

1,4-Di-*n*-octyl-1,2,3,4-tetrahydroquinoxaline-2,3-dione

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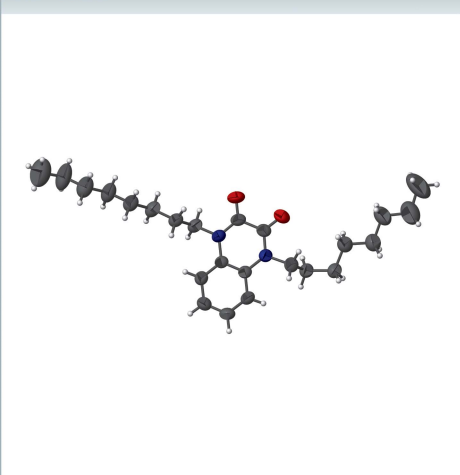
Keywords: crystal structure; π -stacking; quinoxaline.

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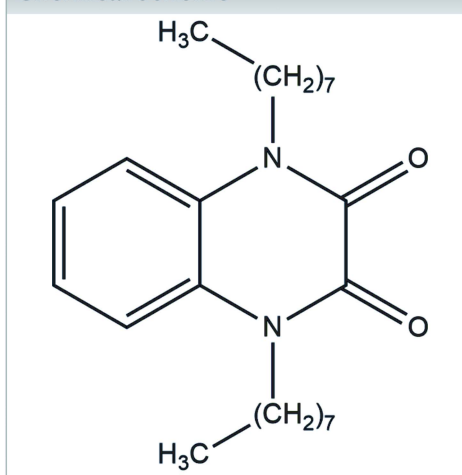
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, C₂₄H₃₈N₂O₂, the heterocyclic ring (r.m.s. = 0.015 Å) deviates from planarity to a greater extent than the benzene ring (r.m.s. deviation = 0.007 Å). In the crystal, the molecules pack to form polar and non-polar regions. The major intermolecular interaction appears to be complementary π -stacking between oppositely oriented tetrahydroquinoxaline units.

3D view



Chemical scheme



Structure description

Quinoxaline derivatives are known as antagonists for the excitatory system (Fray *et al.*, 2001), anticonvulsants, (De Sarro *et al.*, 2003) and as antibacterial and antifungal agents (Tandon *et al.*, 2006; Kotharkar & Shinde, 2006). As a continuation of our work in this area (Mustaphi *et al.*, 2001; Ferfra *et al.*, 2001), we have synthesized the new title compound and determined its crystal structure.

In the title molecule (Fig. 1), the C1–C6 ring is planar to within 0.0109 (16) Å with an r.m.s. deviation of the fitted atoms of 0.007 Å. By contrast, the maximum deviations from the N1/C7/C8/N1/C1/C2 ring are 0.0251 (16) Å (C8) and –0.0228 (15) Å (N2) with an r.m.s. deviation of 0.015 Å. As depicted in Fig. 2, the molecules pack to form polar and non-polar regions. The major intermolecular interaction appears to be complementary π -stacking between oppositely oriented tetrahydroquinoxaline units [$Cg1 \cdots Cg2^i = 3.767$ (2) Å; $Cg1$ and $Cg2$ are the centroids of the N1/C7/C8/N1/C1/C2 and C1–C6 rings, respectively; symmetry code: (i) $-x + \frac{3}{2}, -y + \frac{1}{2}, -z + 1$], which make a dihedral angle of 2.0 (1)°.

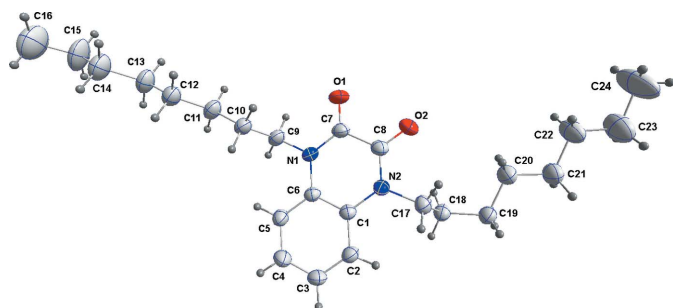


Figure 1
The title molecule with labeling scheme and 30% probability ellipsoids.

