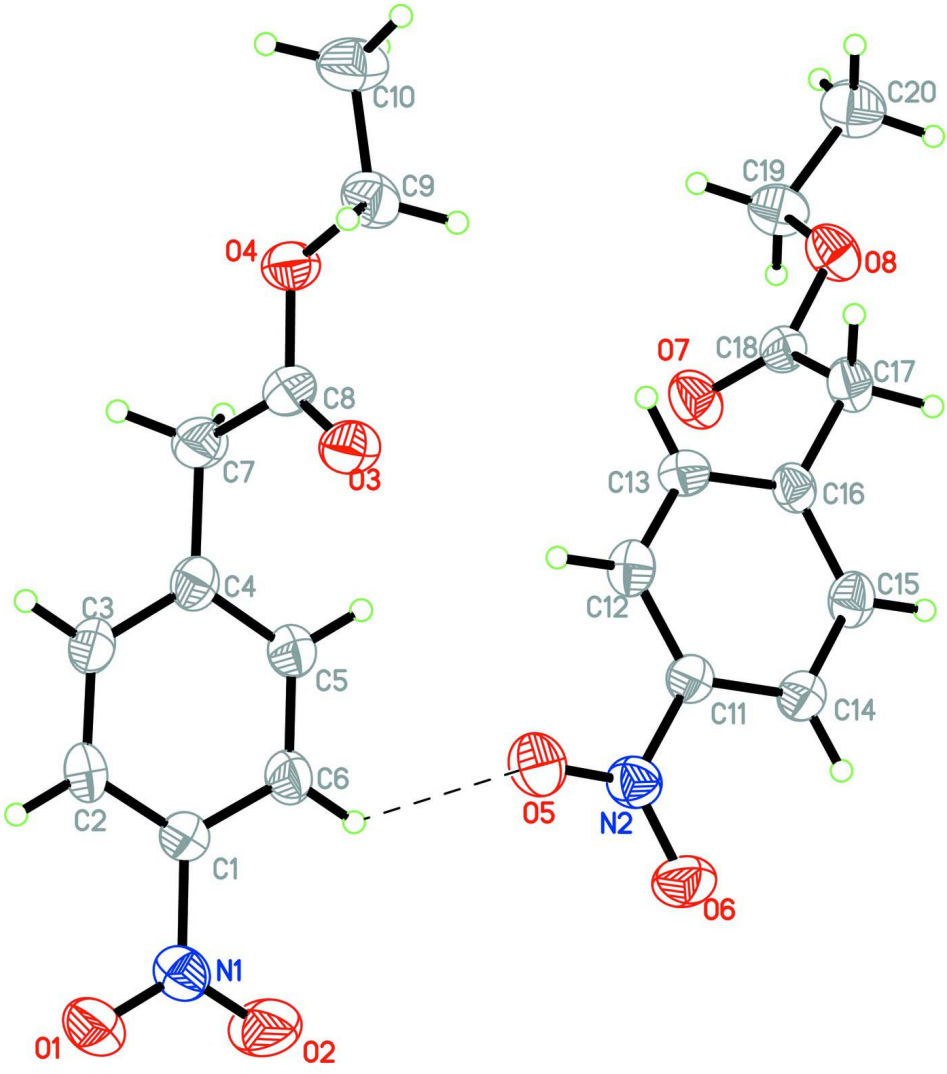

Figure 1

The asymmetric unit of the title compound with the atom numbering, showing displacement ellipsoids at the 50% probability level. The hydrogen bond is shown as a dashed line.

