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4-[2-(Dibenzylaminomethyl)-1*H*-benzimidazol-1-ylmethyl]benzonitrile

Guang-Ju Ping, Ying-Ying Liu, Ting-Ting Han and Jian-Fang Ma*

Department of Chemistry, Northeast Normal University, Changchun 130024, People's Republic of China
Correspondence e-mail: majf247nenu@yahoo.com.cn

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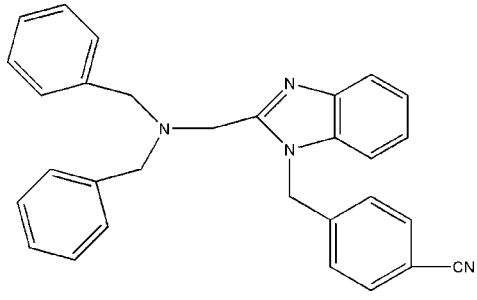
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.120; data-to-parameter ratio = 19.7.

The molecule of the title compound, $C_{30}H_{26}N_4$, is non-planar. The dihedral angles between the two benzene rings of the benzyl groups, and between the benzimidazole and 4-(methyl)benzonitrile ring systems, are 117.9 (2) and 70.3 (3)°, respectively. The bond distances and angles are all in normal ranges.

Related literature

For related literature, see: Spasov *et al.* (1999); Keeffe *et al.* (2000); Feng & Xu (2001); Ferey (2001); Pandiyan *et al.* (1997); Barros-García *et al.* (2005); Maldonado-Rogado *et al.*(2007).



Experimental

Crystal data

$C_{30}H_{26}N_4$
M_r = 442.55
Orthorhombic, *Pbca*
a = 15.364 (1) Å
b = 17.006 (1) Å
c = 18.908 (1) Å
V = 4940.3 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 293 (2) K
0.46 × 0.34 × 0.21 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.971, T_{max} = 0.985
28803 measured reflections
6054 independent reflections
4045 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.120
S = 1.01
6054 reflections
308 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2213).

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supplementary materials

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4-[2-(Dibenzylaminomethyl)-1*H*-benzimidazol-1-ylmethyl]benzonitrile

G.-J. Ping, Y.-Y. Liu, T.-T. Han and J.-F. Ma

Comment

For many years there has been extensive research on the reactions of benzimidazole derivatives with transition metals, as models of some important biological molecules, due to their varied pharmacological activities (Spasov *et al.*, 1999; Keeffe *et al.*, 2000; Feng & Xu, 2001; Ferey, 2001). To further widen the scope of research on the coordination chemistry of benzimidazole derivatives, there is a need to prepare a new series of benzimidazole derivatives. In this paper, the structure of the title compound is described.

As shown in Fig. 1, the molecular skeleton is non-planar. The dihedral angles between the two benzene rings of the benzyl groups, and between the benzimidazole and 4-(methyl)benzonitrile ring systems are 117.9 (2) and 70.3 (3)°, respectively. The bond distances and bond angles are all in normal ranges (Pandiyan *et al.*, 1997; Barros-García *et al.*, 2005; Maldonado-Rogado *et al.*, 2007).

Experimental

A mixture of *N*,*N*-dibenzylglycine (10.2 g, 40 mmol) and *o*-phenylenediamine (4.32 g, 40 mmol) in ethanediol (70 ml) was heated to reflux for 16 h. The mixture was cooled to room temperature, added to hot water and stirred continuously until brown solids were obtained and then filtered. The solid was purified by recrystallization from an ethanol–water solution (1:1 *v*/*v*) to yield *L* (where *L* is (1*H*-benzo[*d*]imidazol-2-yl)-*N*,*N*-dibenzylmethanamine). Sodium hydroxide (1.2 g) was added to a DMF solution (15 ml) of *L* (9.39 g, 30 mmol). The mixture was stirred at room temperature for 2 h in air. 4-(Chloromethyl)benzonitrile (4.55 g, 30 mmol) was then added and the mixture stirred for 1 d. After evaporation of DMF, the mixture was added to hot water. The brown solids obtained were filtered and dried in air. Colorless crystals suitable for X-ray diffraction study were obtained by slow evaporation of an ethanol solution.

