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4-Amino-13-(1-naphthyl)-[2,2]paracyclophane

Junshan Sun,[a] Yanmin Huo,[b] Rentao Wu,[c] Jikun Li[a] and Yudao Ma[d]*

[a]Department of Materials and Chemical Engineering, Taishan University, 271021 Taian, Shandong, People's Republic of China, [b]Shandong Institute of Supervision & Inspection of Product Quality, 250100 Jinan, Shandong, People's Republic of China, [c]Department of Chemistry, Taishan University, 271021 Taian, Shandong, People's Republic of China, and [d]Department of Chemistry, Shandong University, 250100 Jinan, Shandong, People's Republic of China
Correspondence e-mail: ydma@sdu.edu.cn

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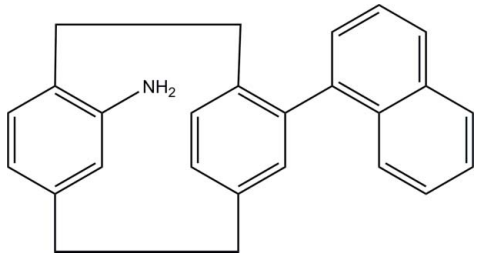
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.054; wR factor = 0.160; data-to-parameter ratio = 7.8.

The title compound [systematic name: 1^2-amino-4^2-(1-naphthyl)-1,4(1,4)-dibenzenacyclohexaphane], $C_{26}H_{23}N$, was synthesized from 4-amino-13-bromo-[2,2]paracyclophane and 1-naphthaleneboronic acid in the presence of 1,4-dioxane. It is a new cyclophane-derived compound which can be regarded as a prospective ligand for asymmetric synthesis and catalysis. The benzene rings of the paracyclophane units are very slightly deformed from planarity as shallow boats.

Related literature

For related literature on paracyclophane chemistry, see: Cipiciani *et al.* (1997); on diphosphanes, see: Pye *et al.* (1997); on oxazoline-phosphanes, see: Wu *et al.* (2003); on oxazoline-imidazolium, see: Bolm *et al.* (2003); on oxazoline-selenides, see: Hou *et al.* (2000); on oxazoline-alcohols, see: Wu *et al.* (2001).



Experimental

Crystal data

$C_{26}H_{23}N$
M_r = 349.45
Orthorhombic, $P2_12_12_1$
a = 8.5261 (5) Å
b = 12.8123 (8) Å
c = 17.2065 (11) Å
V = 1879.6 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 293 (2) K
0.15 × 0.12 × 0.10 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.990, T_{max} = 0.993
9879 measured reflections
1901 independent reflections
1690 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.159
S = 1.00
1901 reflections
245 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Data collection: *APEX2* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KJ2079).

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supplementary materials

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4-Amino-13-(1-naphthyl)-[2,2]paracyclophane

J. Sun, Y. Huo, R. Wu, J. Li and Y. Ma

Comment

The chemistry of [2.2]paracyclophanes has attracted the interest of researchers since the middle of the last century. After a standstill period, investigations in this area have received a new impulse (Cipiciani *et al.*, 1997) and recently there has been notable progress especially regarding the synthesis of new derivatives. [2.2]paracyclophane is unique as the strain in the molecule has become so large that the benzene rings have been substantially bent from planarity. The configurationally rigid [2. 2]paracyclophanyl unit makes the design of chiral ligands of different types possible. The [2.2]paracyclophane ligand has previously been included in diphosphanes, (Pye *et al.*, 1997) oxazoline-phosphanes,(Wu *et al.*, 2003) oxazoline-imidazolium,(Bolm *et al.*, 2003) oxazoline-selenides, (Hou *et al.*, 2000) oxazoline-alcohols,(Wu *et al.*, 2001) and Schiff base phenols.

The benzene rings in the [2,2] paracyclophane are not planar. Their conformation can be described as an asymmetric boat conformation. The benzene C atoms which are directly bonded to the ethylene links of the paracyclophane deviate significantly from the least-squares planes running through the other four benzene C atoms. The largest deviations are found for the atoms C3 [0.117 (5) Å] and C12 [0.146 (4) Å], which are the atoms closest to the amino and naphtyl substituents of the benzene rings. The angle between the planes through the benzene rings is 6.0 (2) °. The N1—C1 bond length lies between the expected values for a C—N and a C=N bond, which is probably caused by p–π conjugation.