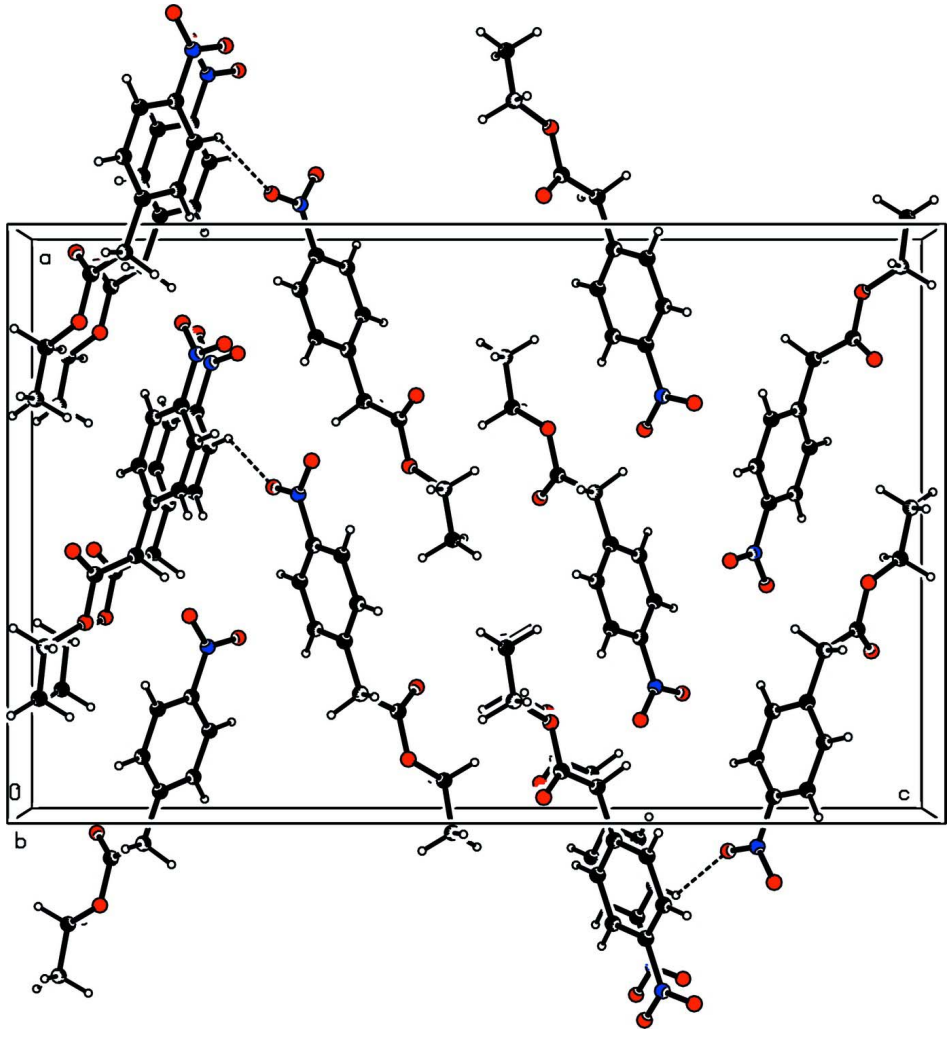

Figure 2

The molecular packing diagram of the title compound, with hydrogen bonds shown as dashed lines.

Ethyl 4-nitrophenylacetate

Crystal data

$C_{10}H_{11}NO_4$
$M_r = 209.20$
Orthorhombic, $Pca2_1$
Hall symbol: P 2c -2ac
$a = 15.9132\ (13)$ Å
$b = 5.2298\ (4)$ Å
$c = 24.878\ (2)$ Å
$V = 2070.4\ (3)$ Å^3
$Z = 8$
$F(000) = 880$
$D_x = 1.342$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1377 reflections
$\theta = 2.7–20.9°$
$\mu = 0.11$ mm^{-1}
$T = 292$ K
Plate, colorless
0.40 × 0.04 × 0.02 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans

Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.959, T_{max} = 0.998
13522 measured reflections
2318 independent reflections
1422 reflections with $I > 2\sigma(I)$