Refinement

All H atoms were positioned geometrically, with C—H = 0.93–0.97 Å, and refined using a riding model with U_{iso}(H) = 1.2U_{eq}(C).

Figures

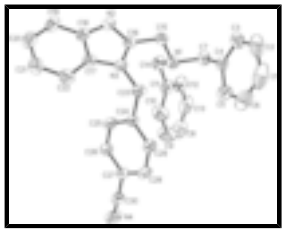


Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. The H atoms have been omitted for clarity.

4-[2-(Dibenzylaminomethyl)-1*H*-benzimidazol-1-ylmethyl]benzonitrile

Crystal data

$C_{30}H_{26}N_4$	F_{000} = 1872
M_r = 442.55	D_x = 1.190 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71069 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 4045 reflections
a = 15.364 (1) Å	θ = 2.1–28.4º
b = 17.006 (1) Å	μ = 0.07 mm^{-1}
c = 18.908 (1) Å	*T* = 293 (2) K
V = 4940.3 (4) Å^3	Block, colourless
Z = 8	0.46 × 0.34 × 0.21 mm

Data collection

Bruker APEX CCD area-detector diffractometer	6054 independent reflections
Radiation source: fine-focus sealed tube	4045 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
T = 293(2) K	θ_{max} = 28.4º
ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −20→18
T_{min} = 0.971, T_{max} = 0.985	*k* = −22→21
28803 measured reflections	*l* = −24→23

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.040	$w = 1/[\sigma^2(F_o^2) + (0.0524P)^2 + 0.5735P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.120	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.01	$\Delta\rho_{max}$ = 0.13 e Å^{-3}
6054 reflections	$\Delta\rho_{min}$ = −0.16 e Å^{-3}
308 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0020 (4)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	−0.08980 (14)	0.47828 (12)	0.62575 (17)	0.1197 (9)
H1	−0.0840	0.5327	0.6250	0.144*
C2	−0.11047 (13)	0.44125 (12)	0.68656 (14)	0.1054 (7)
H2	−0.1173	0.4702	0.7279	0.126*
C3	−0.12144 (10)	0.36140 (9)	0.68776 (8)	0.0747 (4)
H3	−0.1369	0.3368	0.7299	0.090*
C4	−0.10992 (8)	0.31674 (8)	0.62744 (7)	0.0554 (3)
C5	−0.08677 (10)	0.35415 (10)	0.56584 (9)	0.0762 (4)
H5	−0.0775	0.3250	0.5249	0.091*
C6	−0.07719 (13)	0.43496 (13)	0.56432 (14)	0.1084 (7)
H6	−0.0624	0.4602	0.5224	0.130*
C7	−0.12267 (8)	0.22928 (8)	0.62758 (7)	0.0610 (3)
H7A	−0.1489	0.2135	0.6721	0.073*
H7B	−0.1624	0.2150	0.5899	0.073*
C8	−0.17796 (16)	0.06684 (12)	0.40156 (13)	0.1079 (7)
H8	−0.2038	0.0587	0.3577	0.129*
C9	−0.09697 (15)	0.09825 (15)	0.40578 (10)	0.1165 (7)
H9	−0.0673	0.1118	0.3647	0.140*
C10	−0.05855 (12)	0.11010 (13)	0.47080 (9)	0.0982 (6)
H10	−0.0030	0.1316	0.4728	0.118*
C11	−0.10049 (9)	0.09085 (8)	0.53285 (8)	0.0658 (4)
C12	−0.18332 (11)	0.05982 (8)	0.52768 (10)	0.0815 (5)
H12	−0.2140	0.0472	0.5685	0.098*
C13	−0.22112 (13)	0.04736 (10)	0.46157 (14)	0.1022 (7)
H13	−0.2765	0.0255	0.4586	0.123*
C14	−0.05651 (10)	0.10309 (8)	0.60316 (8)	0.0672 (4)
H14A	−0.0929	0.0814	0.6403	0.081*
H14B	−0.0016	0.0749	0.6035	0.081*
C15	0.01235 (8)	0.19572 (8)	0.68250 (6)	0.0548 (3)
H15A	−0.0154	0.1664	0.7203	0.066*
H15B	0.0124	0.2507	0.6960	0.066*
C16	0.10411 (7)	0.16876 (7)	0.67610 (5)	0.0472 (3)
C17	0.24253 (8)	0.16810 (8)	0.64567 (6)	0.0537 (3)

