Author(s): Valkonen, Arto; Kolehmainen, Erkki; Grzegórska, Aleksandra; Osmialowski, Borys; Gawinecki, Ryszard; Rissanen, Kari

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Two (*E*)-2-({[4-(dialkylamino)phenyl]imino}methyl)-4-nitrophenols

Arto Valkonen,[a]* Erkki Kolehmainen,[a] Aleksandra Grzegórska,[b] Borys Ośmiałowski,[b] Ryszard Gawinecki[b] and Kari Rissanen[a]

[a]Department of Chemistry, University of Jyväskylä, PO Box 35, FIN-40014 Jyväskylä, Finland, and [b]Department of Chemistry, University of Technology and Life Sciences, Seminaryjna 3, PL-85-326 Bydgoszcz, Poland
Correspondence e-mail: arto.m.valkonen@jyu.fi

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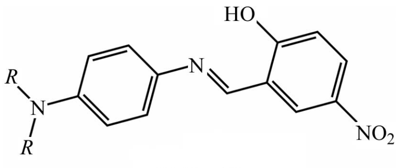
The slow evaporation of analytical NMR samples resulted in the formation of crystals of (*E*)-2-({[4-(dimethylamino)phenyl]imino}methyl)-4-nitrophenol, $C_{15}H_{15}N_3O_3$, (I), and (*E*)-2-({[4-(diethylamino)phenyl]imino}methyl)-4-nitrophenol, $C_{17}H_{19}N_3O_3$, (II). Despite the small structural difference between these two *N*-salicylideneaniline derivatives, they show different space groups and diverse molecular packing. The molecules of both compounds are close to being planar due to an intramolecular O—H⋯N hydrogen bond. The 4-alkylamino-substituted benzene ring is inclined at an angle of 13.44 (19)° in (I) and 2.57 (8)° in (II) with respect to the 4-nitro-substituted phenol ring. Only very weak intermolecular π–π stacking and C—H⋯O interactions were found in these structures.

Comment

(*E*)-2-({[4-(Dimethylamino)phenyl]imino}methyl)-4-nitrophenol, (I), and (*E*)-2-({[4-(diethylamino)phenyl]imino}methyl)-4-nitrophenol, (II), are products from the condensation reaction of *N*,*N*-dimethyl-*p*-phenylenediamine or *N*,*N*-diethyl-*p*-phenylenediamine, respectively, with 2-hydroxy-5-nitrobenzaldehyde. These two compounds have the potential to occur in two tautomeric forms, and they were prepared in order to check whether increased acidity of OH (due to the presence of an NO_2 group in the *para* position) and increased basicity of the –N=CH– N atom would result in the enamine form of these compounds. This study shows that they occur in the solid state in the imine form (Figs. 1 and 2). However, in solution there is a fast H-atom exchange, observed from the chemical shifts of atoms C1, C6, C7 and N4, between the imine (with –OH) and enaminone (with –NH) forms. As previously observed with similar compounds (Gawinecki *et al.*, 2007), the enaminone form predominates in chloroform solution. Recently, (I) was studied to obtain novel Grubbs-type bidentate Schiff base ruthenium catalysts, but its pK_a value was too low for it to be utilized for that method (Drozdzak & Nishioka, 2010). Previously, the electronic properties of (I) were investigated (Avramovici *et al.*, 1973, 1974) and it was also studied for the preparation of organometallic Ga^{III} complexes (Chesnut *et al.*, 1998). To the best of our knowledge, (II) has not been discussed previously in the literature.


(I) *R* = Me
(II) *R* = Et

The crystal structure of (I) is ordered (Fig. 1), but in (II) a small static disorder exists in one ethyl group (Fig. 2), with the occupancy of the major component being 0.789 (6). The molecules of both compounds are rather planar. However, the dihedral angle between the two aromatic rings in (I) is 13.44 (19)°, significantly larger than that in (II) [2.57 (8)°]. Furthermore, the dimethylamino group shows torsion angles of −13.8 (6) (C16—N15—C12—C13) and 5.2 (6)° (C18—N15—C12—C11) with respect to the parent benzene ring in (I). The corresponding angles in (II) are −2.1 (3) [major component; for the minor C16*B*—N15—C12—C13 component the angle is 37.1 (4)°] and −14.6 (3)°, respectively. Overall, the structure of (II) is more planar than that of (I) and the only significant deviation from the plane is found for the diethylamino group.

The presence of an intramolecular hydrogen bond in (I) was predicted according to previous studies on salicylideneanilines

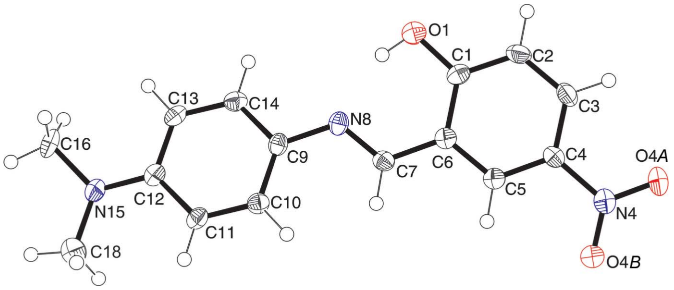


Figure 1
A view of the asymmetric unit of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

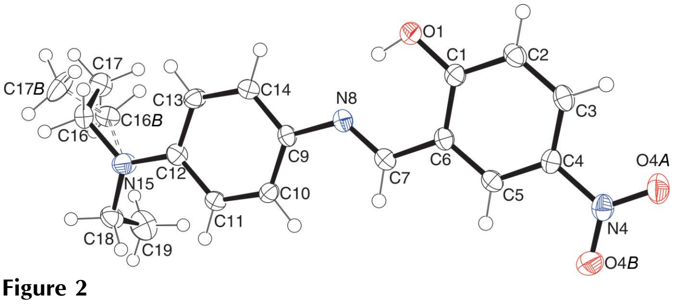


Figure 2
A view of the asymmetric unit of (II), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. Dashed bonds indicate the minor disorder component.

