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N-(4-Methoxy-2-methyl-5-nitrophenyl)acetamide

Rao M. Uppu[a]* and Frank R. Fronczek[b]

[a]Department of Environmental Toxicology, Southern University and A&M College, Baton Rouge, LA 70813, USA, and [b]Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803, USA. *Correspondence e-mail: rao_uppu@subr.edu

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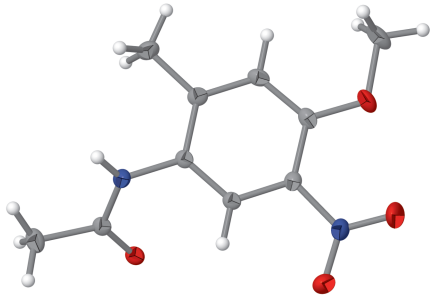
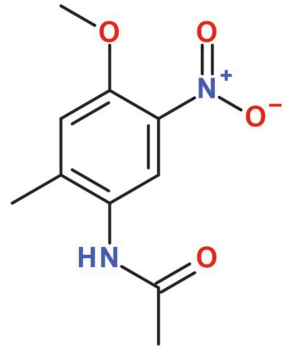
In the title compound, $C_{10}H_{12}N_2O_4$, the four substituents lie out of the phenyl plane by varying degrees. The methyl C atom lies 0.019 (3) Å out of plane, while the methoxy O and C atoms lie 0.067 (2) and 0.042 (3) Å out of plane, respectively, with the C—C—O—C torsion angle being 3.3 (2)°. The plane of the nitro group is twisted out of the phenyl plane, forming a dihedral angle of 12.03 (9)° with it. The acetamide substituent is twisted considerably more out of the phenyl plane, forming a dihedral angle of 47.24 (6)° with it. In the extended structure, the acetamide NH group donates a hydrogen bond to an acetamide carbonyl O atom, thereby forming chains propagating in the [010] direction.

3D view



Chemical scheme



Structure description

The title compound, $C_{10}H_{12}N_2O_4$, is a nitro-derivative of 2-methylmethacetin [*N*-(4-methoxy-2-methylphenyl)acetamide]. It is likely formed during peroxynitrite-mediated oxidation of 2-methylmethacetin under physiologically relevant pH and bicarbonate conditions (Hines *et al.*, 2025). The reaction is consistent with electrophilic nitration initiated by the *in situ* generation of the free-radical oxidants nitrogen dioxide ($^{\cdot}NO_2$) and carbonate radical ($CO_3^{\cdot-}$) from the interaction of the peroxynitrite anion ($ONOO^-$) with CO_2 (Agu *et al.*, 2020; Deere *et al.*, 2020; Lymar & Hurst, 1995; Uppu *et al.*, 2000; Uppu & Pryor, 1996; Uppu & Pryor, 1999).

Phenacetin [*N*-(4-ethoxyphenyl)acetamide, $C_{10}H_{13}NO_2$], methacetin [*N*-(4-methoxyphenyl)acetamide, $C_9H_{11}NO_2$] and propacetin [*N*-(4-propoxyphenyl)acetamide, $C_{11}H_{15}NO_2$] were among the earliest synthetic antipyretic–analgesic agents examined in depth (Merck, 1899). Interest in these congeners grew after their precursor acetanilide (Antifebrin, introduced in 1880) was linked to methemoglobinaemia and cyanosis owing to excessive formation of its aniline metabolite. Comparative studies in the late 19th and early 20th centuries showed that methacetin possessed the strongest antipyretic and analgesic activity, followed by phenacetin and then propacetin, each acting through metabolic release of 4-aminophenol (Starmer *et al.*, 1971). While all three function largely