R_{int} = 0.065
θ_{max} = 27.0°, θ_{min} = 1.6°
h = −15→20
k = −6→6
l = −31→31

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.122
S = 1.01
2318 reflections
273 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0579P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
C1	1.1982 (2)	1.1755 (8)	0.18201 (15)	0.0473 (10)
C2	1.1806 (3)	1.3761 (8)	0.14828 (17)	0.0556 (11)
H2	1.2230	1.4856	0.1368	0.067*
C3	1.0991 (3)	1.4122 (8)	0.13180 (17)	0.0559 (11)
H3	1.0864	1.5479	0.1091	0.067*
C4	1.0354 (3)	1.2492 (8)	0.14854 (17)	0.0521 (10)
C5	1.0559 (3)	1.0479 (8)	0.1821 (2)	0.0578 (12)
H5	1.0139	0.9359	0.1930	0.069*
C6	1.1363 (3)	1.0091 (8)	0.1995 (2)	0.0579 (13)
H6	1.1492	0.8744	0.2225	0.069*
C7	0.9459 (3)	1.2913 (9)	0.13058 (18)	0.0629 (13)
H7A	0.9096	1.2882	0.1619	0.076*
H7B	0.9415	1.4598	0.1145	0.076*
C8	0.9148 (3)	1.0963 (9)	0.09078 (17)	0.0527 (11)
C9	0.7949 (3)	0.9750 (9)	0.0399 (2)	0.0682 (15)
H9A	0.7939	0.8004	0.0531	0.082*
H9B	0.8261	0.9790	0.0064	0.082*
C10	0.7077 (3)	1.0715 (12)	0.0316 (2)	0.0842 (17)
H10A	0.6768	1.0582	0.0646	0.126*

H10B	0.6805	0.9713	0.0043	0.126*
H10C	0.7097	1.2471	0.0204	0.126*
C11	0.9635 (2)	0.3428 (7)	0.32274 (15)	0.0467 (10)
C12	0.9473 (3)	0.1331 (8)	0.35509 (17)	0.0541 (11)
H12	0.9903	0.0220	0.3649	0.065*
C13	0.8662 (3)	0.0924 (8)	0.37249 (18)	0.0556 (11)
H13	0.8547	−0.0456	0.3949	0.067*
C14	0.8017 (2)	0.2530 (8)	0.35717 (15)	0.0469 (10)
C15	0.8203 (3)	0.4571 (9)	0.3234 (2)	0.0570 (12)
H15	0.7772	0.5645	0.3122	0.068*
C16	0.9012 (2)	0.5043 (8)	0.30617 (19)	0.0501 (12)
H16	0.9131	0.6424	0.2839	0.060*
C17	0.7135 (2)	0.2026 (8)	0.37470 (17)	0.0561 (11)
H17A	0.7108	0.0337	0.3908	0.067*
H17B	0.6774	0.2020	0.3433	0.067*
C18	0.6801 (3)	0.3948 (8)	0.41442 (17)	0.0494 (10)
C19	0.5597 (3)	0.5179 (9)	0.4642 (2)	0.0631 (14)
H19A	0.5581	0.6910	0.4503	0.076*
H19B	0.5909	0.5186	0.4977	0.076*
C20	0.4726 (3)	0.4214 (11)	0.4734 (2)	0.0776 (15)
H20A	0.4414	0.4300	0.4404	0.116*
H20B	0.4455	0.5249	0.5002	0.116*
H20C	0.4749	0.2474	0.4856	0.116*
N1	1.2850 (2)	1.1303 (8)	0.19950 (16)	0.0625 (10)
N2	1.0504 (2)	0.3938 (8)	0.30557 (16)	0.0594 (10)
O1	1.3401 (2)	1.2661 (7)	0.18162 (16)	0.0868 (11)
O2	1.2991 (2)	0.9635 (9)	0.23154 (18)	0.1051 (16)
O3	0.95456 (18)	0.9271 (7)	0.07121 (13)	0.0671 (10)
O4	0.83388 (17)	1.1435 (6)	0.07940 (12)	0.0630 (8)
O5	1.0631 (2)	0.5766 (7)	0.27657 (17)	0.0878 (12)
O6	1.1065 (2)	0.2546 (7)	0.32154 (15)	0.0766 (10)
O7	0.71909 (18)	0.5709 (6)	0.43392 (14)	0.0685 (9)
O8	0.59970 (17)	0.3485 (6)	0.42567 (12)	0.0607 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.049 (2)	0.048 (2)	0.045 (2)	0.0003 (19)	0.0007 (19)	−0.0029 (18)
C2	0.064 (3)	0.048 (3)	0.055 (2)	−0.012 (2)	0.006 (2)	0.002 (2)
C3	0.069 (3)	0.043 (2)	0.055 (3)	0.001 (2)	−0.006 (2)	0.003 (2)
C4	0.061 (3)	0.041 (2)	0.054 (2)	0.003 (2)	0.003 (2)	−0.008 (2)
C5	0.054 (3)	0.049 (3)	0.070 (3)	−0.004 (2)	0.004 (2)	0.004 (2)
C6	0.055 (3)	0.051 (3)	0.068 (4)	−0.003 (2)	0.008 (2)	0.005 (2)
C7	0.053 (3)	0.054 (3)	0.082 (4)	0.008 (2)	−0.004 (2)	−0.011 (2)
C8	0.053 (3)	0.055 (3)	0.050 (2)	0.008 (2)	0.003 (2)	0.001 (2)
C9	0.069 (3)	0.072 (4)	0.064 (4)	−0.007 (3)	−0.014 (3)	−0.010 (2)
C10	0.065 (4)	0.104 (4)	0.083 (4)	0.001 (3)	−0.020 (3)	−0.006 (3)
C11	0.046 (2)	0.047 (2)	0.047 (2)	0.0012 (19)	−0.0004 (18)	−0.0049 (18)