doi:10.1107/S0108270112025589

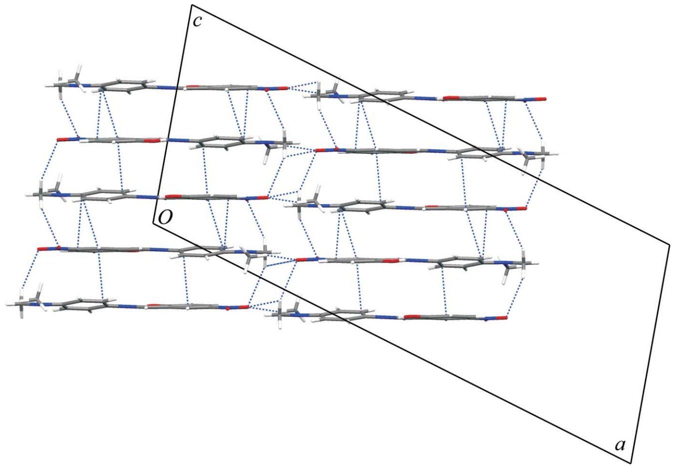


Figure 3
A packing diagram for (I), viewed along the *b* axis, showing the stacked molecules and the C—H⋯O interactions (dashed lines) between methyl and nitro groups.

and proved by spectroscopic methods in solution about 40 years ago (Avramovici *et al.*, 1973). Due to the conjugated system and the intramolecular hydrogen bond with an *S*(6) graph-set motif (Bernstein *et al.*, 1995) in the solid state, the benzylideneamine group becomes closely planar, as demonstrated by the torsion angles of 179.7 (4) (C5—C6—C7—N8) and 0.9 (6)° (C1—C6—C7—N8) between the imine bond and the phenolic ring in (I). In (II), these torsion angles are similar, with values of −178.28 (15) and 0.9 (2)°, respectively.

The hydroxy H atom in both compounds was found from an electron-density map within bonding distance (~1 Å) of the O atom, before being refined at its geometrically idealized position. Although this shows signs of the structures occurring in the imine form, reliable determination of H-atom positions is difficult. More evidence of the predominant imine form can be seen from the bond distances. The O1—C1 distance in both compounds [1.338 (5) Å in (I) and 1.334 (2) Å in (II)] is close to normal values reported for single C—O bonds in phenols and salicylideneamines (*e.g.* Ozeryanskii *et al.*, 2006). Also, the N8—C7 bond is short in both compounds [1.294 (5) Å in (I) and 1.289 (2) Å in (II)], strongly indicating the existence of a conjugated C═N bond, while the long C6—C7 bond [1.446 (5) Å in (I) and 1.457 (2) Å in (II)] implies a single bond. Based on these facts, the presence of an intramolecular O—H⋯N bond (Tables 1 and 2) and the pure *E* isomer in both compounds are justified. These features are similar to what has been observed in related 4-dimethylamino-*N*-salicylideneanilines (Filipenko *et al.*, 1983; Aldoshin *et al.*, 1984; Wozniak *et al.*, 1995; Pizzala *et al.*, 2000; Gül *et al.*, 2007). Whereas these structures, including the present ones, show phenol–imine forms, the related 4,5-bis(dimethylamino)-1-[(2-hydroxy-5-nitrobenzylidene)amino]naphthalene is reported to have the enaminone form (Ozeryanskii *et al.*, 2006).

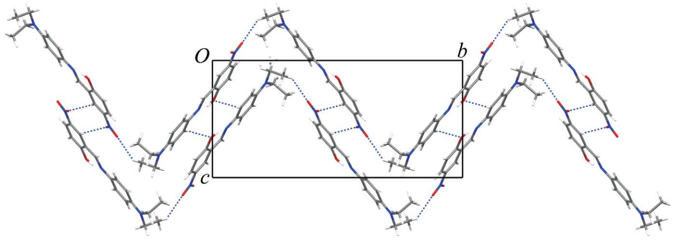


Figure 4
A packing diagram for (II), viewed along the *a* axis, showing two adjacent chains along the *b* axis and the C—H⋯O interactions (dashed lines).

The molecule of (I) has intermolecular C—H⋯O contacts between the methyl groups and the nitro group (Fig. 3), and between atom C2 and the nitro group (Table 1). There are also two different weak *π*–*π* stacking interactions, with rather long centroid–centroid distances between the phenol (C1–C6) ring and the phenylenediamine (C9–C14) rings at $(-x+1, y, -z+\frac{3}{2})$ [3.759 (2) Å] and $(-x+1, -y+1, -z+1)$ [3.878 (2) Å] (Fig. 3). These *π*–*π* interactions and two C—H⋯O interactions connect the molecules into antiparallel stacks. The other three C—H⋯O contacts connect the stacks to neighbouring ones.

There is only one C—H⋯O contact between the methyl groups and the nitro group in (II) (Table 2). Arylic atoms C5 and C14 donate C—H⋯O contacts, which are accepted by nitro and hydroxy groups, respectively. In (II), there are *π*–*π* stacking interactions between the phenol (C1–C6) ring and the phenylenediamine (C9–C14) ring at $(-x+2, -y, -z+1)$ [centroid–centroid distance = 3.5826 (10) Å], and between two phenol (C1–C6) rings [3.6267 (9) Å; symmetry code for the second ring $(-x+2, -y, -z+2)$]. Due to the different intermolecular interactions, the packing in (II) is different, as can be seen in Fig. 4. Furthermore, the only C—H⋯O contact between a methyl (C17) and a nitro group is not sufficiently strong to hold the C16—C17 ethyl group completely in one conformation. The minor component does not show a similar close contact.

Experimental

A solution of *N*,*N*-dimethyl-*p*-phenylenediamine (0.68 g, 5 mmol) and 2-hydroxy-5-nitrobenzaldehyde (0.83 g, 5 mmol) in ethanol (20 ml) was refluxed for 15 min. The solid which precipitated from the cooled reaction mixture was filtered off and recrystallized twice from ethanol to give crystals of (I). Compound (II) was obtained in a similar manner using *N*,*N*-diethyl-1,4-phenylenediamine (0.82 g, 5 mmol) as the starting material.