as pro-drugs, undergoing rapid oxidative *O*-dealkylation to produce the active metabolite 4-hydroxyacetanilide (Brodie & Axelrod, 1948; Kapetanović *et al.*, 1979; Kapetanović & Mieyal, 1979), a minor *N*-deacetylation pathway yields 4-alkoxyanilines that can be further oxidized to reactive 4-*N*-hydroxy and 4-nitroso derivatives, leading to methemoglobinaemia, nephrotoxicity and, in the case of phenacetin, urothelial cancer (Prescott, 1980; Hinson, 1983). Toxicological studies in experimental animals revealed that methacetin, with the shortest alkyl chain, exhibited higher toxicity, while phenacetin, with a moderate chain length, offered a better balance between efficacy and reduced toxicity (Starmer *et al.*, 1971). Consequently, phenacetin remained widely used until it was ultimately replaced by acetaminophen [*N*-(4-hydroxyphenyl)acetamide] in the 1980s as a safer alternative [FDA (Food and Drug Administration), 1983; IARC (International Agency for Research on Cancer), 1987]. There is no evidence that 2-methylmethacetin itself was ever marketed or tested in humans during that era (Merck, 1952). Recent studies show that oxidative *O*-demethylation of methacetin-(methyl-^{13}C) and subsequent conversion of H^{13}CHO to $^{13}CO_2$ in LiMAx/MBT breath testing provide broad diagnostic utility across diverse clinical applications (Buechter & Gerken, 2022; Gairing *et al.*, 2022; Santol *et al.*, 2024).

Non-enzymatic oxidation of 4-alkoxyacetanilides was largely unexplored until reactive oxygen and nitrogen species (RONS) were shown to nitrate 4-hydroxyacetanilide *in vitro* (Uppu & Martin, 2005; Deere *et al.*, 2020). We reasoned that analogous reactions might affect other 4-alkoxy congeners. Indeed, treating 2-methylmethacetin with peroxynitrite in bicarbonate-enriched buffers at and around neutral pH yielded the title compound as the major product (Hines *et al.*, 2025). The electron-donating 4-methoxy group directs nitration *ortho* to itself, whereas the acetamido group weakly deactivates the ring *ortho* to the amide; consequently, nitration occurs preferentially at C5 to give *N*-(4-methoxy-2-methyl-5-nitrophenyl)acetamide rather than the C6 position with little or no detectable formation of *N*-(4-methoxy-2-methyl-6-nitrophenyl)acetamide (Hines *et al.*, 2025; Uppu & Martin, 2005). Towards better understanding of the mechanisms of electrophilic nitration of 4-alkoxyacetanilides by free radical oxidants formed in peroxynitrite/CO_2 reactions (Uppu & Pryor, 1999; Uppu *et al.*, 2000) and to shed light on molecular targets, we grew crystals of *N*-(4-methoxy-2-methyl-5-nitrophenyl)acetamide in water and analyzed them by X-ray diffraction.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O2^{i}	0.84 (2)	2.03 (2)	2.8636 (16)	174 (2)
C9—H9*A*···O2^{ii}	0.98	2.54	3.5009 (19)	166
C9—H9*B*···O2^{i}	0.98	2.47	3.2971 (19)	142

Symmetry codes: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, z$; (ii) $x+\frac{1}{2}, y, -z+\frac{3}{2}$.

Single-crystal X-ray diffraction confirms this regiochemistry. The molecular structure (Fig. 1) shows the C1–C6 aromatic ring, methoxy group (C1–O1–C10H$_3$) and C9 methyl carbon atom to be nearly coplanar (r.m.s. deviation = 0.012 Å), whereas the N2/O3/O4 nitro group at C2 is twisted about the C2—N2 bond such that the plane of the nitro group forms a dihedral angle of 12.03 (9)° with the phenyl plane. The N1/C7/C8/O2 acetamide substituent is twisted considerably more out of the phenyl plane, forming a dihedral angle of 47.24 (6)° with it. In the crystal, N1—H1*N*···O2(carbonyl) hydrogen bonds [N···O = 2.8636 (16) Å] assemble the molecules into [010] chains (Table 1, Fig. 2); weaker C—H···O contacts link these chains into layers, giving the overall