C18	0.22577 (8)	0.11201 (7)	0.69749 (6)	0.0528 (3)
C19	0.29279 (10)	0.06283 (9)	0.72069 (7)	0.0689 (4)
H19	0.2830	0.0248	0.7551	0.083*
C20	0.37359 (10)	0.07248 (11)	0.69101 (9)	0.0821 (5)
H20	0.4188	0.0394	0.7047	0.099*
C21	0.38938 (10)	0.13020 (12)	0.64117 (9)	0.0872 (5)
H21	0.4454	0.1360	0.6234	0.105*
C22	0.32479 (10)	0.17923 (11)	0.61709 (8)	0.0754 (4)
H22	0.3356	0.2179	0.5834	0.090*
C23	0.14828 (9)	0.26609 (7)	0.58130 (6)	0.0560 (3)
H23A	0.1924	0.3063	0.5879	0.067*
H23B	0.0921	0.2898	0.5911	0.067*
C24	0.14997 (7)	0.23942 (7)	0.50493 (6)	0.0489 (3)
C25	0.16991 (9)	0.16342 (8)	0.48514 (6)	0.0601 (3)
H25	0.1829	0.1263	0.5197	0.072*
C26	0.17090 (9)	0.14185 (8)	0.41474 (6)	0.0635 (3)
H26	0.1849	0.0905	0.4021	0.076*
C27	0.15110 (8)	0.19628 (8)	0.36307 (6)	0.0580 (3)
C28	0.13195 (10)	0.27277 (9)	0.38191 (7)	0.0663 (4)
H28	0.1194	0.3099	0.3473	0.080*
C29	0.13160 (9)	0.29372 (8)	0.45235 (6)	0.0606 (3)
H29	0.1188	0.3453	0.4648	0.073*
C30	0.15169 (10)	0.17137 (10)	0.29035 (7)	0.0736 (4)
N1	−0.04017 (7)	0.18681 (6)	0.61800 (5)	0.0527 (2)
N2	0.13861 (7)	0.11413 (6)	0.71633 (5)	0.0536 (3)
N3	0.16329 (6)	0.20334 (6)	0.63191 (5)	0.0504 (2)
N4	0.15204 (12)	0.14906 (10)	0.23346 (7)	0.1052 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0947 (14)	0.0548 (10)	0.210 (3)	0.0029 (10)	−0.0439 (16)	−0.0018 (15)
C2	0.0931 (13)	0.0756 (12)	0.1474 (19)	0.0199 (10)	−0.0303 (13)	−0.0472 (13)
C3	0.0694 (9)	0.0785 (10)	0.0762 (9)	0.0104 (7)	−0.0056 (7)	−0.0214 (8)
C4	0.0467 (6)	0.0582 (7)	0.0614 (7)	0.0042 (5)	−0.0076 (5)	−0.0073 (6)
C5	0.0748 (9)	0.0791 (10)	0.0747 (9)	0.0014 (8)	−0.0051 (7)	0.0069 (8)
C6	0.0946 (13)	0.0875 (14)	0.1432 (19)	−0.0084 (11)	−0.0132 (12)	0.0443 (13)
C7	0.0522 (7)	0.0614 (8)	0.0694 (8)	−0.0022 (6)	−0.0032 (6)	−0.0063 (6)
C8	0.1210 (17)	0.0899 (13)	0.1127 (15)	0.0133 (12)	−0.0526 (14)	−0.0422 (12)
C9	0.1190 (17)	0.155 (2)	0.0754 (11)	−0.0052 (14)	−0.0177 (11)	−0.0345 (12)
C10	0.0801 (11)	0.1364 (17)	0.0782 (11)	−0.0152 (10)	−0.0102 (9)	−0.0273 (11)
C11	0.0706 (8)	0.0475 (7)	0.0793 (9)	0.0028 (6)	−0.0175 (7)	−0.0124 (6)
C12	0.0803 (10)	0.0516 (8)	0.1125 (13)	−0.0067 (7)	−0.0212 (9)	0.0014 (8)
C13	0.0876 (12)	0.0633 (10)	0.1558 (19)	−0.0059 (9)	−0.0520 (13)	−0.0170 (11)
C14	0.0773 (9)	0.0517 (7)	0.0726 (9)	−0.0001 (6)	−0.0143 (7)	−0.0022 (6)
C15	0.0574 (7)	0.0642 (7)	0.0429 (6)	−0.0006 (6)	−0.0003 (5)	−0.0019 (5)
C16	0.0568 (6)	0.0494 (6)	0.0354 (5)	−0.0047 (5)	−0.0034 (5)	−0.0002 (4)
C17	0.0566 (7)	0.0633 (7)	0.0412 (5)	−0.0009 (6)	−0.0036 (5)	−0.0030 (5)