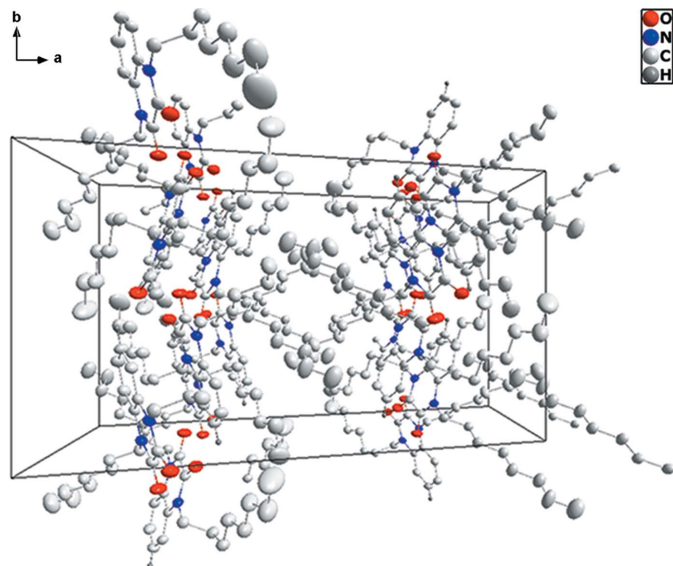


Figure 2
Packing viewed along the *c*-axis direction.

Synthesis and crystallization

A mixture of quinoxaline-2,3-dione (1 g, 6.17 mmol), K_2CO_3 (2.13 g, 15.42 mmol), octyl bromide (2.13 ml, 12.33 mmol) and tetra *n*-butylammonium bromide as a catalyst in dimethylformamide (60 ml), was stirred at room temperature for 48 h. The solution was filtered by suction and the solvent was removed under reduced pressure. The residue was chromatographed on a silica-gel column using hexane and ethyl acetate (90/10) as eluents to afford the title compound as colorless crystals upon recrystallization from ethanol solution.

Refinement

Crystal data, data collection and structure and refinement data are summarized in Table 1.

Acknowledgements

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Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{38}N_2O_2$
M_r	386.56
Crystal system, space group	Monoclinic, $C2/c$
Temperature (K)	298
a, b, c (Å)	26.407 (1), 14.3718 (5), 12.9624 (5)
β (°)	108.312 (2)
V (Å ³)	4670.3 (3)
Z	8
Radiation type	Cu $K\alpha$
μ (mm ⁻¹)	0.54
Crystal size (mm)	0.25 × 0.20 × 0.07
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (SADABS; Bruker, 2016)
T_{min}, T_{max}	0.78, 0.96
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17969, 4687, 2965
R_{int}	0.065
$(\sin \theta/\lambda)_{max}$ (Å ⁻¹)	0.626
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.072, 0.203, 1.02
No. of reflections	4687
No. of parameters	365
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³)	0.34, -0.28

Computer programs: APEX3 and SAINT (Bruker, 2016), SHELXT (Sheldrick, 2015a), SHELXL2014/7 (Sheldrick, 2015b), DIAMOND (Brandenburg & Putz, 2012) and SHELXTL (Sheldrick, 2008).

Tulane Crystallography Laboratory are gratefully acknowledged.