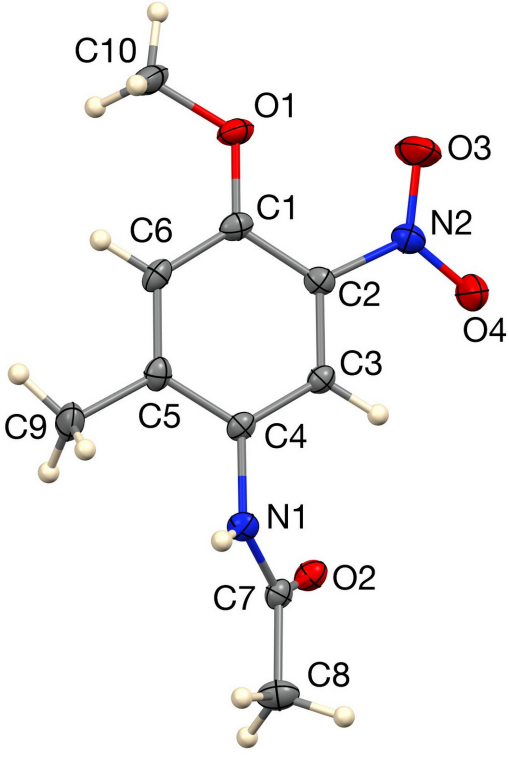


Figure 1
The asymmetric unit of the title compound with 50% probability ellipsoids.

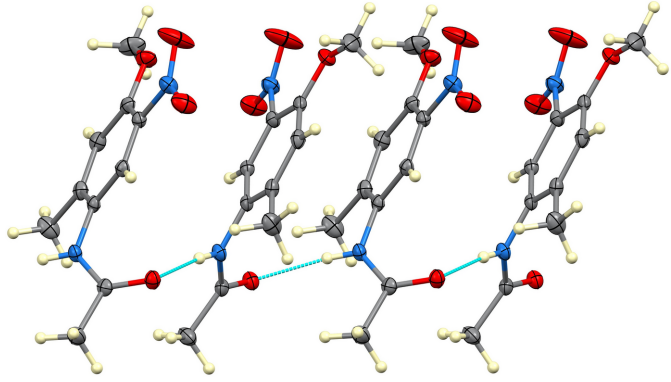


Figure 2
Fragment of a [010] hydrogen-bonded chain.

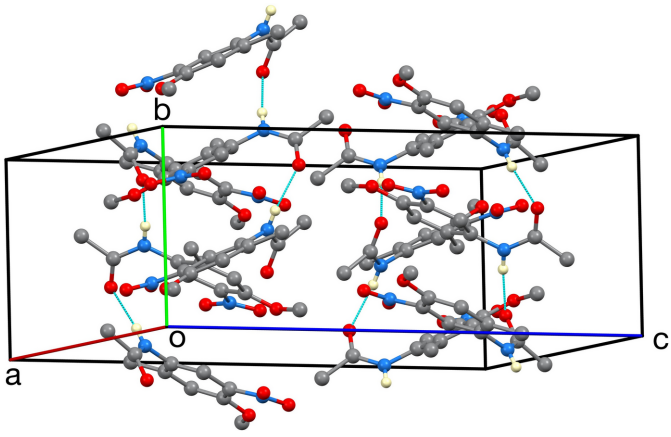


Figure 3
The unit cell. Only N-bound hydrogen atoms are shown.

packing illustrated in Fig. 3. The 2-methyl substituent takes no part in specific intermolecular interactions but influences packing through van der Waals contacts.

The structure of the title compound represents the first crystallographic characterization of a nitrated 4-alkoxyacetanilide formed under biomimetic RONS conditions. Its isolation in peroxynitrite/CO_2-mediated oxidation of *N*-(4-methoxy-2-methyl)acetamide strongly suggests the possibility that analogous nitrated metabolites may arise *in vivo* during oxidative stress, potentially modulating the pharmacology or toxicity of 4-alkoxyacetanilide analgesics.