C18	0.0605 (7)	0.0549 (7)	0.0429 (6)	−0.0009 (5)	−0.0124 (5)	−0.0037 (5)
C19	0.0745 (9)	0.0676 (8)	0.0647 (8)	0.0057 (7)	−0.0247 (7)	−0.0001 (6)
C20	0.0673 (9)	0.1006 (12)	0.0786 (10)	0.0198 (8)	−0.0242 (8)	−0.0130 (9)
C21	0.0541 (8)	0.1271 (15)	0.0804 (10)	0.0065 (9)	−0.0028 (7)	−0.0091 (10)
C22	0.0619 (8)	0.1020 (12)	0.0622 (8)	−0.0049 (8)	0.0044 (6)	0.0049 (8)
C23	0.0727 (8)	0.0505 (7)	0.0448 (6)	−0.0016 (6)	0.0007 (5)	0.0078 (5)
C24	0.0505 (6)	0.0530 (7)	0.0432 (6)	−0.0011 (5)	0.0019 (5)	0.0089 (5)
C25	0.0802 (9)	0.0547 (7)	0.0455 (6)	0.0085 (6)	−0.0031 (6)	0.0119 (5)
C26	0.0827 (9)	0.0584 (8)	0.0494 (7)	0.0141 (7)	0.0002 (6)	0.0038 (6)
C27	0.0605 (7)	0.0709 (8)	0.0426 (6)	0.0110 (6)	0.0019 (5)	0.0084 (5)
C28	0.0843 (9)	0.0670 (9)	0.0477 (7)	0.0148 (7)	−0.0026 (6)	0.0167 (6)
C29	0.0767 (8)	0.0534 (7)	0.0518 (7)	0.0091 (6)	0.0002 (6)	0.0090 (5)
C30	0.0925 (11)	0.0825 (10)	0.0457 (7)	0.0264 (8)	−0.0012 (7)	0.0088 (7)
N1	0.0551 (6)	0.0512 (6)	0.0520 (5)	0.0011 (4)	−0.0081 (4)	−0.0055 (4)
N2	0.0627 (6)	0.0553 (6)	0.0429 (5)	−0.0051 (5)	−0.0079 (4)	0.0071 (4)
N3	0.0575 (6)	0.0545 (6)	0.0391 (5)	0.0007 (4)	−0.0004 (4)	0.0060 (4)
N4	0.1612 (15)	0.1052 (11)	0.0493 (7)	0.0442 (10)	−0.0050 (8)	0.0015 (7)