Analysis for compound (I): yield 91%; red crystals, m.p. 488–491 K. Elemental analysis calculated for $C_{15}H_{15}N_3O_3$: C 63.15, H 5.30, N 14.73%; found: C 63.01, H 5.49, N 14.59%. ^{1}H NMR ($CDCl_3$): δ 15.19 (*br s*, 1H, OH/NH), 8.65 (*s*, 1H, H7), 8.31 (*s*, 1H, H5), 8.19 (*d*, J = 9.0 Hz, 1H, H3), 7.32 (*d*, J = 9.0 Hz, 2H, H10 and H14), 7.02 (*d*, J = 9.2 Hz, 1H, H2), 6.75 (*d*, J = 9.0 Hz, 2H, H11 and H13), 3.03 (*s*, 6H, 2 × CH_3); ^{13}C NMR ($CDCl_3$): δ 167.4 (C1), 154.5 (C7), 150.6 (C12), 139.6 (C9), 134.4 (C4), 127.5 (C5), 127.4 (C3), 122.4 (C10 and C14), 118.5 (C6), 118.2 (C2), 112.6 (C11 and C13), 40.4 (C16 and C18); ^{15}N NMR ($CDCl_3$/ext. CH_3NO_2): δ −13.1 (N4), −93.8 (N8), −331.3 (N15).

Analysis for compound (II): yield 89%; red crystals, m.p. 441–443 K. Elemental analysis calculated for $C_{17}H_{19}N_3O_3$: C 65.16, H 6.11, N 13.41%; found: C 65.11, H 6.17, N 13.37%. ^{1}H NMR ($CDCl_3$): δ 15.30 (*br s*, 1H, OH/NH), 8.63 (*s*, 1H, H7), 8.30 (*s*, 1H, H5), 8.18 (*d*, J =

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1—H1$\cdots$N8	0.84	1.84	2.583 (4)	147
C16—H16$A\cdots$O4$A^{\rm i}$	0.98	2.62	3.495 (5)	148
C16—H16$A\cdots$O4$A^{\rm ii}$	0.98	2.69	3.062 (5)	103
C16—H16$C\cdots$O4$B^{\rm iii}$	0.98	2.60	3.411 (5)	140
C2—H2$\cdots$O4$B^{\rm iv}$	0.95	2.64	3.352 (5)	132

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

Table 2
Hydrogen-bond geometry (Å, °) for (II).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1—H1$\cdots$N8	0.84	1.81	2.557 (2)	148
C14—H14$\cdots$O1$^{\rm i}$	0.95	2.64	3.421 (2)	139
C17—H17$B\cdots$O4$A^{\rm ii}$	0.98	2.60	3.195 (3)	119
C5—H5$\cdots$O4$B^{\rm iii}$	0.95	2.56	3.328 (2)	138

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

9.0 Hz, 1H, H3), 7.30 (*d*, J = 9.0 Hz, 2H, H10 and H14), 7.01 (*d*, J = 9.2 Hz, 1H, H2), 6.70 (*d*, J = 9.0 Hz, 2H, H11 and H13), 3.41 (*q*, J = 7.1 Hz, 4H, 2 × CH$_2$), 1.21 (*t*, J = 7.1 Hz, 6H, 2 × CH$_3$); ^{13}C NMR (CDCl$_3$): δ 167.5 (C1), 153.7 (C7), 148.1 (C12), 139.5 (C9), 133.3 (C4), 127.5 (C5), 127.2 (C3), 122.7 (C10 and C14), 118.6 (C6), 118.2 (C2), 111.9 (C11 and C13), 44.58 (C16 and C18), 12.56 (C17 and C19); ^{15}N NMR (CDCl$_3$/ext. CH$_3$NO$_2$): δ −13.4 (N4), −95.3 (N8), −302.3 (N15).

Single crystals of both compounds suitable for X-ray diffraction were obtained by very slow evaporation of analytical samples from NMR tubes, where CDCl$_3$ was used as solvent.

Compound (I)

Crystal data

$C_{15}H_{15}N_3O_3$
M_r = 285.30
Monoclinic, $C2/c$
a = 31.688 (2) Å
b = 6.7674 (5) Å
c = 13.146 (1) Å
β = 106.545 (6)°

V = 2702.4 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 123 K
0.15 × 0.13 × 0.03 mm

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\rm min}$ = 0.985, $T_{\rm max}$ = 0.997

4611 measured reflections
2467 independent reflections
1242 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.108

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.082
$wR(F^2)$ = 0.167
S = 1.02
2467 reflections

193 parameters
H-atom parameters constrained
$\Delta\rho_{\rm max}$ = 0.27 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.25 e Å^{-3}

Compound (II)

Crystal data

$C_{17}H_{19}N_3O_3$
M_r = 313.35
Monoclinic, $P2_1/c$
a = 6.5848 (1) Å
b = 22.2544 (4) Å
c = 10.8735 (2) Å
β = 106.811 (1)°

V = 1525.31 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 123 K
0.20 × 0.16 × 0.06 mm

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\rm min}$ = 0.981, $T_{\rm max}$ = 0.994

6646 measured reflections
3790 independent reflections
2653 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.123
S = 1.04
3790 reflections
228 parameters

8 restraints
H-atom parameters constrained
$\Delta\rho_{\rm max}$ = 0.38 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.25 e Å^{-3}

All H atoms were located from electron-density maps, but they were calculated at their idealized positions and allowed to ride on their parent atoms, with C—H = 0.95 (aromatic), 0.98 (methyl) or 0.99 Å (methylene) and O—H = 0.84 Å, and with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) for aromatic or methylene groups or 1.5$U_{\rm eq}$(C,O) for methyl or hydroxy groups. The treatment of disorder in (II) required the use of similarity restraints to equalize the bonding distances N15—C16 and N15—C16B, and also the C16—C17 and C16B—C17B distances (s.u. = 0.02 Å). Similarity restraints were also applied for the minor component to make the anisotropic displacement parameters of C16B and C17B more similar (s.u. = 0.02 Å^2).

For both compounds, data collection: *COLLECT* (Bruker, 2008); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: LG3082). Services for accessing these data are described at the back of the journal.

