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[(1*R*,4a*S*)-7-Isopropyl-1,4a-dimethyl-1,2,3,4,4a,9,10,10*a*-octahydrophenanthren-1-yl](piperidin-1-yl)methanone

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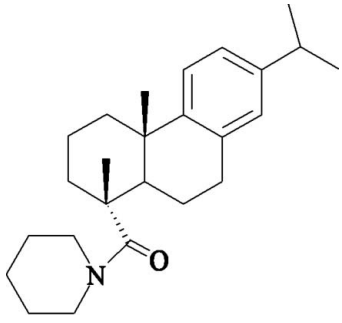
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.051; wR factor = 0.134; data-to-parameter ratio = 9.5.

The title compound, $C_{25}H_{37}NO$, has been synthesized from (+)-dehydroabietic acid. The piperidine ring exhibits a classic chair conformation, whereas the two cyclohexane rings adopt chair and half-chair conformations. The two methyl groups directly attached to the tricyclic nucleus are on the same side of the tricyclic phenanthrene structure.

Related literature

For related literature, see: Fernandez *et al.* (2001); Fonseca *et al.* (2004); Halbrook & Lawrence (1966); Hamodrakas *et al.* (1978); Rao *et al.* (2006); Savluchinske *et al.* (1999); Sepulveda *et al.* (2005); Wada *et al.* (1985).



Experimental

Crystal data

$C_{25}H_{37}NO$
M_r = 367.56
Orthorhombic, $P2_12_12_1$
a = 10.612 (2) Å
b = 11.566 (2) Å
c = 17.067 (3) Å
V = 2094.8 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 293 (2) K
0.40 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scans (North *et al.*, 1968)
T_{min} = 0.932, T_{max} = 0.966
4522 measured reflections
2339 independent reflections
1756 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.134
S = 1.00
2339 reflections
245 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
Selected torsion angles (°).

C8—C7—C16—C17	179.0 (2)	N1—C21—C22—C23	−55.3 (4)

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: OM2152).

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supplementary materials

Acta Cryst. (2007). E**63**, o3886 [**doi:10.1107/S1600536807040998**]

[(1*R*,4a*S*)-7-Isopropyl-1,4a-dimethyl-1,2,3,4,4a,9,10,10*a*-octahydrophenanthren-1-yl](piperidin-1-yl)methanone

X.-P. Rao, Z.-Q. Song, W.-H. Jia and S.-B. Shang

Comment

(+)Dehydroabietic acid is an abietane diterpenic resin acid which can be easily obtained from Pinus resin or commercial rosin (Halbrook & Lawrence, 1966). It is widely used as a starting material for the design and synthesis of biological compounds. Biological activities, such as anti-tumor (Wada *et al.*, 1985), antimicrobial (Savluchinske *et al.*, 1999), anti-inflammatory (Fernandez *et al.*, 2001) and gastroprotective (Sepulveda *et al.*, 2005) effects of dehydroabietic acid derivatives have been reported. Heterocyclic chemistry has attracted great interest in recent years, for those compounds containing heterocyclic rings often exhibit higher biological activities. Heterocyclic rings fused to the aromatic ring of dehydroabietic acid (Fonseca *et al.*, 2004) have been successfully synthesized, and they exhibit antiviral activities against DNA and RNA. Considerable efforts have been devoted to the biological activities of heterocyclic derivatives of dehydroabietic acid, yet the crystal structure of such compounds have seldom been reported. In this work, we describe the crystal structure of the title compound. The overall geometry is comparable to that found for dehydroabietic *N*-methyl anilide (Rao *et al.*, 2006). The tricyclic phenanthrene structure of the title compound exhibits the same conformation as dehydroabietic *N*-methyl anilide, which exhibited planar, classic chair and half-chair conformations, respectively. The two cyclohexane rings form a *trans* ring junction with two methyl groups on the same side of the tricyclic phenanthrene structure (Hamodrakas, *et al.*, 1978). Apart from the planar conformation of the benzene ring, the piperidine ring of the title compound forms a classic chair conformation. The bond lengths and bond angles in the molecule are in normal ranges.

Experimental

All chemicals purchased were of reagent grade and used without further purification. A mixture of (+)dehydroabietic acid (0.1 mol), phosphorus trichloride (6 ml) and chloroform (40 ml) were stirred at 333 K for 3 h, then the solvent was distilled off. The residue was slowly added to piperidine (0.2 mol) in toluene (60 ml) solution. After a further 24 h stirring at room temperature, the resulting mixture was filtered. The precipitate was washed with hydrochloric acid (5%) and water and the solvent was distilled off. Upon recrystallization from acetone, colorless crystals of the title compound were obtained (yield 54.7%, m.p. 342.5 K). Single crystals were grown from acetone.

Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.96Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms, and C—H = 0.97–0.98Å and U_{iso}(H) = 1.2U_{eq}(C) for all other H atoms. In the absence of significant anomalous scattering effects, all Friedel pairs were merged.