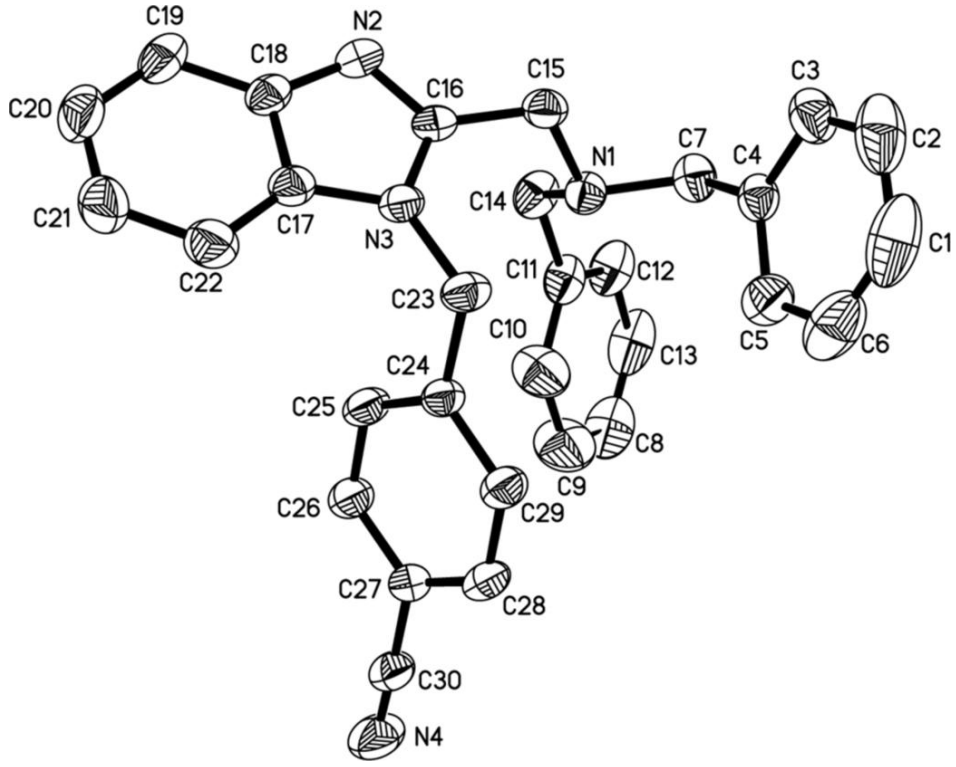
Geometric parameters (Å, °)

C1—C2	1.349 (3)	C15—H15A	0.9700
C1—C6	1.389 (3)	C15—H15B	0.9700
C1—H1	0.9300	C16—N2	1.3124 (14)
C2—C3	1.368 (3)	C16—N3	1.3678 (14)
C2—H2	0.9300	C17—N3	1.3817 (15)
C3—C4	1.3817 (18)	C17—C22	1.3874 (19)
C3—H3	0.9300	C17—C18	1.3916 (17)
C4—C5	1.374 (2)	C18—N2	1.3862 (16)
C4—C7	1.5003 (18)	C18—C19	1.3972 (18)
C5—C6	1.382 (3)	C19—C20	1.372 (2)
C5—H5	0.9300	C19—H19	0.9300
C6—H6	0.9300	C20—C21	1.382 (2)
C7—N1	1.4700 (16)	C20—H20	0.9300
C7—H7A	0.9700	C21—C22	1.374 (2)
C7—H7B	0.9700	C21—H21	0.9300
C8—C13	1.355 (3)	C22—H22	0.9300
C8—C9	1.356 (3)	C23—N3	1.4517 (15)
C8—H8	0.9300	C23—C24	1.5138 (16)
C9—C10	1.378 (2)	C23—H23A	0.9700
C9—H9	0.9300	C23—H23B	0.9700
C10—C11	1.378 (2)	C24—C25	1.3799 (17)
C10—H10	0.9300	C24—C29	1.3860 (16)
C11—C12	1.381 (2)	C25—C26	1.3808 (17)
C11—C14	1.5058 (19)	C25—H25	0.9300
C12—C13	1.395 (3)	C26—C27	1.3797 (17)
C12—H12	0.9300	C26—H26	0.9300
C13—H13	0.9300	C27—C28	1.381 (2)
C14—N1	1.4727 (16)	C27—C30	1.4388 (18)
C14—H14A	0.9700	C28—C29	1.3788 (18)