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supplementary materials

Acta Cryst. (2012). C**68**, o279–o282 [doi:10.1107/S0108270112025589]

Two (*E*)-2-({[4-(dialkylamino)phenyl]imino}methyl)-4-nitrophenols

Arto Valkonen, Erkki Kolehmainen, Aleksandra Grzegórska, Borys Ośmiałowski, Ryszard Gawinecki and Kari Rissanen

(I) (*E*)-2-({[4-(dimethylamino)phenyl]imino}methyl)-4-nitrophenol

Crystal data

$C_{15}H_{15}N_3O_3$
$M_r = 285.30$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 31.688$ (2) Å
$b = 6.7674$ (5) Å
$c = 13.146$ (1) Å
$\beta = 106.545$ (6)°
$V = 2702.4$ (3) Å^3
$Z = 8$
$F(000) = 1200$
$D_x = 1.402$ Mg m^{-3}
Mo *Kα* radiation, $\lambda = 0.71073$ Å
Cell parameters from 3324 reflections
$\theta = 0.4$–28.3°
$\mu = 0.10$ mm^{-1}
$T = 123$ K
Plate, red
0.15 × 0.13 × 0.03 mm

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 9 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.985$, $T_{max} = 0.997$
4611 measured reflections
2467 independent reflections
1242 reflections with $I > 2\sigma(I)$
$R_{int} = 0.108$
$\theta_{max} = 25.4°$, $\theta_{min} = 3.1°$
$h = -38 \rightarrow 37$
$k = -7 \rightarrow 8$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.082$
$wR(F^2) = 0.167$
$S = 1.01$
2467 reflections
193 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
$w = 1/[\sigma^2(F_o^2) + (0.0415P)^2 + 5.4351P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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}
O1	0.52621 (9)	1.0161 (4)	0.6531 (3)	0.0392 (9)
H1	0.5043	0.9460	0.6235	0.059*
O4A	0.71055 (9)	0.6370 (5)	0.8492 (2)	0.0353 (8)
O4B	0.67200 (9)	0.3711 (4)	0.7984 (2)	0.0297 (7)
N4	0.67536 (11)	0.5524 (5)	0.8074 (3)	0.0271 (9)
N8	0.48098 (11)	0.6959 (5)	0.5994 (3)	0.0226 (8)
N15	0.31176 (10)	0.3775 (5)	0.4226 (3)	0.0288 (9)
C1	0.56150 (13)	0.9003 (6)	0.6902 (3)	0.0258 (10)
C2	0.60210 (14)	0.9886 (6)	0.7378 (4)	0.0324 (12)
H2	0.6039	1.1284	0.7440	0.039*
C3	0.63947 (13)	0.8768 (6)	0.7759 (3)	0.0282 (11)
H3	0.6671	0.9379	0.8075	0.034*
C4	0.63598 (12)	0.6738 (6)	0.7670 (3)	0.0203 (10)
C5	0.59640 (12)	0.5812 (6)	0.7212 (3)	0.0203 (10)
H5	0.5953	0.4411	0.7166	0.024*
C6	0.55827 (13)	0.6899 (6)	0.6818 (3)	0.0207 (10)
C7	0.51652 (12)	0.5931 (6)	0.6357 (3)	0.0227 (10)
H7	0.5152	0.4530	0.6319	0.027*
C9	0.43969 (13)	0.6029 (6)	0.5577 (3)	0.0221 (10)
C10	0.43060 (12)	0.4040 (6)	0.5674 (3)	0.0218 (10)
H10	0.4535	0.3171	0.6036	0.026*
C11	0.38834 (13)	0.3317 (6)	0.5246 (3)	0.0237 (10)
H11	0.3828	0.1954	0.5326	0.028*
C12	0.35325 (13)	0.4541 (6)	0.4695 (3)	0.0231 (10)
C13	0.36290 (13)	0.6552 (6)	0.4624 (3)	0.0250 (10)
H13	0.3401	0.7438	0.4276	0.030*
C14	0.40491 (13)	0.7256 (6)	0.5054 (3)	0.0244 (10)
H14	0.4104	0.8624	0.4992	0.029*
C16	0.27433 (12)	0.5130 (7)	0.3847 (4)	0.0320 (12)
H16A	0.2703	0.5892	0.4447	0.048*
H16B	0.2476	0.4368	0.3522	0.048*
H16C	0.2801	0.6034	0.3321	0.048*
C18	0.30268 (15)	0.1728 (6)	0.4367 (4)	0.0378 (12)
H18A	0.3230	0.0898	0.4114	0.057*
H18B	0.2723	0.1425	0.3962	0.057*
H18C	0.3066	0.1464	0.5121	0.057*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0297 (18)	0.0243 (18)	0.057 (2)	0.0043 (14)	0.0009 (17)	0.0084 (16)
O4A	0.0213 (16)	0.040 (2)	0.040 (2)	−0.0061 (15)	0.0006 (14)	−0.0023 (17)
O4B	0.0276 (16)	0.0250 (18)	0.0339 (19)	0.0002 (14)	0.0045 (14)	0.0003 (15)
N4	0.027 (2)	0.026 (2)	0.029 (2)	−0.0033 (17)	0.0082 (17)	−0.0010 (18)
N8	0.0207 (19)	0.030 (2)	0.018 (2)	0.0004 (16)	0.0071 (16)	−0.0013 (17)
N15	0.0203 (19)	0.029 (2)	0.034 (2)	0.0024 (17)	0.0030 (16)	0.0029 (18)
C1	0.028 (2)	0.023 (3)	0.026 (3)	0.005 (2)	0.006 (2)	0.006 (2)
C2	0.034 (3)	0.017 (3)	0.043 (3)	−0.003 (2)	0.006 (2)	0.001 (2)
C3	0.028 (2)	0.023 (2)	0.030 (3)	−0.007 (2)	0.003 (2)	−0.003 (2)
C4	0.027 (2)	0.020 (3)	0.017 (2)	−0.0035 (18)	0.0105 (19)	−0.0048 (19)
C5	0.022 (2)	0.022 (2)	0.020 (2)	0.0014 (18)	0.0109 (19)	−0.0009 (19)
C6	0.021 (2)	0.025 (2)	0.017 (2)	0.0020 (19)	0.0062 (18)	0.004 (2)
C7	0.023 (2)	0.020 (2)	0.027 (3)	−0.0018 (18)	0.010 (2)	−0.0031 (19)
C9	0.021 (2)	0.026 (2)	0.020 (2)	−0.0007 (19)	0.0067 (19)	−0.001 (2)
C10	0.022 (2)	0.021 (2)	0.021 (3)	0.0028 (18)	0.005 (2)	0.0034 (19)
C11	0.022 (2)	0.025 (3)	0.027 (3)	0.0057 (19)	0.0113 (19)	0.004 (2)
C12	0.027 (2)	0.028 (3)	0.016 (2)	0.003 (2)	0.009 (2)	0.0037 (19)
C13	0.023 (2)	0.023 (2)	0.029 (3)	0.0067 (19)	0.0083 (19)	0.000 (2)
C14	0.030 (3)	0.018 (2)	0.025 (3)	0.0023 (19)	0.008 (2)	0.0028 (19)
C16	0.016 (2)	0.047 (3)	0.032 (3)	0.007 (2)	0.005 (2)	0.001 (2)
C18	0.033 (3)	0.036 (3)	0.041 (3)	−0.004 (2)	0.005 (2)	0.000 (2)