References

- Brandenburg, K. & Putz, H. (2012). *DIAMOND*, Crystal Impact GbR, Bonn, Germany.
- Bruker (2016). *APEX3, SAINT and SADABS*. Bruker AXS, Inc., Madison, Wisconsin, USA.
- De Sarro, G., Ferreri, G., Gareri, P., Russo, E., De Sarro, A., Gitto, R. & Chimirì, A. (2003). *Pharmacol. Biochem. Behav.* **74**, 595–602.
- Ferfra, S., Ahabchane, N. H., Mustaphi, N. E., Essassi, E. M., Bellan, J. & Pierrot, M. (2001). *Phosphorus Sulfur Silicon*, **175**, 169–181.
- Fray, M. J., Bull, D. J., Carr, C. L., Gautier, E. C. L., Mowbray, C. E. & Stobie, A. (2001). *J. Med. Chem.* **44**, 1951–1962.
- Kotharkar, S. A. & Shinde, D. B. (2006). *Bioorg. Med. Chem. Lett.* **16**, 6181–6184.
- Mustaphi, N. E., Ferfra, S., Essassi, E. M. & Pierrot, M. (2001). *Acta Cryst. E57*, o176–o177.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sheldrick, G. M. (2015a). *Acta Cryst.* **A71**, 3–8.
- Sheldrick, G. M. (2015b). *Acta Cryst.* **C71**, 3–8.
- Tandon, V. K., Yadav, D. B., Maurya, H. K., Chaturvedi, A. K. & Shukla, P. K. (2006). *Bioorg. Med. Chem.* **14**, 6120–6126.

full crystallographic data

IUCrData (2017). 2, x170520 [https://doi.org/10.1107/S241431461700520X]

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1,4-Di-*n*-octyl-1,2,3,4-tetrahydroquinoxaline-2,3-dione*Crystal data*

$C_{24}H_{38}N_2O_2$

$M_r = 386.56$

Monoclinic, $C2/c$

$a = 26.407$ (1) Å

$b = 14.3718$ (5) Å

$c = 12.9624$ (5) Å

$\beta = 108.312$ (2)°

$V = 4670.3$ (3) Å³

$Z = 8$

$F(000) = 1696$

$D_x = 1.100$ Mg m⁻³

Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å

Cell parameters from 8815 reflections

$\theta = 3.6$ – 74.6 °

$\mu = 0.54$ mm⁻¹

$T = 298$ K

Thick plate, colourless

$0.25 \times 0.20 \times 0.07$ mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS
diffractometer

Radiation source: INCOATEC I μ S micro-focus
source

Mirror monochromator

Detector resolution: 10.4167 pixels mm⁻¹

ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2016)

$T_{\min} = 0.78$, $T_{\max} = 0.96$

17969 measured reflections

4687 independent reflections

2965 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.065$

$\theta_{\max} = 74.9$ °, $\theta_{\min} = 3.6$ °

$h = -30 \rightarrow 33$

$k = -17 \rightarrow 17$

$l = -15 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.072$

$wR(F^2) = 0.203$

$S = 1.02$

4687 reflections

365 parameters

0 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

$w = 1/[\sigma^2(F_o^2) + (0.0811P)^2 + 3.6894P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.34$ e Å⁻³

$\Delta\rho_{\min} = -0.28$ 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. 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. Because of the significant librational motions of the last two carbon atoms of the octyl chains, it was not possible to locate the associated hydrogen atoms with confidence. These were included as riding contributions in idealized positions.