In terms of molecular planarity and substituent orientations, *N*-(4-methoxy-2-nitrophenyl)acetamide (Hines *et al.*, 2022), *N*-(4-methoxy-3-nitrophenyl)acetamide (Hines *et al.*, 2023) and the title compound share a benzene ring with the *para*-methoxy group nearly coplanar to it (C—C—O—C torsion angles on the order of 0–6°). Significant differences emerge in the disposition of the nitro and acetamide substituents. For instance, in *N*-(4-methoxy-3-nitrophenyl)acetamide, the acetamide moiety lies essentially in the aromatic plane (the C—N—C═O dihedral angle is close to 0°), making the entire methoxyphenyl-acetamide fragment nearly planar (r.m.s. deviation ∼0.04 Å). The nitro group at the *meta* position is rotated out of the ring plane (∼30°) and is disordered over two orientations. In *N*-(4-methoxy-3-nitrophenyl)acetamide and *N*-(4-methoxy-2-methyl-5-nitrophenyl)acetamide, with the nitro substituent *ortho* to the anilide nitrogen atom, the phenyl and acetamide groups are not coplanar. The acetamide group is tilted by about 25° in *N*-(4-methoxy-2-nitrophenyl)acetamide and as much as ∼47° in *N*-(4-methoxy-2-methyl-5-nitrophenyl)acetamide, due to steric interference from the *ortho* substituents. Meanwhile, their nitro groups (designated as either 2- or 5-position on the ring) are only moderately twisted out of the plane (on the order of 12°), a considerably smaller deviation than in *N*-(4-methoxy-3-nitrophenyl)acetamide.

Regarding intermolecular interactions, the presence or absence of an *ortho* nitro group governs the hydrogen-bonding patterns. In the 2-nitro compound [*N*-(4-methoxy-2-nitrophenyl)acetamide] (Hines *et al.*, 2022), an intramolecular N—H···O hydrogen bond links the amide N—H group to the *ortho* nitro oxygen atom. This internal hydrogen bond satisfies the donor, so no strong intermolecular N—H bonds occur; instead, packing is consolidated by weaker contacts (*e.g.*, a C—H···O contact between molecules) and exhibits a herringbone motif (adjacent phenyl rings are inclined by ∼65° rather than stacked parallel). In the 3-nitro isomer [*N*-(4-methoxy-3-nitrophenyl)acetamide] (Hines *et al.*, 2023), in contrast, there is no provision for an intramolecular hydrogen bond. Accordingly, each N—H group donates to a nitro oxygen atom on a neighboring molecule, forming N—H···O(nitro) chains in the crystal (the amide carbonyl O is not an acceptor in this structure). The 2-methyl-5-nitro derivative lacks an *ortho* nitro acceptor, and it instead exhibits the conventional amide catemer: the N—H hydrogen bonds to the carbonyl O atom of an adjacent molecule, linking molecules into N—H···O═C chains propagating through the structure. Importantly, none of nitro derivatives shows significant π–π stacking between aromatic rings; for example, the 2-nitro and 2-methyl-5-nitro crystals adopt a crossed herringbone-like packing rather than face-to-face stacks.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{10}H_{12}N_2O_4$
M_r	224.22
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	100
a, *b*, *c* (Å)	14.2323 (6), 7.6198 (3), 19.8463 (8)
V (Å^3)	2152.28 (15)
Z	8
Radiation type	Cu *Kα*
μ (mm^{-1})	0.92
Crystal size (mm)	0.23 × 0.04 × 0.02
Data collection	
Diffractometer	Bruker D8 Venture DUO with Photon III C14
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.722, 0.982
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	25336, 2301, 1853
R_{int}	0.160
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.638
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.053, 0.136, 1.04
No. of reflections	2301
No. of parameters	151
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.37, −0.41

Computer programs: *APEX5* and *SAINT* (Bruker, 2016), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2019/1* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2020), *publCIF* (Westrip, 2010).