Geometric parameters (Å, º)

O1—C1	1.338 (5)	C6—C7	1.446 (5)
O1—H1	0.8400	C7—H7	0.9500
O4A—N4	1.235 (4)	C9—C10	1.390 (5)
O4B—N4	1.234 (4)	C9—C14	1.395 (5)
N4—C4	1.462 (5)	C10—C11	1.386 (5)
N8—C7	1.294 (5)	C10—H10	0.9500
N8—C9	1.414 (5)	C11—C12	1.410 (6)
N15—C12	1.384 (5)	C11—H11	0.9500
N15—C18	1.438 (5)	C12—C13	1.404 (6)
N15—C16	1.470 (5)	C13—C14	1.374 (6)
C1—C2	1.395 (6)	C13—H13	0.9500
C1—C6	1.430 (6)	C14—H14	0.9500
C2—C3	1.374 (6)	C16—H16A	0.9800
C2—H2	0.9500	C16—H16B	0.9800
C3—C4	1.380 (6)	C16—H16C	0.9800
C3—H3	0.9500	C18—H18A	0.9800
C4—C5	1.378 (5)	C18—H18B	0.9800
C5—C6	1.383 (5)	C18—H18C	0.9800
C5—H5	0.9500		
C1—O1—H1	109.5	C10—C9—N8	126.1 (4)
O4B—N4—O4A	123.1 (4)	C14—C9—N8	116.1 (4)
O4B—N4—C4	118.9 (3)	C11—C10—C9	120.4 (4)

O4A—N4—C4	118.0 (3)	C11—C10—H10	119.8
C7—N8—C9	121.1 (4)	C9—C10—H10	119.8
C12—N15—C18	120.2 (4)	C10—C11—C12	122.0 (4)
C12—N15—C16	119.3 (4)	C10—C11—H11	119.0
C18—N15—C16	118.2 (3)	C12—C11—H11	119.0
O1—C1—C2	118.7 (4)	N15—C12—C13	122.1 (4)
O1—C1—C6	121.4 (4)	N15—C12—C11	121.2 (4)
C2—C1—C6	119.9 (4)	C13—C12—C11	116.7 (4)
C3—C2—C1	121.1 (4)	C14—C13—C12	120.8 (4)
C3—C2—H2	119.4	C14—C13—H13	119.6
C1—C2—H2	119.4	C12—C13—H13	119.6
C2—C3—C4	118.5 (4)	C13—C14—C9	122.2 (4)
C2—C3—H3	120.7	C13—C14—H14	118.9
C4—C3—H3	120.7	C9—C14—H14	118.9
C5—C4—C3	122.0 (4)	N15—C16—H16A	109.5
C5—C4—N4	118.7 (4)	N15—C16—H16B	109.5
C3—C4—N4	119.3 (4)	H16A—C16—H16B	109.5
C4—C5—C6	120.7 (4)	N15—C16—H16C	109.5
C4—C5—H5	119.6	H16A—C16—H16C	109.5
C6—C5—H5	119.6	H16B—C16—H16C	109.5
C5—C6—C1	117.7 (4)	N15—C18—H18A	109.5
C5—C6—C7	120.9 (4)	N15—C18—H18B	109.5
C1—C6—C7	121.4 (4)	H18A—C18—H18B	109.5
N8—C7—C6	120.5 (4)	N15—C18—H18C	109.5
N8—C7—H7	119.7	H18A—C18—H18C	109.5
C6—C7—H7	119.7	H18B—C18—H18C	109.5
C10—C9—C14	117.8 (4)		

O1—C1—C2—C3	−179.1 (4)	C5—C6—C7—N8	179.7 (4)
C6—C1—C2—C3	0.9 (7)	C1—C6—C7—N8	0.9 (6)
C1—C2—C3—C4	−0.7 (7)	C7—N8—C9—C10	12.4 (6)
C2—C3—C4—C5	0.2 (6)	C7—N8—C9—C14	−169.9 (4)
C2—C3—C4—N4	−179.8 (4)	C14—C9—C10—C11	1.0 (6)
O4B—N4—C4—C5	0.5 (6)	N8—C9—C10—C11	178.6 (4)
O4A—N4—C4—C5	−179.3 (4)	C9—C10—C11—C12	0.4 (6)
O4B—N4—C4—C3	−179.5 (4)	C18—N15—C12—C13	−176.6 (4)
O4A—N4—C4—C3	0.7 (6)	C16—N15—C12—C13	−13.8 (6)
C3—C4—C5—C6	0.0 (6)	C18—N15—C12—C11	5.2 (6)
N4—C4—C5—C6	−179.9 (3)	C16—N15—C12—C11	168.0 (4)
C4—C5—C6—C1	0.1 (6)	C10—C11—C12—N15	176.7 (4)
C4—C5—C6—C7	−178.7 (4)	C10—C11—C12—C13	−1.7 (6)
O1—C1—C6—C5	179.4 (4)	N15—C12—C13—C14	−176.8 (4)
C2—C1—C6—C5	−0.6 (6)	C11—C12—C13—C14	1.5 (6)
O1—C1—C6—C7	−1.8 (6)	C12—C13—C14—C9	−0.1 (6)
C2—C1—C6—C7	178.3 (4)	C10—C9—C14—C13	−1.1 (6)
C9—N8—C7—C6	−177.6 (4)	N8—C9—C14—C13	−179.0 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N8	0.84	1.84	2.583 (4)	147
C16—H16*A*···O4*A*^{i}	0.98	2.62	3.495 (5)	148
C16—H16*A*···O4*A*^{ii}	0.98	2.69	3.062 (5)	103
C16—H16*C*···O4*B*^{iii}	0.98	2.60	3.411 (5)	140
C2—H2···O4*B*^{iv}	0.95	2.64	3.352 (5)	132