Experimental

A solution of 4-amino-13-bromo [2,2]paracyclophane (501.3 mg, 1.66 mmol), 1-naphthaleneboronic acid (428.3 mg, 2.49 mmol), KF (289.7 mg, 4.98 mmol), Pd-DPPF (13.6 mg, 0.0166 mmol) in 1,4-dioxane (5 ml) was stirred at 353–363k for 24 h under a slight overpressure of nitrogen. After this, reagents were added to the mixture at 24 h intervals. 1-naphthaleneboronic acid (0.55 mmol), KF (72.4 mg, 1.245 mmol), Pd-DPPF (13.6 mg, 0.0166 mmol) were added to the flask in the first two times, in the last two times, 1-naphthaleneboronic acid (0.55 mmol), KF (72.4 mg, 1.245 mmol), Pd-DPPF (6.78 mg, 0.0083 mmol) were added. The flask was kept at 353–363 K and stirred the whole time. After completion of the reaction, as indicated by TLC, water (5 ml) was added and the solution was filtered. The solution was extracted by dichloromethane (30 ml) and the solvent was removed on a rotary evaporator. The solid was subjected to chromatography on silica gel (eluent: petroleum ether / ethyl acetate =20:1). Pure product was isolated (yield 84.6%). Analysis, calculated for $C_{26}H_{23}N$: C, 89.36; H, 6.63; N, 4.01. Found: C, 89.03; H, 6.62; N, 3.93. The elemental analyses were performed with a Perkin Elmer PE2400II.

Refinement

All the H atoms could be found in the difference Fourier maps. Nevertheless, they were placed into the idealized positions and refined in a riding atom approximation with following constraints: C—H = 0.93, 0.97 Å and N—H = 0.86 Å, and with U_{iso}(H) = 1.2U_{eq}(C-aromatic and methylene and *N*-amido) in all the cases. In the absence of significant anomalous scattering effects, 1406 Friedel pairs were merged. The absolute configuration was determined by synthesis.

Figures

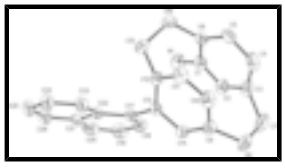


Fig. 1. The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme. The H atoms are omitted.

1^2-amino-4^2-(1-naphthyl)-1,4(1,4)-dibenzenacyclohexaphane

Crystal data

$C_{26}H_{23}N$	$D_x = 1.235$ Mg m^{-3}
$M_r = 349.45$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Orthorhombic, $P2_12_12_1$	Cell parameters from 3936 reflections
$a = 8.5261$ (5) Å	$\theta = 2.7$–25.1º
$b = 12.8123$ (8) Å	$\mu = 0.07$ mm^{-1}
$c = 17.2065$ (11) Å	$T = 293$ (2) K
$V = 1879.6$ (2) Å^3	Block, colorless
$Z = 4$	0.15 × 0.12 × 0.10 mm
$F_{000} = 744$	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	1901 independent reflections
Radiation source: fine-focus sealed tube	1690 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.026$
$T = 293$(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 2.0$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -8\rightarrow10$
$T_{min} = 0.990$, $T_{max} = 0.993$	$k = -14\rightarrow15$
9879 measured reflections	$l = -12\rightarrow20$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.054$	H-atom parameters constrained
$wR(F^2) = 0.159$	$w = 1/[\sigma^2(F_o^2) + (0.0986P)^2 + 0.8216P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.005$
1901 reflections	$\Delta\rho_{max} = 0.37$ e Å^{-3}

245 parameters

6 restraints

Primary atom site location: structure-invariant direct methods

$\Delta\rho_{min} = -0.32$ e Å^{-3}

Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.022 (5)