Figures

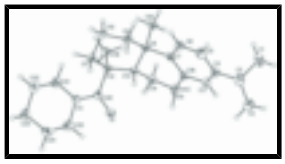


Fig. 1. The molecular structure of the title compound, with H atoms represented by small spheres of arbitrary radius and displacement ellipsoids at the 30% probability level.

[(1*R*,4a*S*)-7-Isopropyl-1,4a-dimethyl-1,2,3,4,4a,9,10,10*a*- octahydrophenanthren-1-yl](piperidin-1-yl)methanone

Crystal data

$C_{25}H_{37}NO$	$D_x = 1.165$ Mg m^{-3}
$M_r = 367.56$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Orthorhombic, $P2_12_12_1$	Cell parameters from 25 reflections
$a = 10.612$ (2) Å	$\theta = 10$–13º
$b = 11.566$ (2) Å	$\mu = 0.07$ mm^{-1}
$c = 17.067$ (3) Å	$T = 293$ (2) K
$V = 2094.8$ (7) Å^3	Block, white
$Z = 4$	0.40 × 0.20 × 0.10 mm
$F_{000} = 808$	

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.043$
Radiation source: fine-focus sealed tube	$\theta_{max} = 26.0$º
Monochromator: graphite	$\theta_{min} = 2.1$º
$T = 293(2)$ K	$h = 0 \rightarrow 13$
$\omega/2\theta$ scans	$k = 0 \rightarrow 14$
Absorption correction: ψ scans (North *et al.*, 1968)	$l = -21 \rightarrow 21$
$T_{min} = 0.932$, $T_{max} = 0.966$	3 standard reflections
4522 measured reflections	every 200 reflections
2339 independent reflections	intensity decay: none
1756 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.08P)^2 + 0.1P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.051$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.134$	$\Delta\rho_{max} = 0.17$ e Å^{-3}
$S = 1.00$	$\Delta\rho_{min} = -0.19$ e Å^{-3}

2339 reflections
245 parameters
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
Extinction correction: none

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}
O1	0.6299 (2)	0.8464 (2)	0.82631 (14)	0.0531 (6)
N1	0.7308 (3)	0.9998 (2)	0.77919 (15)	0.0441 (7)
C1	0.7437 (5)	0.1750 (3)	1.1017 (3)	0.0815 (14)
H1A	0.7027	0.1077	1.1227	0.122*
H1B	0.8050	0.2027	1.1386	0.122*
H1C	0.7848	0.1553	1.0535	0.122*
C2	0.5402 (4)	0.2221 (4)	1.0376 (3)	0.0845 (14)
H2A	0.5062	0.1541	1.0620	0.127*
H2B	0.5712	0.2028	0.9864	0.127*
H2C	0.4754	0.2796	1.0331	0.127*
C3	0.6465 (4)	0.2686 (3)	1.0868 (2)	0.0586 (10)
H3	0.6106	0.2895	1.1377	0.070*
C4	0.7086 (3)	0.3767 (3)	1.0541 (2)	0.0455 (8)
C5	0.7801 (4)	0.4453 (3)	1.1025 (2)	0.0549 (9)
H5	0.7889	0.4248	1.1550	0.066*
C6	0.8393 (3)	0.5436 (3)	1.07563 (19)	0.0484 (8)
H6	0.8881	0.5871	1.1101	0.058*
C7	0.8278 (3)	0.5796 (3)	0.99782 (17)	0.0361 (7)
C8	0.8948 (3)	0.6890 (2)	0.96851 (17)	0.0351 (7)
C9	0.9003 (3)	0.7812 (3)	1.03387 (18)	0.0416 (8)
H9A	0.8172	0.7902	1.0567	0.050*
H9B	0.9570	0.7551	1.0748	0.050*
C10	0.9451 (3)	0.8968 (3)	1.00311 (19)	0.0450 (8)
H10A	1.0296	0.8886	0.9821	0.054*
H10B	0.9483	0.9520	1.0459	0.054*
C11	0.8584 (3)	0.9420 (3)	0.93971 (18)	0.0394 (7)