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	0.74116 (9)	0.54364 (12)	0.59734 (18)	0.0900 (7)
O2	0.77845 (9)	0.45664 (13)	0.79053 (15)	0.0833 (6)
N1	0.70490 (8)	0.40936 (13)	0.51553 (16)	0.0557 (5)
N2	0.73887 (8)	0.32196 (12)	0.71746 (14)	0.0532 (5)
C1	0.71139 (9)	0.26985 (14)	0.62490 (18)	0.0492 (5)
C2	0.70215 (10)	0.17526 (17)	0.6314 (2)	0.0595 (6)
H2	0.7170 (10)	0.1495 (16)	0.697 (2)	0.056 (7)*
C3	0.67539 (12)	0.12529 (18)	0.5395 (2)	0.0708 (8)
H3	0.6691 (10)	0.062 (2)	0.545 (2)	0.076 (8)*
C4	0.65768 (12)	0.16928 (19)	0.4408 (3)	0.0728 (8)
H4	0.6376 (12)	0.138 (2)	0.380 (3)	0.089 (10)*
C5	0.66673 (11)	0.26283 (17)	0.4326 (2)	0.0621 (7)
H5	0.6520 (10)	0.2918 (18)	0.365 (2)	0.067 (8)*
C6	0.69430 (9)	0.31416 (15)	0.52398 (18)	0.0503 (5)
C7	0.73204 (10)	0.46110 (16)	0.6031 (2)	0.0626 (7)
C8	0.75199 (10)	0.41277 (16)	0.7119 (2)	0.0604 (6)
C9	0.69058 (11)	0.4552 (2)	0.4085 (2)	0.0644 (7)
H9A	0.7150 (11)	0.507 (2)	0.419 (2)	0.079 (8)*
H9B	0.6974 (10)	0.4120 (19)	0.356 (2)	0.070 (8)*
C10	0.63381 (11)	0.48941 (19)	0.3665 (2)	0.0619 (7)
H10A	0.6284 (10)	0.5282 (18)	0.422 (2)	0.064 (7)*
H10B	0.6084 (10)	0.4385 (19)	0.360 (2)	0.069 (7)*
C11	0.62461 (12)	0.5370 (2)	0.2581 (3)	0.0745 (8)
H11A	0.6500 (13)	0.589 (2)	0.269 (2)	0.099 (10)*
H11B	0.6350 (15)	0.492 (3)	0.203 (3)	0.121 (12)*
C12	0.56892 (13)	0.5723 (2)	0.2037 (3)	0.0769 (8)
H12A	0.5564 (13)	0.612 (2)	0.255 (3)	0.105 (11)*
H12B	0.5409 (13)	0.523 (2)	0.194 (2)	0.096 (10)*
C13	0.56333 (15)	0.6179 (3)	0.0948 (3)	0.0942 (11)
H13A	0.5897 (17)	0.668 (3)	0.112 (3)	0.136 (16)*
H13B	0.5719 (16)	0.566 (3)	0.044 (3)	0.143 (16)*
C14	0.50903 (18)	0.6512 (3)	0.0323 (3)	0.1102 (13)
H14B	0.4791 (18)	0.598 (3)	0.030 (3)	0.157 (17)*
H14A	0.4975 (10)	0.6937 (18)	0.085 (2)	0.063 (7)*
C15	0.50677 (19)	0.6956 (4)	-0.0776 (4)	0.1469 (19)
H15A	0.5305	0.7506	-0.0632	0.176*
H15B	0.5211	0.6503	-0.1190	0.176*
C16	0.4567 (2)	0.7227 (5)	-0.1415 (4)	0.177 (2)