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}
N1	0.2691 (6)	0.4913 (3)	0.2196 (3)	0.0659 (12)
H1A	0.2007	0.5066	0.2545	0.079*
H1B	0.3499	0.5306	0.2131	0.079*
C1	0.2490 (5)	0.4028 (3)	0.1733 (2)	0.0497 (11)
C2	0.1199 (5)	0.3383 (4)	0.1826 (3)	0.0561 (12)
H2	0.0486	0.3532	0.2219	0.067*
C3	0.0935 (6)	0.2543 (4)	0.1365 (3)	0.0628 (13)
C4	0.1940 (7)	0.2352 (4)	0.0744 (3)	0.0683 (15)
H4	0.1728	0.1820	0.0392	0.082*
C5	0.3267 (7)	0.2972 (4)	0.0662 (3)	0.0628 (14)
H5	0.3937	0.2856	0.0244	0.075*
C6	0.3618 (6)	0.3758 (4)	0.1187 (2)	0.0515 (11)
C7	0.0003 (7)	0.1612 (5)	0.1707 (4)	0.0833 (19)
H7A	−0.0545	0.1263	0.1287	0.100*
H7B	−0.0782	0.1882	0.2063	0.100*
C8	0.1025 (7)	0.0790 (4)	0.2147 (4)	0.0692 (15)
H8A	0.0486	0.0596	0.2622	0.083*
H8B	0.1106	0.0169	0.1827	0.083*
C9	0.2692 (6)	0.1156 (3)	0.2358 (3)	0.0517 (11)
C10	0.3837 (6)	0.1093 (3)	0.1808 (3)	0.0539 (12)
H10	0.3753	0.0595	0.1417	0.065*
C11	0.5102 (6)	0.1742 (3)	0.1817 (3)	0.0515 (11)
H11	0.5909	0.1640	0.1461	0.062*
C12	0.5201 (5)	0.2548 (3)	0.2347 (2)	0.0417 (10)
C13	0.4179 (5)	0.2553 (3)	0.2981 (2)	0.0394 (9)
C14	0.2894 (5)	0.1865 (3)	0.2960 (2)	0.0465 (10)
H14	0.2162	0.1885	0.3361	0.056*
C15	0.6056 (5)	0.3547 (4)	0.2093 (3)	0.0504 (11)

H15A	0.7152	0.3386	0.2001	0.061*
H15B	0.6005	0.4055	0.2510	0.061*
C16	0.5336 (6)	0.4041 (4)	0.1335 (3)	0.0585 (13)
H16A	0.5423	0.4794	0.1370	0.070*
H16B	0.5955	0.3816	0.0892	0.070*
C17	0.4316 (5)	0.3268 (3)	0.3660 (2)	0.0442 (10)
C18	0.3029 (6)	0.3795 (4)	0.3928 (3)	0.0567 (12)
H18	0.2071	0.3686	0.3683	0.068*
C19	0.3088 (8)	0.4494 (5)	0.4558 (3)	0.0711 (16)
H19	0.2190	0.4849	0.4713	0.085*
C20	0.4445 (9)	0.4643 (5)	0.4931 (3)	0.0748 (18)
H20	0.4484	0.5109	0.5345	0.090*
C21	0.5830 (7)	0.4106 (4)	0.4706 (3)	0.0630 (15)
C22	0.5777 (6)	0.3395 (4)	0.4069 (2)	0.0479 (11)
C23	0.7156 (6)	0.2835 (4)	0.3886 (3)	0.0599 (13)
H23	0.7143	0.2352	0.3482	0.072*
C24	0.8502 (7)	0.2994 (5)	0.4293 (4)	0.0771 (18)
H24	0.9397	0.2614	0.4170	0.093*
C25	0.8549 (10)	0.3729 (6)	0.4899 (4)	0.091 (2)
H25	0.9485	0.3850	0.5162	0.109*
C26	0.7244 (9)	0.4258 (5)	0.5102 (3)	0.080 (2)
H26	0.7285	0.4732	0.5512	0.096*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.069 (3)	0.048 (2)	0.081 (3)	0.005 (2)	−0.001 (2)	−0.009 (2)
C1	0.055 (3)	0.042 (2)	0.052 (2)	0.007 (2)	−0.010 (2)	0.009 (2)
C2	0.044 (2)	0.055 (3)	0.069 (3)	0.007 (2)	−0.011 (2)	0.005 (2)
C3	0.054 (3)	0.062 (3)	0.073 (3)	−0.001 (3)	−0.022 (3)	0.002 (3)
C4	0.084 (4)	0.060 (3)	0.061 (3)	−0.001 (3)	−0.033 (3)	−0.006 (3)
C5	0.081 (3)	0.072 (3)	0.036 (2)	−0.002 (3)	−0.005 (2)	0.002 (2)
C6	0.063 (3)	0.051 (2)	0.041 (2)	−0.006 (2)	−0.003 (2)	0.012 (2)
C7	0.059 (3)	0.075 (4)	0.116 (5)	−0.024 (3)	−0.026 (4)	0.002 (4)
C8	0.072 (3)	0.052 (3)	0.083 (3)	−0.026 (3)	−0.013 (3)	−0.002 (3)
C9	0.062 (3)	0.035 (2)	0.058 (2)	−0.008 (2)	−0.011 (2)	0.0041 (19)
C10	0.068 (3)	0.034 (2)	0.060 (3)	0.005 (2)	−0.011 (2)	−0.009 (2)
C11	0.055 (3)	0.044 (2)	0.055 (2)	0.011 (2)	0.000 (2)	−0.007 (2)
C12	0.0367 (19)	0.039 (2)	0.049 (2)	0.0018 (18)	−0.0046 (18)	−0.0019 (18)
C13	0.043 (2)	0.0339 (19)	0.042 (2)	0.0011 (17)	−0.0071 (17)	0.0002 (16)
C14	0.052 (2)	0.042 (2)	0.045 (2)	−0.006 (2)	−0.004 (2)	0.0073 (19)
C15	0.042 (2)	0.049 (2)	0.060 (3)	−0.008 (2)	0.010 (2)	−0.003 (2)
C16	0.065 (3)	0.062 (3)	0.049 (2)	−0.016 (3)	0.013 (2)	0.006 (2)
C17	0.054 (2)	0.039 (2)	0.040 (2)	−0.0040 (19)	−0.001 (2)	0.0009 (18)
C18	0.063 (3)	0.055 (3)	0.052 (2)	−0.003 (2)	0.009 (2)	−0.007 (2)
C19	0.087 (4)	0.066 (3)	0.060 (3)	0.004 (3)	0.015 (3)	−0.014 (3)
C20	0.117 (5)	0.060 (3)	0.047 (3)	−0.017 (3)	0.016 (3)	−0.013 (2)
C21	0.096 (4)	0.055 (3)	0.038 (2)	−0.028 (3)	−0.010 (3)	0.009 (2)