Symmetry codes: (i) $-x+1, y, -z+3/2$; (ii) $x-1/2, -y+3/2, z-1/2$; (iii) $-x+1, -y+1, -z+1$; (iv) $x, y+1, z$.

(II) (*E*)-2-({[4-(diethylamino)phenyl]imino}methyl)-4-nitrophenol

Crystal data

$C_{17}H_{19}N_3O_3$	$F(000) = 664$
$M_r = 313.35$	$D_x = 1.365$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 3812 reflections
$a = 6.5848$ (1) Å	$\theta = 0.4$–28.3°
$b = 22.2544$ (4) Å	$\mu = 0.10$ mm^{-1}
$c = 10.8735$ (2) Å	$T = 123$ K
$\beta = 106.811$ (1)°	Plate, red
$V = 1525.31$ (5) Å^3	0.20 × 0.16 × 0.06 mm
$Z = 4$	

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer	6646 measured reflections
Radiation source: fine-focus sealed tube	3790 independent reflections
Graphite monochromator	2653 reflections with $I > 2\sigma(I)$
Detector resolution: 9 pixels mm^{-1}	$R_{\text{int}} = 0.030$
φ and ω scans	$\theta_{\max} = 28.3°$, $\theta_{\min} = 2.7°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -8 \rightarrow 8$
$T_{\min} = 0.981$, $T_{\max} = 0.994$	$k = -29 \rightarrow 25$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.056$	H-atom parameters constrained
$wR(F^2) = 0.123$	$w = 1/[\sigma^2(F_o^2) + (0.0343P)^2 + 0.8927P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{\max} < 0.001$
3790 reflections	$\Delta\rho_{\max} = 0.38$ e Å^{-3}
228 parameters	$\Delta\rho_{\min} = -0.25$ e Å^{-3}
8 restraints	
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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	$U_{\rm iso}$*/$U_{\rm eq}$	Occ. (<1)
O1	0.62487 (19)	−0.00420 (6)	0.65774 (11)	0.0292 (3)	
H1	0.6717	0.0187	0.6108	0.044*	
O4A	1.2373 (2)	−0.11842 (6)	1.14921 (12)	0.0369 (3)	
O4B	1.4676 (2)	−0.07660 (6)	1.06910 (13)	0.0371 (3)	
N4	1.2831 (2)	−0.08873 (7)	1.06541 (14)	0.0272 (3)	
N8	0.8984 (2)	0.05530 (6)	0.58184 (13)	0.0219 (3)	
N15	0.9700 (2)	0.21352 (7)	0.19249 (16)	0.0344 (4)	
C1	0.7858 (3)	−0.02429 (8)	0.75424 (15)	0.0224 (4)	
C2	0.7423 (3)	−0.06292 (8)	0.84506 (16)	0.0253 (4)	
H2	0.6000	−0.0745	0.8365	0.030*	
C3	0.9037 (3)	−0.08426 (8)	0.94667 (16)	0.0246 (4)	
H3	0.8736	−0.1102	1.0086	0.029*	
C4	1.1114 (3)	−0.06732 (7)	0.95727 (15)	0.0221 (4)	
C5	1.1597 (3)	−0.02930 (7)	0.86918 (16)	0.0219 (4)	
H5	1.3029	−0.0184	0.8788	0.026*	
C6	0.9984 (3)	−0.00712 (7)	0.76660 (15)	0.0210 (4)	
C7	1.0492 (3)	0.03371 (7)	0.67494 (16)	0.0223 (4)	
H7	1.1925	0.0443	0.6838	0.027*	
C9	0.9309 (3)	0.09557 (7)	0.48881 (15)	0.0206 (3)	
C10	1.1272 (3)	0.11697 (8)	0.48217 (16)	0.0223 (4)	
H10	1.2536	0.1042	0.5441	0.027*	
C11	1.1391 (3)	0.15641 (7)	0.38660 (16)	0.0230 (4)	
H11	1.2742	0.1705	0.3846	0.028*	
C12	0.9561 (3)	0.17650 (8)	0.29146 (17)	0.0245 (4)	
C13	0.7602 (3)	0.15488 (8)	0.30041 (17)	0.0260 (4)	
H13	0.6329	0.1676	0.2393	0.031*	
C14	0.7495 (3)	0.11537 (8)	0.39666 (16)	0.0240 (4)	
H14	0.6148	0.1014	0.3998	0.029*	
C16	0.7773 (4)	0.23028 (11)	0.0887 (3)	0.0257 (7)	0.789 (6)
H16A	0.6813	0.1952	0.0666	0.031*	0.789 (6)
H16B	0.8178	0.2419	0.0111	0.031*	0.789 (6)
C17	0.6615 (5)	0.28215 (12)	0.1294 (2)	0.0313 (7)	0.789 (6)
H17A	0.5351	0.2923	0.0591	0.047*	0.789 (6)
H17B	0.7557	0.3171	0.1500	0.047*	0.789 (6)
H17C	0.6191	0.2705	0.2053	0.047*	0.789 (6)
C16B	0.7851 (15)	0.2594 (4)	0.1507 (9)	0.029 (3)	0.211 (6)
H16C	0.7019	0.2614	0.2133	0.034*	0.211 (6)
H16D	0.8367	0.3001	0.1382	0.034*	0.211 (6)
C17B	0.658 (2)	0.2316 (5)	0.0247 (11)	0.051 (3)	0.211 (6)
H17D	0.5326	0.2562	−0.0137	0.076*	0.211 (6)
H17E	0.6143	0.1909	0.0404	0.076*	0.211 (6)
H17F	0.7465	0.2296	−0.0341	0.076*	0.211 (6)

