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N,*N*-Diethyl-5-nitropyridin-2-amine

Dmitry S. Yufit,* Michael J. Turner and Judith A. K. Howard

Chemistry Department, University of Durham, South Road, Durham DH1 3LE, England

Correspondence e-mail: d.s.yufit@durham.ac.uk

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Key indicators

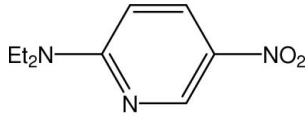
Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.002 Å
R factor = 0.040
wR factor = 0.112
Data-to-parameter ratio = 15.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $C_9H_{13}N_3O_2$, the asymmetric unit contains two almost identical but crystallographically independent molecules. The molecules are linked together by pairs of weak C—H···O interactions into zigzag chains, which, in turn, form corrugated layers perpendicular to the *a* axis.

Comment

In continuation of our studies of organic molecules with non-linear optical properties (Yufit *et al.*, 2006), an attempt to grow crystals of 2-adamantylamino-5-nitropyridine (AANP) (Tomaru *et al.*, 1991; Antipin *et al.*, 2001) by sublimation has been made. As a result, two types of crystals formed in the reaction vessel. An X-ray study of the small cubic-shaped ones revealed that they are, in fact, crystals of *N*,*N*-diethyl-5-nitropyridine-2-amine, (I), which is a side product in the synthesis of AANP. Here, we briefly describe the structural features of this compound.



(I)

The asymmetric unit of (I) contains two virtually identical but crystallographically independent molecules (Fig. 1). These molecules differ slightly in the positions of the terminal C atoms of the ethyl groups (Fig. 2).

The packing of the molecules of (I) is quite different from that of its benzene analogue *N*,*N*-diethyl-*p*-nitroaniline (Maurin & Krygowski, 1988), in which numerous C—H···π interactions are present.

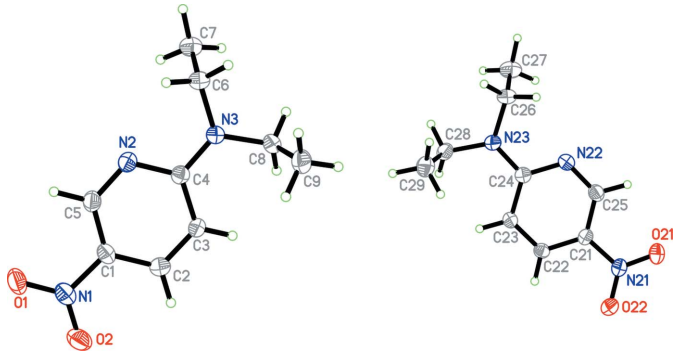


Figure 1
The asymmetric unit of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

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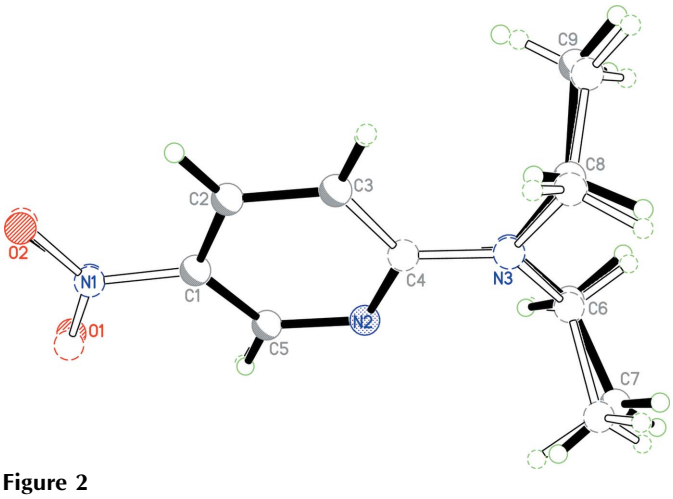

Figure 2
A least-squares fit of the pyridine rings of the two independent molecules.