H16A	0.4590	0.7499	-0.2092	0.266*
H16B	0.4330	0.6684	-0.1583	0.266*
H16C	0.4424	0.7690	-0.1025	0.266*
C17	0.75789 (12)	0.2801 (2)	0.8271 (2)	0.0619 (7)
H17A	0.7569 (10)	0.327 (2)	0.873 (2)	0.071 (8)*
H17B	0.7347 (11)	0.2350 (19)	0.827 (2)	0.069 (8)*
C18	0.81408 (12)	0.2432 (2)	0.8558 (2)	0.0640 (7)
H18A	0.8340 (11)	0.285 (2)	0.827 (2)	0.081 (9)*
H18B	0.8127 (10)	0.1829 (19)	0.819 (2)	0.064 (7)*
C19	0.84036 (14)	0.2334 (2)	0.9775 (2)	0.0696 (7)
H19A	0.8744 (11)	0.195 (2)	0.990 (2)	0.077 (8)*
H19B	0.8182 (12)	0.201 (2)	1.009 (2)	0.086 (10)*
C20	0.85371 (18)	0.3267 (2)	1.0348 (3)	0.0858 (9)
H20B	0.8221 (13)	0.361 (2)	1.027 (2)	0.089 (10)*
H20A	0.8800 (15)	0.362 (2)	1.013 (3)	0.113 (13)*
C21	0.88719 (16)	0.3219 (3)	1.1508 (3)	0.0897 (10)
H21B	0.8680 (13)	0.276 (2)	1.190 (3)	0.099 (10)*
H21A	0.9239 (16)	0.288 (3)	1.155 (3)	0.134 (14)*
C22	0.8982 (2)	0.4168 (3)	1.2046 (4)	0.1124 (14)
H22A	0.9188 (14)	0.453 (3)	1.168 (3)	0.102 (13)*
H22B	0.8648 (17)	0.445 (3)	1.199 (3)	0.136 (16)*
C23	0.9322 (2)	0.4163 (4)	1.3191 (4)	0.1512 (19)
H23A	0.9674	0.3896	1.3240	0.181*
H23B	0.9157	0.3762	1.3618	0.181*
C24	0.9397 (3)	0.5124 (5)	1.3667 (5)	0.233 (4)
H24A	0.9624	0.5095	1.4426	0.349*
H24B	0.9566	0.5520	1.3254	0.349*
H24C	0.9049	0.5386	1.3631	0.349*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1099 (17)	0.0429 (10)	0.1054 (16)	-0.0037 (9)	0.0169 (13)	0.0042 (9)
O2	0.1063 (16)	0.0604 (11)	0.0740 (13)	-0.0030 (10)	0.0151 (11)	-0.0195 (10)
N1	0.0601 (12)	0.0460 (10)	0.0617 (12)	0.0050 (8)	0.0200 (10)	0.0052 (9)
N2	0.0612 (12)	0.0481 (10)	0.0517 (11)	0.0075 (8)	0.0199 (10)	-0.0027 (8)
C1	0.0497 (12)	0.0458 (11)	0.0546 (13)	0.0056 (9)	0.0198 (11)	-0.0015 (10)
C2	0.0661 (16)	0.0495 (13)	0.0618 (16)	0.0061 (11)	0.0185 (13)	0.0081 (12)
C3	0.0801 (19)	0.0443 (13)	0.0819 (19)	-0.0054 (12)	0.0168 (15)	-0.0018 (13)
C4	0.081 (2)	0.0570 (15)	0.0701 (18)	-0.0004 (13)	0.0087 (16)	-0.0105 (14)
C5	0.0685 (16)	0.0571 (14)	0.0566 (15)	0.0097 (12)	0.0139 (13)	0.0004 (12)
C6	0.0515 (13)	0.0448 (11)	0.0568 (14)	0.0062 (9)	0.0199 (11)	-0.0008 (10)
C7	0.0680 (16)	0.0432 (12)	0.0752 (17)	0.0056 (11)	0.0208 (14)	-0.0004 (12)
C8	0.0656 (16)	0.0497 (13)	0.0654 (16)	0.0062 (11)	0.0200 (13)	-0.0092 (12)
C9	0.0667 (17)	0.0571 (14)	0.0695 (17)	0.0029 (12)	0.0215 (14)	0.0145 (13)
C10	0.0627 (16)	0.0545 (14)	0.0685 (17)	0.0045 (12)	0.0204 (14)	0.0072 (12)
C11	0.0706 (19)	0.0750 (18)	0.0780 (19)	0.0070 (15)	0.0235 (16)	0.0205 (15)
C12	0.0704 (19)	0.0771 (19)	0.080 (2)	0.0067 (15)	0.0189 (16)	0.0140 (16)