C12	0.055 (3)	0.049 (3)	0.058 (2)	0.002 (2)	−0.002 (2)	0.005 (2)
C13	0.064 (3)	0.046 (3)	0.057 (3)	−0.001 (2)	0.010 (2)	0.007 (2)
C14	0.050 (3)	0.040 (2)	0.050 (2)	−0.004 (2)	0.0009 (19)	−0.0081 (19)
C15	0.047 (3)	0.058 (3)	0.066 (3)	0.004 (2)	−0.002 (2)	−0.002 (2)
C16	0.066 (3)	0.047 (3)	0.037 (2)	−0.002 (2)	0.003 (2)	0.0023 (17)
C17	0.057 (3)	0.048 (3)	0.063 (3)	−0.007 (2)	0.006 (2)	−0.007 (2)
C18	0.048 (3)	0.044 (3)	0.056 (3)	0.003 (2)	0.004 (2)	0.001 (2)
C19	0.057 (3)	0.077 (4)	0.056 (3)	0.002 (2)	0.007 (2)	−0.004 (2)
C20	0.066 (3)	0.096 (4)	0.071 (3)	−0.001 (3)	0.013 (3)	−0.001 (3)
N1	0.061 (3)	0.069 (3)	0.058 (2)	−0.008 (2)	−0.002 (2)	0.003 (2)
N2	0.052 (2)	0.065 (3)	0.061 (2)	0.001 (2)	0.0045 (19)	0.001 (2)
O1	0.059 (2)	0.094 (3)	0.107 (3)	−0.0180 (19)	−0.0037 (19)	0.018 (2)
O2	0.077 (3)	0.126 (3)	0.112 (4)	−0.001 (2)	−0.013 (2)	0.061 (3)
O3	0.059 (2)	0.067 (2)	0.076 (3)	0.0100 (17)	−0.0050 (16)	−0.023 (2)
O4	0.0493 (18)	0.066 (2)	0.074 (2)	0.0083 (15)	−0.0097 (15)	−0.0110 (16)
O5	0.072 (2)	0.087 (3)	0.104 (3)	−0.0159 (19)	0.015 (2)	0.041 (2)
O6	0.055 (2)	0.081 (3)	0.094 (2)	0.0124 (17)	0.0080 (18)	0.007 (2)
O7	0.066 (2)	0.062 (2)	0.078 (2)	−0.0127 (15)	0.0025 (16)	−0.0180 (19)
O8	0.0560 (18)	0.065 (2)	0.0611 (17)	−0.0103 (15)	0.0146 (15)	−0.0113 (16)