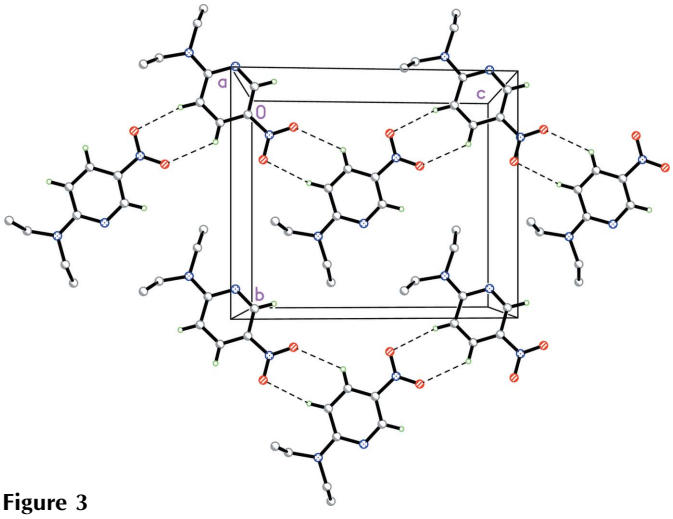

Figure 3
The chains of molecules of (I) in a single layer. H atoms of ethyl groups have been omitted for clarity. Dashed lines indicate hydrogen bonds.

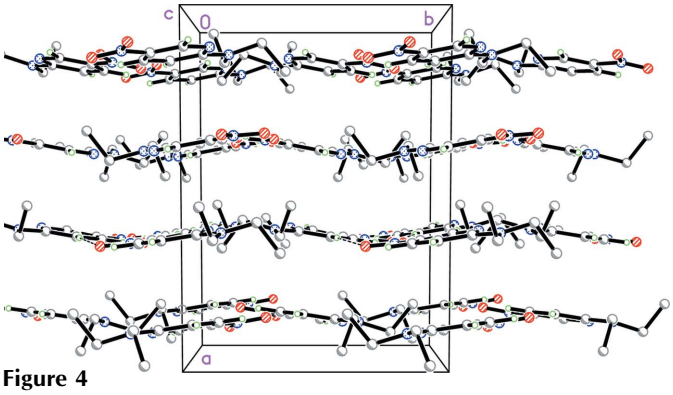

Figure 4
A packing diagram for (I), viewed down the *a* axis.

In the crystal structure, molecules are linked together by pairs of C—H···O [$O1^{i}\cdots H2(-C2)$ = 2.74 (1) Å, $O2^{i}\cdots H3(-C3)$ = 2.63 (1) Å, $O21^{ii}\cdots H22(-C22)$ = 2.67 (1) Å and $O22^{ii}\cdots H23(-C23)$ = 2.51 (1) Å; symmetry codes: (i) $x, \frac{5}{2}-y, \frac{1}{2}+z$, (ii) $x, \frac{5}{2}-y, -\frac{1}{2}+z$] interactions in zigzag chains parallel to the *c* axis (Fig. 3); each independent molecule forms separate chains. These chains form corrugated layers perpendicular to *a* axis (Fig. 4). The pyridine rings of the molecules in adjacent layers are partially overlapped, the shortest interplanar distance being 3.42 Å, which is within the normal range for π–π aromatic interactions (Janiak, 2000).

Experimental

The title compound, (I), was isolated by chromatography from the mixture of products of the reaction between 2-chloronitropyridine (0.948 g, 5.979 mmol) and adamantylamine (0.984 g, 6.594 mmol). The crystals of (I) were formed on heating the powder sample at 343 K for 3 d (yield 0.99 g, 61%; m.p. 440 K).

Crystal data

$C_9H_{13}N_3O_2$
M_r = 195.22
Monoclinic, $P2_1/c$
a = 14.6723 (7) Å
b = 10.6920 (5) Å
c = 12.4224 (5) Å
β = 96.820 (1)°
V = 1934.99 (15) Å^3
Z = 8
D_x = 1.340 Mg m^{-3}
Mo- $K\alpha$ radiation
Cell parameters from 4483 reflections
θ = 2.4–30.4°
μ = 0.10 mm^{-1}
T = 120 (2) K
Block, yellow
0.26 × 0.14 × 0.12 mm