C22	0.061 (3)	0.043 (2)	0.040 (2)	−0.013 (2)	−0.009 (2)	0.0080 (18)
C23	0.061 (3)	0.061 (3)	0.057 (3)	−0.004 (2)	−0.017 (2)	0.009 (2)
C24	0.062 (3)	0.085 (4)	0.084 (4)	−0.012 (3)	−0.026 (3)	0.029 (3)
C25	0.101 (5)	0.105 (5)	0.068 (4)	−0.048 (5)	−0.044 (4)	0.026 (4)
C26	0.104 (5)	0.083 (4)	0.054 (3)	−0.035 (4)	−0.028 (3)	0.013 (3)

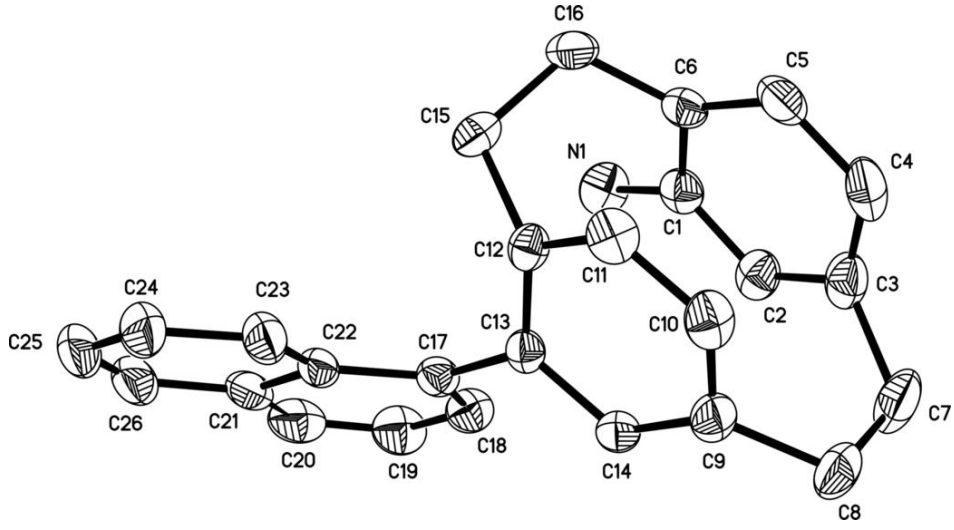
Geometric parameters (Å, °)