C13	0.083 (2)	0.109 (3)	0.083 (2)	0.014 (2)	0.0160 (19)	0.029 (2)
C14	0.098 (3)	0.127 (3)	0.098 (3)	0.022 (3)	0.021 (2)	0.026 (2)
C15	0.113 (3)	0.205 (5)	0.107 (3)	0.038 (3)	0.011 (3)	0.058 (3)
C16	0.163 (5)	0.228 (7)	0.139 (4)	0.051 (5)	0.044 (4)	0.034 (4)
C17	0.0705 (18)	0.0654 (16)	0.0525 (15)	0.0023 (13)	0.0234 (13)	-0.0026 (13)
C18	0.0739 (18)	0.0602 (15)	0.0580 (16)	0.0107 (13)	0.0210 (14)	0.0002 (13)
C19	0.080 (2)	0.0648 (16)	0.0616 (17)	0.0072 (15)	0.0191 (15)	0.0048 (13)
C20	0.099 (3)	0.076 (2)	0.074 (2)	0.0035 (19)	0.0147 (19)	-0.0045 (16)
C21	0.093 (2)	0.091 (2)	0.076 (2)	0.0020 (19)	0.0146 (19)	-0.0038 (18)
C22	0.107 (3)	0.109 (3)	0.102 (3)	0.002 (3)	0.006 (3)	-0.032 (2)
C23	0.138 (4)	0.164 (5)	0.127 (4)	0.012 (3)	0.007 (3)	-0.034 (3)
C24	0.242 (8)	0.192 (6)	0.202 (6)	0.013 (5)	-0.021 (6)	-0.111 (5)

Geometric parameters (Å, °)

O1—C7	1.217 (3)	C14—C15	1.545 (6)
O2—C8	1.215 (3)	C14—H14B	1.10 (5)
N1—C7	1.358 (3)	C14—H14A	1.03 (3)
N1—C6	1.408 (3)	C15—C16	1.378 (6)
N1—C9	1.474 (3)	C15—H15A	0.9900
N2—C8	1.358 (3)	C15—H15B	0.9900
N2—C1	1.407 (3)	C16—H16A	0.9800
N2—C17	1.478 (3)	C16—H16B	0.9800
C1—C2	1.388 (3)	C16—H16C	0.9800
C1—C6	1.396 (3)	C17—C18	1.508 (4)
C2—C3	1.380 (4)	C17—H17A	0.91 (3)
C2—H2	0.90 (2)	C17—H17B	0.89 (3)
C3—C4	1.371 (4)	C18—C19	1.518 (4)
C3—H3	0.93 (3)	C18—H18A	0.95 (3)
C4—C5	1.376 (4)	C18—H18B	0.98 (3)
C4—H4	0.91 (3)	C19—C20	1.519 (4)
C5—C6	1.391 (3)	C19—H19A	1.03 (3)
C5—H5	0.94 (3)	C19—H19B	0.94 (3)
C7—C8	1.511 (4)	C20—C21	1.488 (5)
C9—C10	1.507 (4)	C20—H20B	0.95 (3)
C9—H9A	0.97 (3)	C20—H20A	0.97 (4)
C9—H9B	0.98 (3)	C21—C22	1.518 (5)
C10—C11	1.512 (4)	C21—H21B	1.05 (3)
C10—H10A	0.96 (3)	C21—H21A	1.07 (4)
C10—H10B	0.98 (3)	C22—C23	1.473 (6)
C11—C12	1.505 (4)	C22—H22A	0.98 (3)
C11—H11A	0.98 (3)	C22—H22B	0.96 (4)
C11—H11B	1.06 (4)	C23—C24	1.500 (7)
C12—C13	1.520 (4)	C23—H23A	0.9900
C12—H12A	1.01 (3)	C23—H23B	0.9900
C12—H12B	1.01 (3)	C24—H24A	0.9800
C13—C14	1.487 (5)	C24—H24B	0.9800
C13—H13A	0.98 (4)	C24—H24C	0.9800