Synthesis and crystallization

N-(4-Methoxy-2-methyl-5-nitrophenyl)acetamide (CAS 196194–97-5), was obtained from AmBeed (Arlington Heights, Illinois, USA) and was used without further purification. Crystals in the form of colorless laths were prepared by

slow cooling of a nearly saturated solution of the title compound in boiling deionized water (resistance *ca*. 18 $M\Omega.cm^{-1}$).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

IUCrData (2025). **10**, x250470 [https://doi.org/10.1107/S2414314625004705]

N-(4-Methoxy-2-methyl-5-nitrophenyl)acetamide

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N-(4-Methoxy-2-methyl-5-nitrophenyl)acetamide

Crystal data

$C_{10}H_{12}N_2O_4$
M_r = 224.22
Orthorhombic, *Pbca*
a = 14.2323 (6) Å
b = 7.6198 (3) Å
c = 19.8463 (8) Å
V = 2152.28 (15) Å^3
Z = 8
F(000) = 944
D_x = 1.384 Mg m^{-3}
Cu *Kα* radiation, λ = 1.54184 Å
Cell parameters from 8628 reflections
θ = 4.5–79.4°
μ = 0.92 mm^{-1}
T = 100 K
Lath, colourless
0.23 × 0.04 × 0.02 mm

Data collection

Bruker D8 Venture DUO with Photon III C14 diffractometer
Radiation source: I*μ*S 3.0 microfocus
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.722, T_{max} = 0.982
25336 measured reflections
2301 independent reflections
1853 reflections with $I > 2\sigma(I)$
R_{int} = 0.160
θ_{max} = 79.5°, θ_{min} = 4.5°
h = −18→16
k = −9→9
l = −24→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.136
S = 1.04
2301 reflections
151 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0839P)^2 + 0.5117P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 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.