Data collection

Bruker SMART CCD 6000 diffractometer
ω scans
Absorption correction: none
19597 measured reflections
5389 independent reflections
3536 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 29.5°
$h = -20 \rightarrow 20$
$k = -14 \rightarrow 14$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.112
S = 0.97
5389 reflections
357 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.06P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—N1	1.2387 (14)	N3—C8	1.4658 (15)
O2—N1	1.2378 (15)	N3—C6	1.4692 (16)
O21—N21	1.2368 (14)	N21—C21	1.4333 (15)
O22—N21	1.2356 (14)	N22—C25	1.3276 (17)
N1—C1	1.4365 (16)	N22—C24	1.3612 (16)
N2—C5	1.3263 (16)	N23—C24	1.3509 (15)
N2—C4	1.3626 (15)	N23—C28	1.4620 (17)
N3—C4	1.3455 (15)	N23—C26	1.4660 (16)
O2—N1—O1	122.69 (11)	O22—N21—C21	118.76 (10)
O2—N1—C1	118.57 (11)	O21—N21—C21	118.83 (11)
O1—N1—C1	118.74 (11)	C25—N22—C24	117.57 (11)
C5—N2—C4	117.73 (11)	C24—N23—C28	121.83 (10)
C4—N3—C8	121.56 (10)	C24—N23—C26	121.11 (11)
C4—N3—C6	121.56 (10)	C28—N23—C26	117.04 (10)
C8—N3—C6	116.44 (10)	N3—C4—N2	116.80 (11)
O22—N21—O21	122.40 (11)	N3—C4—C3	121.76 (11)

H atoms were located in a difference synthesis and refined isotropically [C—H = 0.922 (14)–0.976 (14) for CH, 0.965 (13)–1.007 (14) for CH_2 and 0.970 (17)–1.028 (16) Å for CH_3].

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2003); program(s) used to refine

structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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supporting information

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Graphite monochromator
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$k = -14 \rightarrow 14$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.112$
$S = 0.97$
5389 reflections
357 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.06P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ 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}
O1	0.88641 (7)	1.16690 (10)	−0.20267 (7)	0.0395 (3)
O2	0.85357 (7)	1.31005 (9)	−0.08920 (8)	0.0394 (2)
O21	0.35252 (8)	1.16353 (10)	1.18822 (7)	0.0408 (3)
O22	0.34599 (7)	1.31229 (9)	1.06912 (7)	0.0336 (2)
N1	0.86987 (8)	1.20006 (11)	−0.11143 (9)	0.0296 (2)
N2	0.88886 (7)	0.89231 (10)	0.02259 (8)	0.0268 (2)
N3	0.87939 (7)	0.83105 (9)	0.19895 (8)	0.0236 (2)
N21	0.35337 (7)	1.20055 (10)	1.09402 (8)	0.0273 (2)
N22	0.39111 (7)	0.89809 (9)	0.96485 (9)	0.0262 (2)
N23	0.38857 (7)	0.83972 (9)	0.78584 (8)	0.0260 (2)
C1	0.86994 (8)	1.10729 (12)	−0.02779 (10)	0.0244 (3)
C2	0.85663 (8)	1.14175 (12)	0.07749 (10)	0.0251 (3)
C3	0.85941 (8)	1.05069 (11)	0.15475 (10)	0.0234 (3)
C4	0.87580 (8)	0.92429 (11)	0.12583 (10)	0.0223 (2)
C5	0.88623 (9)	0.98302 (12)	−0.05055 (10)	0.0268 (3)
C6	0.90970 (9)	0.70469 (12)	0.17327 (11)	0.0262 (3)
C7	0.83026 (10)	0.61517 (13)	0.14346 (12)	0.0309 (3)
C8	0.86461 (9)	0.85407 (13)	0.31190 (10)	0.0260 (3)
C9	0.95032 (10)	0.89981 (14)	0.38086 (11)	0.0328 (3)
C21	0.36342 (8)	1.11063 (11)	1.01067 (9)	0.0229 (3)
C22	0.35764 (8)	1.14762 (11)	0.90234 (10)	0.0224 (2)
C23	0.36722 (8)	1.05862 (11)	0.82571 (10)	0.0226 (2)
C24	0.38215 (8)	0.93229 (11)	0.85857 (10)	0.0230 (3)
C25	0.38127 (8)	0.98655 (12)	1.03757 (10)	0.0262 (3)
C26	0.41529 (9)	0.71269 (12)	0.82107 (12)	0.0283 (3)
C27	0.33357 (10)	0.62959 (14)	0.83556 (14)	0.0362 (3)
C28	0.37213 (10)	0.86210 (13)	0.66905 (10)	0.0287 (3)
C29	0.45757 (11)	0.90510 (15)	0.62215 (12)	0.0361 (3)
H2	0.8458 (9)	1.2287 (13)	0.0962 (11)	0.025 (3)*
H3	0.8547 (10)	1.0713 (13)	0.2259 (11)	0.029 (4)*
H5	0.8977 (9)	0.9588 (14)	−0.1233 (12)	0.035 (4)*
H61	0.9503 (10)	0.6739 (13)	0.2380 (12)	0.034 (4)*
H62	0.9477 (9)	0.7122 (12)	0.1149 (11)	0.025 (3)*
H71	0.7969 (11)	0.6413 (14)	0.0736 (13)	0.040 (4)*
H72	0.8559 (10)	0.5284 (15)	0.1329 (12)	0.042 (4)*
H73	0.7881 (10)	0.6140 (13)	0.1993 (12)	0.036 (4)*
H81	0.8431 (9)	0.7764 (13)	0.3393 (10)	0.023 (3)*
H82	0.8137 (9)	0.9168 (13)	0.3140 (10)	0.027 (4)*
H91	0.9978 (12)	0.8369 (16)	0.3803 (13)	0.052 (5)*
H92	0.9758 (10)	0.9807 (15)	0.3509 (12)	0.041 (4)*