C18	1.1665 (3)	0.24487 (8)	0.19747 (19)	0.0305 (4)
H18A	1.1560	0.2607	0.1107	0.037*
H18B	1.2844	0.2155	0.2198	0.037*
C19	1.2213 (4)	0.29653 (10)	0.2927 (2)	0.0458 (6)
H19A	1.3548	0.3150	0.2897	0.069*
H19B	1.2368	0.2813	0.3795	0.069*
H19C	1.1077	0.3266	0.2704	0.069*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0257 (7)	0.0352 (7)	0.0249 (7)	−0.0052 (6)	0.0046 (5)	0.0048 (5)
O4A	0.0429 (8)	0.0383 (8)	0.0310 (7)	0.0053 (6)	0.0132 (6)	0.0119 (6)
O4B	0.0272 (7)	0.0400 (8)	0.0424 (8)	0.0031 (6)	0.0072 (6)	0.0113 (6)
N4	0.0342 (9)	0.0231 (8)	0.0251 (8)	0.0033 (7)	0.0098 (7)	0.0021 (6)
N8	0.0271 (8)	0.0187 (7)	0.0207 (7)	−0.0018 (6)	0.0083 (6)	−0.0021 (6)
N15	0.0257 (8)	0.0366 (9)	0.0404 (9)	−0.0002 (7)	0.0087 (7)	0.0178 (7)
C1	0.0251 (9)	0.0228 (8)	0.0192 (8)	−0.0020 (7)	0.0065 (7)	−0.0044 (6)
C2	0.0268 (9)	0.0270 (9)	0.0238 (9)	−0.0067 (7)	0.0099 (7)	−0.0038 (7)
C3	0.0333 (10)	0.0211 (8)	0.0221 (9)	−0.0025 (7)	0.0125 (7)	−0.0012 (7)
C4	0.0282 (9)	0.0196 (8)	0.0181 (8)	0.0020 (7)	0.0059 (7)	−0.0018 (6)
C5	0.0225 (8)	0.0201 (8)	0.0244 (8)	−0.0012 (7)	0.0091 (7)	−0.0023 (7)
C6	0.0266 (9)	0.0188 (8)	0.0193 (8)	−0.0010 (7)	0.0092 (7)	−0.0032 (6)
C7	0.0241 (9)	0.0198 (8)	0.0242 (8)	−0.0009 (7)	0.0088 (7)	−0.0016 (7)
C9	0.0252 (9)	0.0188 (8)	0.0191 (8)	−0.0011 (7)	0.0084 (7)	−0.0019 (6)
C10	0.0215 (8)	0.0225 (8)	0.0213 (8)	0.0020 (7)	0.0036 (7)	−0.0003 (7)
C11	0.0220 (8)	0.0225 (8)	0.0256 (9)	−0.0020 (7)	0.0089 (7)	−0.0002 (7)
C12	0.0270 (9)	0.0196 (8)	0.0280 (9)	0.0005 (7)	0.0098 (7)	0.0028 (7)
C13	0.0211 (9)	0.0251 (9)	0.0299 (9)	0.0015 (7)	0.0045 (7)	0.0057 (7)
C14	0.0219 (8)	0.0243 (9)	0.0264 (9)	−0.0020 (7)	0.0079 (7)	−0.0010 (7)
C16	0.0341 (16)	0.0242 (13)	0.0203 (14)	−0.0001 (11)	0.0100 (12)	0.0004 (11)
C17	0.0333 (16)	0.0263 (13)	0.0343 (14)	0.0031 (12)	0.0099 (11)	0.0045 (10)
C16B	0.031 (6)	0.021 (5)	0.038 (5)	0.008 (4)	0.016 (4)	−0.003 (4)
C17B	0.049 (7)	0.045 (6)	0.042 (7)	−0.002 (5)	−0.012 (6)	0.011 (5)
C18	0.0297 (10)	0.0283 (9)	0.0362 (10)	−0.0006 (8)	0.0139 (8)	0.0077 (8)
C19	0.0578 (15)	0.0337 (11)	0.0497 (13)	−0.0057 (10)	0.0217 (11)	−0.0002 (10)

Geometric parameters (Å, º)

O1—C1	1.334 (2)	C10—H10	0.9500
O1—H1	0.8400	C11—C12	1.414 (2)
O4A—N4	1.2316 (19)	C11—H11	0.9500
O4B—N4	1.233 (2)	C12—C13	1.406 (2)
N4—C4	1.456 (2)	C13—C14	1.384 (2)
N8—C7	1.289 (2)	C13—H13	0.9500
N8—C9	1.413 (2)	C14—H14	0.9500
N15—C12	1.379 (2)	C16—C17	1.518 (4)
N15—C18	1.457 (2)	C16—H16A	0.9900
N15—C16	1.481 (3)	C16—H16B	0.9900
N15—C16B	1.553 (9)	C17—H17A	0.9800

C1—C2	1.400 (2)	C17—H17B	0.9800
C1—C6	1.420 (2)	C17—H17C	0.9800
C2—C3	1.377 (2)	C16B—C17B	1.515 (13)
C2—H2	0.9500	C16B—H16C	0.9900
C3—C4	1.391 (2)	C16B—H16D	0.9900
C3—H3	0.9500	C17B—H17D	0.9800
C4—C5	1.382 (2)	C17B—H17E	0.9800
C5—C6	1.389 (2)	C17B—H17F	0.9800
C5—H5	0.9500	C18—C19	1.519 (3)
C6—C7	1.457 (2)	C18—H18A	0.9900
C7—H7	0.9500	C18—H18B	0.9900
C9—C14	1.390 (2)	C19—H19A	0.9800
C9—C10	1.399 (2)	C19—H19B	0.9800
C10—C11	1.380 (2)	C19—H19C	0.9800