Refinement. All H atoms were located in difference maps and those on C were thereafter treated as riding in geometrically idealized positions with C—H distances 0.95 Å for phenyl and 0.98 Å for methyl. Coordinates of the N—H atom were refined. U_{iso}(H) values were assigned as 1.2U_{eq} for the attached atom (1.5 for methyl). Torsional parameters were refined for the methyl groups.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.34418 (8)	0.78233 (14)	0.55179 (6)	0.0238 (3)
O2	0.14170 (7)	0.65326 (13)	0.83184 (5)	0.0199 (3)
O3	0.16525 (11)	0.7593 (3)	0.52701 (8)	0.0556 (5)
O4	0.07202 (8)	0.71866 (19)	0.61014 (6)	0.0326 (3)
N1	0.25448 (9)	0.46222 (15)	0.79712 (6)	0.0173 (3)
H1N	0.2850 (15)	0.370 (3)	0.8043 (11)	0.021*
N2	0.15115 (9)	0.72149 (17)	0.58592 (7)	0.0222 (3)
C1	0.32443 (10)	0.70066 (17)	0.61038 (7)	0.0177 (3)
C2	0.23007 (10)	0.67361 (18)	0.62915 (7)	0.0169 (3)
C3	0.20741 (9)	0.59707 (17)	0.69062 (7)	0.0159 (3)
H3	0.143309	0.580561	0.702360	0.019*
C4	0.27693 (10)	0.54469 (17)	0.73487 (7)	0.0154 (3)
C5	0.37149 (10)	0.56655 (18)	0.71717 (7)	0.0181 (3)
C6	0.39333 (10)	0.64377 (18)	0.65543 (8)	0.0192 (3)
H6	0.457538	0.658219	0.643570	0.023*
C7	0.18799 (10)	0.51835 (18)	0.84076 (7)	0.0174 (3)
C8	0.17255 (12)	0.4061 (2)	0.90199 (8)	0.0263 (3)
H8A	0.221118	0.315107	0.904041	0.039*
H8B	0.110504	0.350799	0.899344	0.039*
H8C	0.175971	0.479260	0.942536	0.039*
C9	0.44939 (11)	0.5085 (2)	0.76307 (9)	0.0274 (4)
H9A	0.510092	0.538858	0.742883	0.041*
H9B	0.445817	0.381196	0.769593	0.041*
H9C	0.443105	0.567589	0.806702	0.041*
C10	0.44162 (13)	0.8017 (3)	0.53463 (8)	0.0313 (4)
H10A	0.447058	0.860973	0.490986	0.047*
H10B	0.471040	0.685593	0.531880	0.047*
H10C	0.473279	0.871596	0.569293	0.047*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0276 (6)	0.0242 (6)	0.0196 (5)	−0.0065 (4)	0.0059 (4)	0.0035 (4)
O2	0.0197 (5)	0.0166 (5)	0.0235 (5)	0.0003 (4)	0.0032 (4)	0.0017 (4)
O3	0.0339 (7)	0.1045 (14)	0.0285 (7)	0.0073 (8)	0.0004 (5)	0.0335 (8)
O4	0.0196 (6)	0.0494 (8)	0.0288 (6)	0.0028 (5)	−0.0025 (4)	0.0087 (5)
N1	0.0186 (6)	0.0131 (6)	0.0201 (6)	0.0017 (4)	0.0001 (4)	0.0031 (4)
N2	0.0238 (6)	0.0227 (6)	0.0203 (6)	0.0004 (5)	−0.0014 (5)	0.0045 (5)
C1	0.0230 (7)	0.0121 (6)	0.0182 (6)	−0.0033 (5)	0.0036 (5)	−0.0009 (5)
C2	0.0192 (7)	0.0138 (6)	0.0177 (6)	0.0008 (5)	−0.0007 (5)	0.0009 (5)
C3	0.0162 (6)	0.0130 (6)	0.0185 (6)	−0.0010 (5)	0.0015 (5)	0.0002 (5)
C4	0.0171 (7)	0.0105 (6)	0.0185 (7)	−0.0014 (5)	0.0011 (5)	0.0002 (4)
C5	0.0172 (7)	0.0136 (6)	0.0235 (7)	−0.0025 (5)	−0.0011 (5)	−0.0006 (5)
C6	0.0161 (6)	0.0165 (6)	0.0251 (7)	−0.0035 (5)	0.0033 (5)	−0.0015 (5)
C7	0.0180 (6)	0.0144 (6)	0.0198 (6)	−0.0036 (5)	−0.0002 (5)	−0.0001 (5)

C8	0.0339 (8)	0.0213 (7)	0.0236 (7)	0.0013 (6)	0.0056 (6)	0.0052 (6)
C9	0.0170 (7)	0.0314 (8)	0.0340 (8)	−0.0035 (6)	−0.0047 (6)	0.0080 (6)
C10	0.0318 (9)	0.0375 (9)	0.0245 (7)	−0.0168 (7)	0.0098 (6)	−0.0017 (6)

Geometric parameters (Å, º)