Geometric parameters (Å, º)

C1—C2	1.372 (6)	C11—N2	1.471 (5)
C1—C6	1.385 (5)	C12—C13	1.378 (5)
C1—N1	1.468 (5)	C12—H12	0.9300
C2—C3	1.373 (5)	C13—C14	1.380 (5)
C2—H2	0.9300	C13—H13	0.9300
C3—C4	1.388 (6)	C14—C15	1.390 (6)
C3—H3	0.9300	C14—C17	1.494 (5)
C4—C5	1.382 (6)	C15—C16	1.380 (6)
C4—C7	1.510 (5)	C15—H15	0.9300
C5—C6	1.366 (6)	C16—H16	0.9300
C5—H5	0.9300	C17—C18	1.506 (6)
C6—H6	0.9300	C17—H17A	0.9700
C7—C8	1.505 (6)	C17—H17B	0.9700
C7—H7A	0.9700	C18—O7	1.212 (5)
C7—H7B	0.9700	C18—O8	1.332 (5)
C8—O3	1.192 (5)	C19—O8	1.452 (6)
C8—O4	1.341 (5)	C19—C20	1.493 (6)
C9—O4	1.458 (5)	C19—H19A	0.9700
C9—C10	1.491 (5)	C19—H19B	0.9700
C9—H9A	0.9700	C20—H20A	0.9600
C9—H9B	0.9700	C20—H20B	0.9600
C10—H10A	0.9600	C20—H20C	0.9600
C10—H10B	0.9600	N1—O2	1.202 (5)
C10—H10C	0.9600	N1—O1	1.212 (4)
C11—C16	1.365 (5)	N2—O5	1.215 (5)
C11—C12	1.385 (6)	N2—O6	1.219 (4)

C2—C1—C6	121.8 (4)	C11—C12—H12	120.7
C2—C1—N1	119.8 (4)	C12—C13—C14	121.0 (4)
C6—C1—N1	118.4 (4)	C12—C13—H13	119.5
C3—C2—C1	118.7 (4)	C14—C13—H13	119.5
C3—C2—H2	120.6	C13—C14—C15	118.4 (4)
C1—C2—H2	120.6	C13—C14—C17	120.7 (4)
C2—C3—C4	121.0 (4)	C15—C14—C17	120.8 (4)
C2—C3—H3	119.5	C16—C15—C14	121.6 (4)
C4—C3—H3	119.5	C16—C15—H15	119.2
C5—C4—C3	118.4 (4)	C14—C15—H15	119.2
C5—C4—C7	120.8 (4)	C11—C16—C15	118.2 (4)
C3—C4—C7	120.7 (4)	C11—C16—H16	120.9
C6—C5—C4	121.7 (4)	C15—C16—H16	120.9
C6—C5—H5	119.1	C14—C17—C18	113.9 (3)
C4—C5—H5	119.1	C14—C17—H17A	108.8
C5—C6—C1	118.2 (4)	C18—C17—H17A	108.8
C5—C6—H6	120.9	C14—C17—H17B	108.8
C1—C6—H6	120.9	C18—C17—H17B	108.8
C8—C7—C4	114.0 (3)	H17A—C17—H17B	107.7
C8—C7—H7A	108.8	O7—C18—O8	123.1 (4)
C4—C7—H7A	108.8	O7—C18—C17	126.1 (4)
C8—C7—H7B	108.8	O8—C18—C17	110.8 (4)
C4—C7—H7B	108.8	O8—C19—C20	107.6 (4)
H7A—C7—H7B	107.7	O8—C19—H19A	110.2
O3—C8—O4	124.0 (4)	C20—C19—H19A	110.2
O3—C8—C7	126.7 (4)	O8—C19—H19B	110.2
O4—C8—C7	109.3 (4)	C20—C19—H19B	110.2
O4—C9—C10	106.5 (4)	H19A—C19—H19B	108.5
O4—C9—H9A	110.4	C19—C20—H20A	109.5
C10—C9—H9A	110.4	C19—C20—H20B	109.5
O4—C9—H9B	110.4	H20A—C20—H20B	109.5
C10—C9—H9B	110.4	C19—C20—H20C	109.5
H9A—C9—H9B	108.6	H20A—C20—H20C	109.5
C9—C10—H10A	109.5	H20B—C20—H20C	109.5
C9—C10—H10B	109.5	O2—N1—O1	122.3 (4)
H10A—C10—H10B	109.5	O2—N1—C1	119.2 (4)
C9—C10—H10C	109.5	O1—N1—C1	118.5 (4)
H10A—C10—H10C	109.5	O5—N2—O6	122.8 (4)
H10B—C10—H10C	109.5	O5—N2—C11	118.1 (4)
C16—C11—C12	122.0 (4)	O6—N2—C11	119.1 (4)
C16—C11—N2	118.8 (4)	C8—O4—C9	116.1 (3)
C12—C11—N2	119.1 (4)	N2—O5—H6	155.7
C13—C12—C11	118.6 (4)	C18—O8—C19	116.7 (3)
C13—C12—H12	120.7		