C13—H13B	1.06 (4)		
C7—N1—C6	122.2 (2)	C13—C14—H14A	105.3 (15)
C7—N1—C9	117.0 (2)	C15—C14—H14A	115.7 (15)
C6—N1—C9	120.6 (2)	H14B—C14—H14A	94 (3)
C8—N2—C1	122.6 (2)	C16—C15—C14	115.0 (4)
C8—N2—C17	115.3 (2)	C16—C15—H15A	108.5
C1—N2—C17	122.1 (2)	C14—C15—H15A	108.5
C2—C1—C6	119.5 (2)	C16—C15—H15B	108.5
C2—C1—N2	121.5 (2)	C14—C15—H15B	108.5
C6—C1—N2	119.0 (2)	H15A—C15—H15B	107.5
C3—C2—C1	120.6 (3)	C15—C16—H16A	109.5
C3—C2—H2	123.8 (15)	C15—C16—H16B	109.5
C1—C2—H2	115.3 (15)	H16A—C16—H16B	109.5
C4—C3—C2	119.8 (3)	C15—C16—H16C	109.5
C4—C3—H3	120.0 (17)	H16A—C16—H16C	109.5
C2—C3—H3	120.2 (17)	H16B—C16—H16C	109.5
C3—C4—C5	120.4 (3)	N2—C17—C18	113.0 (2)
C3—C4—H4	121.1 (19)	N2—C17—H17A	105.4 (17)
C5—C4—H4	118.4 (19)	C18—C17—H17A	109.1 (17)
C4—C5—C6	120.7 (3)	N2—C17—H17B	105.8 (17)
C4—C5—H5	118.4 (16)	C18—C17—H17B	111.4 (18)
C6—C5—H5	120.8 (16)	H17A—C17—H17B	112 (2)
C5—C6—C1	119.0 (2)	C17—C18—C19	112.5 (2)
C5—C6—N1	120.9 (2)	C17—C18—H18A	107.5 (17)
C1—C6—N1	120.2 (2)	C19—C18—H18A	109.9 (17)
O1—C7—N1	123.1 (2)	C17—C18—H18B	107.8 (15)
O1—C7—C8	119.2 (2)	C19—C18—H18B	111.0 (14)
N1—C7—C8	117.8 (2)	H18A—C18—H18B	108 (2)
O2—C8—N2	122.9 (2)	C18—C19—C20	112.8 (2)
O2—C8—C7	119.0 (2)	C18—C19—H19A	107.6 (15)
N2—C8—C7	118.1 (2)	C20—C19—H19A	110.4 (16)
N1—C9—C10	114.7 (2)	C18—C19—H19B	110.5 (18)
N1—C9—H9A	104.7 (17)	C20—C19—H19B	108.4 (18)
C10—C9—H9A	110.1 (16)	H19A—C19—H19B	107 (2)
N1—C9—H9B	108.5 (15)	C21—C20—C19	115.2 (3)
C10—C9—H9B	109.7 (15)	C21—C20—H20B	111.0 (19)
H9A—C9—H9B	109 (2)	C19—C20—H20B	110.3 (19)
C9—C10—C11	109.6 (2)	C21—C20—H20A	94 (2)
C9—C10—H10A	106.5 (15)	C19—C20—H20A	113 (2)
C11—C10—H10A	114.7 (15)	H20B—C20—H20A	112 (3)
C9—C10—H10B	111.3 (15)	C20—C21—C22	112.9 (3)
C11—C10—H10B	110.9 (15)	C20—C21—H21B	107.0 (18)
H10A—C10—H10B	104 (2)	C22—C21—H21B	113.2 (18)
C12—C11—C10	115.9 (3)	C20—C21—H21A	108 (2)
C12—C11—H11A	109.4 (19)	C22—C21—H21A	110 (2)
C10—C11—H11A	108.2 (19)	H21B—C21—H21A	105 (3)
C12—C11—H11B	108 (2)	C23—C22—C21	115.2 (4)