C14—H14B	0.9700	C28—H28	0.9300
C15—N1	1.4703 (14)	C29—H29	0.9300
C15—C16	1.4874 (17)	C30—N4	1.1406 (18)
C2—C1—C6	119.87 (19)	N2—C16—N3	112.95 (10)
C2—C1—H1	120.1	N2—C16—C15	123.63 (10)
C6—C1—H1	120.1	N3—C16—C15	123.18 (10)
C1—C2—C3	120.42 (19)	N3—C17—C22	132.08 (12)
C1—C2—H2	119.8	N3—C17—C18	105.48 (10)
C3—C2—H2	119.8	C22—C17—C18	122.43 (12)
C2—C3—C4	121.06 (18)	N2—C18—C17	109.99 (10)
C2—C3—H3	119.5	N2—C18—C19	130.31 (12)
C4—C3—H3	119.5	C17—C18—C19	119.67 (12)
C5—C4—C3	118.58 (14)	C20—C19—C18	117.83 (14)
C5—C4—C7	119.63 (12)	C20—C19—H19	121.1
C3—C4—C7	121.79 (13)	C18—C19—H19	121.1
C4—C5—C6	120.36 (18)	C19—C20—C21	121.51 (14)
C4—C5—H5	119.8	C19—C20—H20	119.2
C6—C5—H5	119.8	C21—C20—H20	119.2
C5—C6—C1	119.7 (2)	C22—C21—C20	122.02 (15)
C5—C6—H6	120.2	C22—C21—H21	119.0
C1—C6—H6	120.2	C20—C21—H21	119.0
N1—C7—C4	111.98 (10)	C21—C22—C17	116.50 (15)
N1—C7—H7A	109.2	C21—C22—H22	121.8
C4—C7—H7A	109.2	C17—C22—H22	121.8
N1—C7—H7B	109.2	N3—C23—C24	113.93 (10)
C4—C7—H7B	109.2	N3—C23—H23A	108.8
H7A—C7—H7B	107.9	C24—C23—H23A	108.8
C13—C8—C9	119.73 (18)	N3—C23—H23B	108.8
C13—C8—H8	120.1	C24—C23—H23B	108.8
C9—C8—H8	120.1	H23A—C23—H23B	107.7
C8—C9—C10	120.2 (2)	C25—C24—C29	118.34 (11)
C8—C9—H9	119.9	C25—C24—C23	122.90 (10)
C10—C9—H9	119.9	C29—C24—C23	118.76 (11)
C11—C10—C9	121.63 (18)	C24—C25—C26	120.84 (11)
C11—C10—H10	119.2	C24—C25—H25	119.6
C9—C10—H10	119.2	C26—C25—H25	119.6
C10—C11—C12	117.48 (14)	C27—C26—C25	120.14 (12)
C10—C11—C14	120.61 (14)	C27—C26—H26	119.9
C12—C11—C14	121.91 (15)	C25—C26—H26	119.9
C11—C12—C13	120.35 (18)	C26—C27—C28	119.76 (11)
C11—C12—H12	119.8	C26—C27—C30	118.55 (13)
C13—C12—H12	119.8	C28—C27—C30	121.69 (12)
C8—C13—C12	120.63 (18)	C29—C28—C27	119.57 (11)
C8—C13—H13	119.7	C29—C28—H28	120.2
C12—C13—H13	119.7	C27—C28—H28	120.2
N1—C14—C11	112.22 (11)	C28—C29—C24	121.34 (12)
N1—C14—H14A	109.2	C28—C29—H29	119.3
C11—C14—H14A	109.2	C24—C29—H29	119.3
N1—C14—H14B	109.2	N4—C30—C27	177.69 (18)