H93	0.9373 (11)	0.9131 (15)	0.4526 (14)	0.048 (5)*
H22	0.3491 (9)	1.2342 (12)	0.8839 (10)	0.019 (3)*
H23	0.3659 (9)	1.0812 (13)	0.7504 (11)	0.029 (4)*
H25	0.3891 (9)	0.9642 (13)	1.1136 (11)	0.030 (4)*
H261	0.4578 (10)	0.7189 (13)	0.8895 (11)	0.028 (4)*
H262	0.4534 (10)	0.6804 (13)	0.7657 (12)	0.031 (4)*
H271	0.3047 (11)	0.6582 (15)	0.8981 (13)	0.045 (5)*
H272	0.3546 (11)	0.5419 (17)	0.8529 (13)	0.050 (5)*
H273	0.2913 (11)	0.6265 (15)	0.7689 (13)	0.044 (4)*
H281	0.3220 (10)	0.9221 (13)	0.6533 (11)	0.030 (4)*
H282	0.3488 (10)	0.7821 (14)	0.6362 (11)	0.030 (4)*
H291	0.5053 (12)	0.8409 (16)	0.6329 (13)	0.052 (5)*
H292	0.4821 (11)	0.9817 (16)	0.6565 (12)	0.044 (4)*
H293	0.4438 (10)	0.9218 (14)	0.5436 (13)	0.038 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0501 (6)	0.0455 (6)	0.0230 (5)	−0.0122 (5)	0.0038 (4)	0.0050 (4)
O2	0.0465 (6)	0.0308 (5)	0.0411 (6)	0.0025 (4)	0.0057 (5)	0.0107 (5)
O21	0.0614 (7)	0.0411 (6)	0.0210 (5)	0.0002 (5)	0.0086 (5)	−0.0017 (4)
O22	0.0426 (6)	0.0275 (5)	0.0300 (5)	0.0021 (4)	0.0020 (4)	−0.0050 (4)
N1	0.0276 (6)	0.0330 (6)	0.0274 (6)	−0.0054 (5)	−0.0001 (4)	0.0061 (5)
N2	0.0316 (6)	0.0256 (5)	0.0235 (5)	−0.0018 (4)	0.0051 (4)	−0.0023 (4)
N3	0.0273 (5)	0.0211 (5)	0.0228 (5)	0.0006 (4)	0.0041 (4)	0.0002 (4)
N21	0.0286 (6)	0.0303 (6)	0.0230 (5)	−0.0007 (4)	0.0030 (4)	−0.0028 (5)
N22	0.0293 (6)	0.0239 (5)	0.0253 (5)	0.0002 (4)	0.0029 (4)	0.0024 (4)
N23	0.0304 (6)	0.0212 (5)	0.0260 (5)	0.0019 (4)	0.0018 (4)	−0.0005 (4)
C1	0.0232 (6)	0.0273 (6)	0.0224 (6)	−0.0033 (5)	0.0018 (5)	0.0047 (5)
C2	0.0227 (6)	0.0233 (6)	0.0294 (7)	−0.0002 (5)	0.0027 (5)	−0.0009 (5)
C3	0.0262 (6)	0.0238 (6)	0.0205 (6)	−0.0001 (5)	0.0041 (5)	−0.0022 (5)
C4	0.0212 (6)	0.0229 (6)	0.0226 (6)	−0.0015 (5)	0.0019 (5)	−0.0010 (5)
C5	0.0299 (7)	0.0296 (7)	0.0209 (6)	−0.0045 (5)	0.0038 (5)	−0.0016 (5)
C6	0.0268 (6)	0.0222 (6)	0.0296 (7)	0.0019 (5)	0.0031 (5)	0.0001 (5)
C7	0.0308 (7)	0.0252 (7)	0.0361 (8)	−0.0012 (5)	0.0019 (6)	−0.0005 (6)
C8	0.0300 (7)	0.0257 (6)	0.0227 (6)	−0.0004 (5)	0.0051 (5)	0.0033 (5)
C9	0.0347 (8)	0.0377 (8)	0.0252 (7)	−0.0005 (6)	0.0000 (6)	0.0011 (6)
C21	0.0229 (6)	0.0246 (6)	0.0212 (6)	−0.0017 (5)	0.0029 (5)	−0.0025 (5)
C22	0.0213 (6)	0.0214 (6)	0.0245 (6)	−0.0006 (5)	0.0026 (5)	0.0011 (5)
C23	0.0235 (6)	0.0235 (6)	0.0209 (6)	0.0006 (5)	0.0028 (5)	0.0019 (5)
C24	0.0207 (6)	0.0235 (6)	0.0248 (6)	−0.0008 (5)	0.0030 (5)	−0.0002 (5)
C25	0.0280 (7)	0.0272 (6)	0.0234 (6)	−0.0015 (5)	0.0025 (5)	0.0032 (5)
C26	0.0288 (7)	0.0209 (6)	0.0354 (7)	0.0013 (5)	0.0041 (6)	−0.0007 (6)
C27	0.0317 (8)	0.0271 (7)	0.0493 (9)	−0.0018 (6)	0.0034 (7)	0.0003 (7)
C28	0.0327 (7)	0.0280 (7)	0.0250 (6)	0.0014 (6)	0.0016 (5)	−0.0047 (5)
C29	0.0405 (8)	0.0386 (8)	0.0304 (8)	0.0005 (7)	0.0097 (6)	−0.0023 (7)