O1—C1	1.3485 (17)	C4—C5	1.4009 (19)
O1—C10	1.436 (2)	C5—C6	1.394 (2)
O2—C7	1.2338 (18)	C5—C9	1.502 (2)
O3—N2	1.221 (2)	C6—H6	0.9500
O4—N2	1.225 (2)	C7—C8	1.502 (2)
N1—C7	1.3522 (19)	C8—H8A	0.9800
N1—C4	1.4224 (17)	C8—H8B	0.9800
N1—H1N	0.84 (2)	C8—H8C	0.9800
N2—C2	1.4597 (19)	C9—H9A	0.9800
C1—C6	1.396 (2)	C9—H9B	0.9800
C1—C2	1.409 (2)	C9—H9C	0.9800
C2—C3	1.3902 (19)	C10—H10A	0.9800
C3—C4	1.3818 (19)	C10—H10B	0.9800
C3—H3	0.9500	C10—H10C	0.9800
C1—O1—C10	116.96 (13)	C5—C6—H6	118.8
C7—N1—C4	125.01 (12)	C1—C6—H6	118.8
C7—N1—H1N	121.3 (15)	O2—C7—N1	123.05 (13)
C4—N1—H1N	113.7 (15)	O2—C7—C8	120.82 (13)
O3—N2—O4	122.09 (14)	N1—C7—C8	116.13 (13)
O3—N2—C2	119.70 (14)	C7—C8—H8A	109.5
O4—N2—C2	118.20 (13)	C7—C8—H8B	109.5
O1—C1—C6	123.30 (13)	H8A—C8—H8B	109.5
O1—C1—C2	119.62 (14)	C7—C8—H8C	109.5
C6—C1—C2	117.06 (13)	H8A—C8—H8C	109.5
C3—C2—C1	120.96 (13)	H8B—C8—H8C	109.5
C3—C2—N2	116.25 (12)	C5—C9—H9A	109.5
C1—C2—N2	122.79 (13)	C5—C9—H9B	109.5
C4—C3—C2	120.86 (13)	H9A—C9—H9B	109.5
C4—C3—H3	119.6	C5—C9—H9C	109.5
C2—C3—H3	119.6	H9A—C9—H9C	109.5
C3—C4—C5	119.62 (13)	H9B—C9—H9C	109.5
C3—C4—N1	121.25 (12)	O1—C10—H10A	109.5
C5—C4—N1	119.08 (13)	O1—C10—H10B	109.5
C6—C5—C4	118.99 (13)	H10A—C10—H10B	109.5
C6—C5—C9	119.53 (13)	O1—C10—H10C	109.5
C4—C5—C9	121.48 (13)	H10A—C10—H10C	109.5
C5—C6—C1	122.49 (13)	H10B—C10—H10C	109.5
C10—O1—C1—C6	3.3 (2)	C2—C3—C4—N1	−178.38 (12)
C10—O1—C1—C2	−178.34 (13)	C7—N1—C4—C3	−46.4 (2)
O1—C1—C2—C3	−177.04 (12)	C7—N1—C4—C5	136.18 (15)

C6—C1—C2—C3	1.4 (2)	C3—C4—C5—C6	1.1 (2)
O1—C1—C2—N2	3.6 (2)	N1—C4—C5—C6	178.54 (12)
C6—C1—C2—N2	−177.98 (13)	C3—C4—C5—C9	−178.84 (14)
O3—N2—C2—C3	−166.83 (17)	N1—C4—C5—C9	−1.4 (2)
O4—N2—C2—C3	11.7 (2)	C4—C5—C6—C1	0.1 (2)
O3—N2—C2—C1	12.6 (2)	C9—C5—C6—C1	179.99 (14)
O4—N2—C2—C1	−168.90 (14)	O1—C1—C6—C5	177.07 (13)
C1—C2—C3—C4	−0.3 (2)	C2—C1—C6—C5	−1.3 (2)
N2—C2—C3—C4	179.11 (12)	C4—N1—C7—O2	−2.9 (2)
C2—C3—C4—C5	−1.0 (2)	C4—N1—C7—C8	177.03 (13)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O2^{i}	0.84 (2)	2.03 (2)	2.8636 (16)	174 (2)
C9—H9*A*···O2^{ii}	0.98	2.54	3.5009 (19)	166
C9—H9*B*···O2^{i}	0.98	2.47	3.2971 (19)	142

Symmetry codes: (i) −*x*+1/2, *y*−1/2, *z*; (ii) *x*+1/2, *y*, −*z*+3/2.