C11—C14—H14B	109.2	C7—N1—C15	108.68 (9)
H14A—C14—H14B	107.9	C7—N1—C14	110.58 (10)
N1—C15—C16	114.89 (9)	C15—N1—C14	110.55 (10)
N1—C15—H15A	108.5	C16—N2—C18	105.05 (10)
C16—C15—H15A	108.5	C16—N3—C17	106.51 (9)
N1—C15—H15B	108.5	C16—N3—C23	127.82 (10)
C16—C15—H15B	108.5	C17—N3—C23	125.66 (10)
H15A—C15—H15B	107.5		
C6—C1—C2—C3	−1.8 (3)	N3—C23—C24—C25	−4.22 (17)
C1—C2—C3—C4	1.4 (3)	N3—C23—C24—C29	176.46 (11)
C2—C3—C4—C5	0.2 (2)	C29—C24—C25—C26	−0.48 (19)
C2—C3—C4—C7	−179.29 (14)	C23—C24—C25—C26	−179.80 (13)
C3—C4—C5—C6	−1.4 (2)	C24—C25—C26—C27	−0.5 (2)
C7—C4—C5—C6	178.15 (14)	C25—C26—C27—C28	1.3 (2)
C4—C5—C6—C1	1.0 (3)	C25—C26—C27—C30	−179.20 (14)
C2—C1—C6—C5	0.6 (3)	C26—C27—C28—C29	−0.9 (2)
C5—C4—C7—N1	69.27 (16)	C30—C27—C28—C29	179.54 (14)
C3—C4—C7—N1	−111.21 (14)	C27—C28—C29—C24	−0.1 (2)
C13—C8—C9—C10	0.2 (3)	C25—C24—C29—C28	0.8 (2)
C8—C9—C10—C11	−0.1 (4)	C23—C24—C29—C28	−179.83 (12)
C9—C10—C11—C12	−0.7 (3)	C4—C7—N1—C15	70.58 (13)
C9—C10—C11—C14	178.95 (18)	C4—C7—N1—C14	−167.90 (11)
C10—C11—C12—C13	1.3 (2)	C16—C15—N1—C7	−169.13 (10)
C14—C11—C12—C13	−178.29 (14)	C16—C15—N1—C14	69.34 (14)
C9—C8—C13—C12	0.4 (3)	C11—C14—N1—C7	66.68 (15)
C11—C12—C13—C8	−1.3 (3)	C11—C14—N1—C15	−172.91 (11)
C10—C11—C14—N1	64.75 (19)	N3—C16—N2—C18	−0.32 (13)
C12—C11—C14—N1	−115.64 (15)	C15—C16—N2—C18	−174.81 (10)
N1—C15—C16—N2	−121.66 (12)	C17—C18—N2—C16	1.09 (13)
N1—C15—C16—N3	64.40 (15)	C19—C18—N2—C16	−176.82 (12)
N3—C17—C18—N2	−1.42 (13)	N2—C16—N3—C17	−0.56 (13)
C22—C17—C18—N2	179.73 (12)	C15—C16—N3—C17	173.96 (10)
N3—C17—C18—C19	176.75 (11)	N2—C16—N3—C23	−179.14 (10)
C22—C17—C18—C19	−2.10 (19)	C15—C16—N3—C23	−4.62 (17)
N2—C18—C19—C20	178.03 (13)	C22—C17—N3—C16	179.87 (14)
C17—C18—C19—C20	0.29 (19)	C18—C17—N3—C16	1.17 (12)
C18—C19—C20—C21	1.7 (2)	C22—C17—N3—C23	−1.5 (2)
C19—C20—C21—C22	−2.1 (3)	C18—C17—N3—C23	179.80 (10)
C20—C21—C22—C17	0.3 (2)	C24—C23—N3—C16	−107.46 (13)
N3—C17—C22—C21	−176.71 (14)	C24—C23—N3—C17	74.22 (15)
C18—C17—C22—C21	1.8 (2)		

Fig. 1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