Geometric parameters (Å, º)

O1—N1	1.2387 (14)	C7—H72	1.015 (16)
O2—N1	1.2378 (15)	C7—H73	0.983 (15)
O21—N21	1.2368 (14)	C8—C9	1.516 (2)
O22—N21	1.2356 (14)	C8—H81	0.965 (13)
N1—C1	1.4365 (16)	C8—H82	1.007 (14)
N2—C5	1.3263 (16)	C9—H91	0.970 (17)
N2—C4	1.3626 (15)	C9—H92	1.028 (16)
N3—C4	1.3455 (15)	C9—H93	0.944 (17)
N3—C8	1.4658 (15)	C21—C25	1.3855 (17)
N3—C6	1.4692 (16)	C21—C22	1.3955 (16)
N21—C21	1.4333 (15)	C22—C23	1.3650 (17)
N22—C25	1.3276 (17)	C22—H22	0.958 (13)
N22—C24	1.3612 (16)	C23—C24	1.4205 (17)
N23—C24	1.3509 (15)	C23—H23	0.964 (14)
N23—C28	1.4620 (17)	C25—H25	0.968 (14)
N23—C26	1.4660 (16)	C26—C27	1.5201 (19)
C1—C5	1.3851 (18)	C26—H261	0.995 (14)
C1—C2	1.3946 (18)	C26—H262	0.997 (14)
C2—C3	1.3644 (18)	C27—H271	0.977 (16)
C2—H2	0.976 (14)	C27—H272	1.003 (17)
C3—C4	1.4261 (17)	C27—H273	0.974 (17)
C3—H3	0.922 (14)	C28—C29	1.515 (2)
C5—H5	0.974 (14)	C28—H281	0.978 (14)
C6—C7	1.5197 (19)	C28—H282	0.991 (15)
C6—H61	0.997 (15)	C29—H291	0.978 (18)
C6—H62	0.970 (13)	C29—H292	0.973 (17)
C7—H71	0.985 (16)	C29—H293	0.989 (15)