N1—C1	1.396 (6)	C12—C15	1.537 (6)
N1—H1A	0.8600	C13—C14	1.406 (6)
N1—H1B	0.8600	C13—C17	1.489 (6)
C1—C2	1.386 (7)	C14—H14	0.9300
C1—C6	1.389 (7)	C15—C16	1.574 (7)
C2—C3	1.354 (7)	C15—H15A	0.9700
C2—H2	0.9300	C15—H15B	0.9700
C3—C4	1.391 (8)	C16—H16A	0.9700
C3—C7	1.549 (8)	C16—H16B	0.9700
C4—C5	1.390 (8)	C17—C18	1.369 (6)
C4—H4	0.9300	C17—C22	1.440 (6)
C5—C6	1.385 (7)	C18—C19	1.406 (7)
C5—H5	0.9300	C18—H18	0.9300
C6—C16	1.530 (7)	C19—C20	1.337 (9)
C7—C8	1.563 (8)	C19—H19	0.9300
C7—H7A	0.9700	C20—C21	1.421 (9)
C7—H7B	0.9700	C20—H20	0.9300
C8—C9	1.539 (7)	C21—C26	1.398 (8)
C8—H8A	0.9700	C21—C22	1.426 (7)
C8—H8B	0.9700	C22—C23	1.413 (7)
C9—C10	1.362 (7)	C23—C24	1.360 (7)
C9—C14	1.390 (6)	C23—H23	0.9300
C10—C11	1.362 (7)	C24—C25	1.405 (10)
C10—H10	0.9300	C24—H24	0.9300
C11—C12	1.381 (6)	C25—C26	1.349 (10)
C11—H11	0.9300	C25—H25	0.9300
C12—C13	1.395 (6)	C26—H26	0.9300
C1—N1—H1A	120.0	C14—C13—C17	117.8 (4)
C1—N1—H1B	120.0	C9—C14—C13	121.7 (4)
H1A—N1—H1B	120.0	C9—C14—H14	119.2
C2—C1—C6	118.7 (4)	C13—C14—H14	119.2
C2—C1—N1	121.1 (5)	C12—C15—C16	112.7 (4)
C6—C1—N1	120.2 (4)	C12—C15—H15A	109.0
C3—C2—C1	122.6 (5)	C16—C15—H15A	109.0
C3—C2—H2	118.7	C12—C15—H15B	109.0
C1—C2—H2	118.7	C16—C15—H15B	109.0
C2—C3—C4	119.1 (5)	H15A—C15—H15B	107.8
C2—C3—C7	118.3 (5)	C6—C16—C15	114.6 (4)
C4—C3—C7	118.1 (5)	C6—C16—H16A	108.6
C5—C4—C3	118.6 (5)	C15—C16—H16A	108.6
C5—C4—H4	120.7	C6—C16—H16B	108.6