C10—C11—H11B	110 (2)	C23—C22—H22A	104 (2)
H11A—C11—H11B	104 (3)	C21—C22—H22A	108 (2)
C11—C12—C13	112.1 (3)	C23—C22—H22B	109 (3)
C11—C12—H12A	111.0 (19)	C21—C22—H22B	108 (3)
C13—C12—H12A	114.1 (19)	H22A—C22—H22B	112 (4)
C11—C12—H12B	113.0 (18)	C22—C23—C24	111.7 (5)
C13—C12—H12B	109.6 (18)	C22—C23—H23A	109.3
H12A—C12—H12B	96 (3)	C24—C23—H23A	109.3
C14—C13—C12	116.1 (3)	C22—C23—H23B	109.3
C14—C13—H13A	112 (3)	C24—C23—H23B	109.3
C12—C13—H13A	105 (2)	H23A—C23—H23B	107.9
C14—C13—H13B	104 (2)	C23—C24—H24A	109.5
C12—C13—H13B	107 (2)	C23—C24—H24B	109.5
H13A—C13—H13B	113 (3)	H24A—C24—H24B	109.5
C13—C14—C15	112.7 (4)	C23—C24—H24C	109.5
C13—C14—H14B	111 (2)	H24A—C24—H24C	109.5
C15—C14—H14B	117 (2)	H24B—C24—H24C	109.5
C8—N2—C1—C2	174.8 (2)	C17—N2—C8—O2	1.5 (4)
C17—N2—C1—C2	-2.0 (3)	C1—N2—C8—C7	5.3 (3)
C8—N2—C1—C6	-3.6 (3)	C17—N2—C8—C7	-177.7 (2)
C17—N2—C1—C6	179.6 (2)	O1—C7—C8—O2	-2.8 (4)
C6—C1—C2—C3	-1.3 (4)	N1—C7—C8—O2	176.7 (2)
N2—C1—C2—C3	-179.6 (2)	O1—C7—C8—N2	176.5 (2)
C1—C2—C3—C4	0.0 (4)	N1—C7—C8—N2	-4.0 (3)
C2—C3—C4—C5	0.4 (5)	C7—N1—C9—C10	-99.8 (3)
C3—C4—C5—C6	0.5 (4)	C6—N1—C9—C10	85.0 (3)
C4—C5—C6—C1	-1.8 (4)	N1—C9—C10—C11	178.6 (3)
C4—C5—C6—N1	178.3 (2)	C9—C10—C11—C12	178.1 (3)
C2—C1—C6—C5	2.1 (3)	C10—C11—C12—C13	-179.3 (3)
N2—C1—C6—C5	-179.5 (2)	C11—C12—C13—C14	177.3 (4)
C2—C1—C6—N1	-177.9 (2)	C12—C13—C14—C15	-179.4 (4)
N2—C1—C6—N1	0.5 (3)	C13—C14—C15—C16	176.4 (5)
C7—N1—C6—C5	-179.5 (2)	C8—N2—C17—C18	-85.7 (3)
C9—N1—C6—C5	-4.6 (3)	C1—N2—C17—C18	91.4 (3)
C7—N1—C6—C1	0.6 (3)	N2—C17—C18—C19	159.0 (2)
C9—N1—C6—C1	175.5 (2)	C17—C18—C19—C20	-70.9 (4)
C6—N1—C7—O1	-179.4 (2)	C18—C19—C20—C21	-170.6 (3)
C9—N1—C7—O1	5.5 (4)	C19—C20—C21—C22	-178.7 (4)
C6—N1—C7—C8	1.2 (3)	C20—C21—C22—C23	-178.7 (4)
C9—N1—C7—C8	-173.9 (2)	C21—C22—C23—C24	-178.3 (5)
C1—N2—C8—O2	-175.5 (2)		