O2—N1—O1	122.69 (11)	H81—C8—H82	106.9 (11)
O2—N1—C1	118.57 (11)	C8—C9—H91	108.7 (10)
O1—N1—C1	118.74 (11)	C8—C9—H92	112.3 (8)
C5—N2—C4	117.73 (11)	H91—C9—H92	106.8 (13)
C4—N3—C8	121.56 (10)	C8—C9—H93	109.6 (10)
C4—N3—C6	121.56 (10)	H91—C9—H93	109.7 (13)
C8—N3—C6	116.44 (10)	H92—C9—H93	109.7 (13)
O22—N21—O21	122.40 (11)	C25—C21—C22	119.48 (11)
O22—N21—C21	118.76 (10)	C25—C21—N21	120.05 (11)
O21—N21—C21	118.83 (11)	C22—C21—N21	120.45 (11)
C25—N22—C24	117.57 (11)	C23—C22—C21	118.39 (11)
C24—N23—C28	121.83 (10)	C23—C22—H22	121.9 (8)
C24—N23—C26	121.11 (11)	C21—C22—H22	119.7 (8)
C28—N23—C26	117.04 (10)	C22—C23—C24	119.18 (11)
C5—C1—C2	119.45 (11)	C22—C23—H23	120.7 (8)
C5—C1—N1	120.00 (11)	C24—C23—H23	120.1 (8)
C2—C1—N1	120.51 (11)	N23—C24—N22	116.45 (11)
C3—C2—C1	118.38 (12)	N23—C24—C23	121.68 (11)

C3—C2—H2	120.3 (8)	N22—C24—C23	121.87 (11)
C1—C2—H2	121.3 (8)	N22—C25—C21	123.42 (12)
C2—C3—C4	119.40 (11)	N22—C25—H25	118.6 (8)
C2—C3—H3	120.3 (9)	C21—C25—H25	118.0 (8)
C4—C3—H3	120.1 (9)	N23—C26—C27	112.96 (11)
N3—C4—N2	116.80 (11)	N23—C26—H261	108.2 (8)
N3—C4—C3	121.76 (11)	C27—C26—H261	111.1 (8)
N2—C4—C3	121.44 (11)	N23—C26—H262	105.5 (8)
N2—C5—C1	123.59 (11)	C27—C26—H262	113.1 (8)
N2—C5—H5	116.6 (9)	H261—C26—H262	105.5 (11)
C1—C5—H5	119.8 (9)	C26—C27—H271	109.5 (9)
N3—C6—C7	112.89 (11)	C26—C27—H272	110.2 (10)
N3—C6—H61	107.2 (8)	H271—C27—H272	105.9 (13)
C7—C6—H61	110.9 (8)	C26—C27—H273	110.5 (10)
N3—C6—H62	107.6 (8)	H271—C27—H273	113.2 (13)
C7—C6—H62	111.3 (8)	H272—C27—H273	107.5 (13)
H61—C6—H62	106.8 (12)	N23—C28—C29	112.63 (12)
C6—C7—H71	108.8 (9)	N23—C28—H281	109.7 (8)
C6—C7—H72	108.8 (9)	C29—C28—H281	111.2 (8)
H71—C7—H72	107.4 (12)	N23—C28—H282	106.0 (8)
C6—C7—H73	111.4 (9)	C29—C28—H282	111.4 (8)
H71—C7—H73	109.8 (12)	H281—C28—H282	105.6 (11)
H72—C7—H73	110.7 (12)	C28—C29—H291	110.2 (10)
N3—C8—C9	112.83 (11)	C28—C29—H292	111.5 (9)
N3—C8—H81	106.5 (8)	H291—C29—H292	108.0 (14)
C9—C8—H81	111.2 (8)	C28—C29—H293	110.7 (9)
N3—C8—H82	109.4 (7)	H291—C29—H293	108.7 (12)
C9—C8—H82	109.8 (8)	H292—C29—H293	107.6 (12)