C3—C4—H4	120.7	C15—C16—H16B	108.6
C6—C5—C4	121.7 (5)	H16A—C16—H16B	107.6
C6—C5—H5	119.2	C18—C17—C22	118.2 (4)
C4—C5—H5	119.2	C18—C17—C13	120.4 (4)
C5—C6—C1	118.2 (5)	C22—C17—C13	121.4 (4)
C5—C6—C16	119.2 (5)	C17—C18—C19	123.1 (5)
C1—C6—C16	119.4 (4)	C17—C18—H18	118.5
C3—C7—C8	114.6 (4)	C19—C18—H18	118.5
C3—C7—H7A	108.6	C20—C19—C18	119.4 (6)
C8—C7—H7A	108.6	C20—C19—H19	120.3
C3—C7—H7B	108.6	C18—C19—H19	120.3
C8—C7—H7B	108.6	C19—C20—C21	121.3 (5)
H7A—C7—H7B	107.6	C19—C20—H20	119.3
C9—C8—C7	115.1 (4)	C21—C20—H20	119.3
C9—C8—H8A	108.5	C26—C21—C20	121.1 (5)
C7—C8—H8A	108.5	C26—C21—C22	119.5 (6)
C9—C8—H8B	108.5	C20—C21—C22	119.5 (5)
C7—C8—H8B	108.5	C23—C22—C21	118.0 (4)
H8A—C8—H8B	107.5	C23—C22—C17	123.6 (4)
C10—C9—C14	117.9 (4)	C21—C22—C17	118.4 (5)
C10—C9—C8	118.7 (4)	C24—C23—C22	120.7 (5)
C14—C9—C8	119.3 (5)	C24—C23—H23	119.6
C11—C10—C9	121.6 (4)	C22—C23—H23	119.6
C11—C10—H10	119.2	C23—C24—C25	120.5 (7)
C9—C10—H10	119.2	C23—C24—H24	119.8
C10—C11—C12	120.8 (4)	C25—C24—H24	119.8
C10—C11—H11	119.6	C26—C25—C24	120.3 (6)
C12—C11—H11	119.6	C26—C25—H25	119.8
C11—C12—C13	118.8 (4)	C24—C25—H25	119.8
C11—C12—C15	117.6 (4)	C25—C26—C21	120.9 (6)
C13—C12—C15	121.0 (4)	C25—C26—H26	119.5
C12—C13—C14	117.7 (4)	C21—C26—H26	119.5
C12—C13—C17	124.5 (4)		
C6—C1—C2—C3	−5.0 (3)	C11—C12—C15—C16	56.6 (5)
N1—C1—C2—C3	177.2 (4)	C13—C12—C15—C16	−104.9 (5)
C1—C2—C3—C4	−4.0 (3)	C5—C6—C16—C15	−99.3 (5)
C1—C2—C3—C7	152.0 (4)	C1—C6—C16—C15	60.0 (6)
C2—C3—C4—C5	6.0 (5)	C12—C15—C16—C6	24.3 (6)
C7—C3—C4—C5	−150.0 (5)	C12—C13—C17—C18	132.4 (4)
C3—C4—C5—C6	1.0 (6)	C14—C13—C17—C18	−44.7 (5)
C4—C5—C6—C1	−9.9 (6)	C12—C13—C17—C22	−50.0 (6)
C4—C5—C6—C16	149.7 (4)	C14—C13—C17—C22	132.9 (4)
C2—C1—C6—C5	11.8 (5)	C22—C17—C18—C19	3.4 (7)
N1—C1—C6—C5	−170.4 (4)	C13—C17—C18—C19	−178.9 (4)
C2—C1—C6—C16	−147.8 (4)	C17—C18—C19—C20	−1.6 (8)
N1—C1—C6—C16	30.0 (6)	C18—C19—C20—C21	−0.3 (9)
C2—C3—C7—C8	−87.2 (6)	C19—C20—C21—C26	−179.5 (5)
C4—C3—C7—C8	69.0 (7)	C19—C20—C21—C22	0.3 (8)
C3—C7—C8—C9	15.1 (8)	C26—C21—C22—C23	2.8 (7)

C7—C8—C9—C10	−82.7 (6)	C20—C21—C22—C23	−176.9 (5)
C7—C8—C9—C14	74.1 (7)	C26—C21—C22—C17	−178.7 (4)
C14—C9—C10—C11	−3.8 (3)	C20—C21—C22—C17	1.6 (7)
C8—C9—C10—C11	153.4 (4)	C18—C17—C22—C23	175.1 (4)
C9—C10—C11—C12	−5.6 (3)	C13—C17—C22—C23	−2.6 (7)
C10—C11—C12—C13	14.2 (5)	C18—C17—C22—C21	−3.3 (6)
C10—C11—C12—C15	−147.7 (3)	C13—C17—C22—C21	179.0 (4)
C11—C12—C13—C14	−13.1 (5)	C21—C22—C23—C24	−1.8 (7)
C15—C12—C13—C14	148.2 (4)	C17—C22—C23—C24	179.8 (5)
C11—C12—C13—C17	169.7 (4)	C22—C23—C24—C25	−0.7 (8)
C15—C12—C13—C17	−29.0 (6)	C23—C24—C25—C26	2.4 (9)
C10—C9—C14—C13	4.5 (5)	C24—C25—C26—C21	−1.4 (9)
C8—C9—C14—C13	−152.5 (4)	C20—C21—C26—C25	178.5 (5)
C12—C13—C14—C9	4.0 (5)	C22—C21—C26—C25	−1.3 (8)
C17—C13—C14—C9	−178.7 (4)		

Fig. 1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