C6—C1—C2—C3	0.3 (6)	N2—C11—C16—C15	−178.7 (4)
N1—C1—C2—C3	179.0 (3)	C14—C15—C16—C11	0.6 (6)

C1—C2—C3—C4	−0.3 (6)	C13—C14—C17—C18	110.9 (4)
C2—C3—C4—C5	−0.4 (6)	C15—C14—C17—C18	−71.5 (5)
C2—C3—C4—C7	179.5 (4)	C14—C17—C18—O7	−3.5 (6)
C3—C4—C5—C6	1.1 (7)	C14—C17—C18—O8	176.0 (3)
C7—C4—C5—C6	−178.9 (4)	C2—C1—N1—O2	175.6 (5)
C4—C5—C6—C1	−1.0 (7)	C6—C1—N1—O2	−5.7 (6)
C2—C1—C6—C5	0.3 (7)	C2—C1—N1—O1	−3.2 (6)
N1—C1—C6—C5	−178.4 (4)	C6—C1—N1—O1	175.5 (4)
C5—C4—C7—C8	−71.4 (5)	C16—C11—N2—O5	−1.0 (6)
C3—C4—C7—C8	108.6 (4)	C12—C11—N2—O5	179.0 (4)
C4—C7—C8—O3	−3.9 (7)	C16—C11—N2—O6	177.9 (4)
C4—C7—C8—O4	177.1 (4)	C12—C11—N2—O6	−2.2 (6)
C16—C11—C12—C13	−2.3 (6)	O3—C8—O4—C9	−0.9 (6)
N2—C11—C12—C13	177.7 (4)	C7—C8—O4—C9	178.2 (4)
C11—C12—C13—C14	1.5 (6)	C10—C9—O4—C8	−176.9 (4)
C12—C13—C14—C15	0.3 (6)	O6—N2—O5—H6	0.9
C12—C13—C14—C17	177.9 (4)	C11—N2—O5—H6	179.7
C13—C14—C15—C16	−1.4 (6)	O7—C18—O8—C19	−1.4 (6)
C17—C14—C15—C16	−179.0 (4)	C17—C18—O8—C19	179.1 (4)
C12—C11—C16—C15	1.3 (6)	C20—C19—O8—C18	−176.3 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O5	0.93	2.47	3.186 (6)	134