C1—O1—H1	109.5	C14—C13—C12	121.18 (16)
O4A—N4—O4B	122.88 (15)	C14—C13—H13	119.4
O4A—N4—C4	118.29 (15)	C12—C13—H13	119.4
O4B—N4—C4	118.83 (14)	C13—C14—C9	121.70 (16)
C7—N8—C9	123.82 (15)	C13—C14—H14	119.2
C12—N15—C18	121.03 (15)	C9—C14—H14	119.2
C12—N15—C16	120.63 (16)	N15—C16—C17	111.1 (2)
C18—N15—C16	117.62 (16)	N15—C16—H16A	109.4
C12—N15—C16B	113.4 (4)	C17—C16—H16A	109.4
C18—N15—C16B	108.0 (4)	N15—C16—H16B	109.4
O1—C1—C2	118.84 (15)	C17—C16—H16B	109.4
O1—C1—C6	121.43 (15)	H16A—C16—H16B	108.0
C2—C1—C6	119.73 (15)	C16—C17—H17A	109.5
C3—C2—C1	120.65 (16)	C16—C17—H17B	109.5
C3—C2—H2	119.7	H17A—C17—H17B	109.5
C1—C2—H2	119.7	C16—C17—H17C	109.5
C2—C3—C4	119.03 (16)	H17A—C17—H17C	109.5
C2—C3—H3	120.5	H17B—C17—H17C	109.5
C4—C3—H3	120.5	C17B—C16B—N15	100.1 (8)
C5—C4—C3	121.75 (16)	C17B—C16B—H16C	111.8
C5—C4—N4	118.65 (15)	N15—C16B—H16C	111.8
C3—C4—N4	119.59 (15)	C17B—C16B—H16D	111.8
C4—C5—C6	119.89 (16)	N15—C16B—H16D	111.8
C4—C5—H5	120.1	H16C—C16B—H16D	109.5
C6—C5—H5	120.1	C16B—C17B—H17D	109.5
C5—C6—C1	118.95 (15)	C16B—C17B—H17E	109.5
C5—C6—C7	119.82 (15)	H17D—C17B—H17E	109.5
C1—C6—C7	121.22 (15)	C16B—C17B—H17F	109.5
N8—C7—C6	119.51 (15)	H17D—C17B—H17F	109.5
N8—C7—H7	120.2	H17E—C17B—H17F	109.5
C6—C7—H7	120.2	N15—C18—C19	114.89 (16)
C14—C9—C10	117.97 (15)	N15—C18—H18A	108.5
C14—C9—N8	116.11 (15)	C19—C18—H18A	108.5
C10—C9—N8	125.91 (15)	N15—C18—H18B	108.5

C11—C10—C9	120.65 (16)	C19—C18—H18B	108.5
C11—C10—H10	119.7	H18A—C18—H18B	107.5
C9—C10—H10	119.7	C18—C19—H19A	109.5
C10—C11—C12	122.02 (16)	C18—C19—H19B	109.5
C10—C11—H11	119.0	H19A—C19—H19B	109.5
C12—C11—H11	119.0	C18—C19—H19C	109.5
N15—C12—C13	121.84 (16)	H19A—C19—H19C	109.5
N15—C12—C11	121.65 (16)	H19B—C19—H19C	109.5
C13—C12—C11	116.47 (15)		

O1—C1—C2—C3	−179.48 (15)	N8—C9—C10—C11	−179.88 (15)
C6—C1—C2—C3	0.3 (3)	C9—C10—C11—C12	−0.5 (3)
C1—C2—C3—C4	−0.6 (3)	C18—N15—C12—C13	167.89 (17)
C2—C3—C4—C5	0.5 (3)	C16—N15—C12—C13	−2.1 (3)
C2—C3—C4—N4	178.95 (15)	C16B—N15—C12—C13	37.1 (4)
O4A—N4—C4—C5	173.99 (15)	C18—N15—C12—C11	−14.6 (3)
O4B—N4—C4—C5	−6.2 (2)	C16—N15—C12—C11	175.41 (18)
O4A—N4—C4—C3	−4.5 (2)	C16B—N15—C12—C11	−145.4 (4)
O4B—N4—C4—C3	175.30 (15)	C10—C11—C12—N15	−176.66 (16)
C3—C4—C5—C6	−0.1 (2)	C10—C11—C12—C13	1.0 (2)
N4—C4—C5—C6	−178.58 (14)	N15—C12—C13—C14	176.75 (17)
C4—C5—C6—C1	−0.2 (2)	C11—C12—C13—C14	−0.9 (3)
C4—C5—C6—C7	179.04 (15)	C12—C13—C14—C9	0.3 (3)
O1—C1—C6—C5	179.86 (15)	C10—C9—C14—C13	0.2 (2)
C2—C1—C6—C5	0.1 (2)	N8—C9—C14—C13	179.99 (15)
O1—C1—C6—C7	0.6 (2)	C12—N15—C16—C17	82.2 (2)
C2—C1—C6—C7	−179.09 (15)	C18—N15—C16—C17	−88.1 (2)
C9—N8—C7—C6	179.41 (14)	C12—N15—C16B—C17B	−106.0 (6)
C5—C6—C7—N8	−178.28 (15)	C18—N15—C16B—C17B	117.0 (6)
C1—C6—C7—N8	0.9 (2)	C12—N15—C18—C19	−72.0 (2)
C7—N8—C9—C14	−178.65 (15)	C16—N15—C18—C19	98.3 (2)
C7—N8—C9—C10	1.1 (3)	C16B—N15—C18—C19	61.1 (4)
C14—C9—C10—C11	−0.1 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N8	0.84	1.81	2.557 (2)	148
C14—H14···O1$^{\rm i}$	0.95	2.64	3.421 (2)	139
C17—H17*B*···O4*A*$^{\rm ii}$	0.98	2.60	3.195 (3)	119
C5—H5···O4*B*$^{\rm iii}$	0.95	2.56	3.328 (2)	138

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