H11A	0.8898	1.0162	0.9217	0.047*
H11B	0.7754	0.9545	0.9620	0.047*
C12	0.8463 (3)	0.8601 (2)	0.86874 (16)	0.0342 (7)
C13	0.8157 (3)	0.7368 (2)	0.89906 (15)	0.0315 (6)
H13A	0.7299	0.7428	0.9199	0.038*
C14	0.8065 (3)	0.6461 (3)	0.83505 (17)	0.0399 (7)
H14A	0.7647	0.6789	0.7897	0.048*
H14B	0.8905	0.6225	0.8194	0.048*
C15	0.7339 (4)	0.5422 (3)	0.86324 (19)	0.0516 (9)
H15A	0.6446	0.5572	0.8566	0.062*
H15B	0.7554	0.4766	0.8305	0.062*
C16	0.7576 (3)	0.5105 (3)	0.94744 (17)	0.0360 (7)
C17	0.6993 (3)	0.4097 (3)	0.97657 (19)	0.0422 (7)
H17A	0.6530	0.3638	0.9423	0.051*
C18	1.0309 (3)	0.6521 (3)	0.9484 (2)	0.0503 (9)
H18A	1.0721	0.6245	0.9948	0.076*
H18B	1.0764	0.7172	0.9279	0.076*
H18C	1.0290	0.5916	0.9098	0.076*
C19	0.9654 (3)	0.8588 (3)	0.8168 (2)	0.0470 (8)
H19A	0.9961	0.7810	0.8121	0.071*
H19B	1.0293	0.9065	0.8402	0.071*
H19C	0.9450	0.8882	0.7657	0.071*
C20	0.7282 (3)	0.9018 (3)	0.82255 (18)	0.0374 (7)
C21	0.8260 (3)	1.0905 (3)	0.7773 (2)	0.0471 (8)
H21A	0.8521	1.1040	0.7236	0.057*
H21B	0.8994	1.0659	0.8069	0.057*
C22	0.7745 (3)	1.2020 (3)	0.8121 (2)	0.0547 (9)
H22A	0.7576	1.1907	0.8674	0.066*
H22B	0.8372	1.2626	0.8071	0.066*
C23	0.6547 (4)	1.2390 (3)	0.7712 (2)	0.0635 (11)
H23A	0.6193	1.3057	0.7978	0.076*
H23B	0.6737	1.2612	0.7177	0.076*
C24	0.5606 (3)	1.1423 (3)	0.7712 (2)	0.0590 (10)
H24A	0.4873	1.1648	0.7409	0.071*
H24B	0.5335	1.1269	0.8244	0.071*
C25	0.6176 (4)	1.0337 (3)	0.7364 (2)	0.0557 (10)
H25A	0.5564	0.9715	0.7384	0.067*
H25B	0.6387	1.0474	0.6818	0.067*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0383 (12)	0.0497 (13)	0.0714 (15)	−0.0063 (11)	−0.0142 (11)	0.0160 (13)
N1	0.0447 (15)	0.0370 (13)	0.0505 (15)	−0.0036 (13)	−0.0108 (13)	0.0038 (13)
C1	0.088 (3)	0.050 (2)	0.106 (3)	−0.001 (2)	−0.003 (3)	0.029 (2)
C2	0.067 (3)	0.065 (3)	0.121 (4)	−0.021 (2)	−0.008 (3)	0.026 (3)
C3	0.066 (2)	0.0497 (19)	0.060 (2)	−0.006 (2)	0.009 (2)	0.0077 (18)
C4	0.0407 (17)	0.0417 (17)	0.0540 (18)	0.0018 (16)	0.0019 (16)	0.0101 (16)

C5	0.064 (2)	0.058 (2)	0.0425 (18)	−0.003 (2)	−0.0047 (18)	0.0130 (17)
C6	0.050 (2)	0.0485 (18)	0.0466 (18)	−0.0065 (17)	−0.0117 (16)	0.0032 (15)
C7	0.0294 (14)	0.0360 (16)	0.0431 (16)	0.0071 (13)	−0.0007 (13)	0.0017 (14)
C8	0.0269 (14)	0.0385 (16)	0.0398 (16)	0.0006 (13)	0.0003 (13)	0.0000 (14)
C9	0.0381 (16)	0.0468 (18)	0.0397 (16)	−0.0040 (15)	−0.0073 (14)	−0.0008 (15)
C10	0.0404 (17)	0.0468 (19)	0.0477 (19)	−0.0090 (16)	−0.0051 (14)	−0.0069 (16)
C11	0.0351 (15)	0.0358 (16)	0.0473 (17)	−0.0049 (14)	0.0016 (14)	0.0003 (14)
C12	0.0309 (15)	0.0362 (15)	0.0355 (15)	0.0002 (14)	0.0016 (12)	0.0005 (13)
C13	0.0268 (13)	0.0336 (14)	0.0340 (14)	−0.0010 (13)	0.0000 (12)	−0.0028 (12)
C14	0.0442 (17)	0.0371 (16)	0.0383 (15)	0.0017 (15)	0.0046 (14)	0.0002 (13)
C15	0.070 (2)	0.0382 (17)	0.0464 (17)	−0.0110 (18)	−0.0088 (17)	−0.0014 (15)
C16	0.0329 (14)	0.0341 (15)	0.0409 (15)	0.0065 (13)	0.0006 (13)	0.0006 (13)
C17	0.0388 (17)	0.0361 (16)	0.0517 (18)	0.0029 (15)	−0.0046 (15)	0.0004 (14)
C18	0.0271 (15)	0.057 (2)	0.067 (2)	0.0074 (16)	−0.0019 (15)	0.0048 (19)
C19	0.0370 (16)	0.0455 (18)	0.058 (2)	0.0024 (16)	0.0118 (15)	0.0059 (17)
C20	0.0398 (16)	0.0333 (15)	0.0392 (16)	−0.0008 (14)	−0.0012 (13)	−0.0039 (13)
C21	0.0485 (19)	0.0438 (18)	0.0490 (18)	−0.0056 (16)	0.0081 (16)	0.0087 (15)
C22	0.057 (2)	0.0395 (18)	0.067 (2)	−0.0076 (18)	−0.0050 (19)	−0.0012 (17)
C23	0.078 (3)	0.0381 (19)	0.074 (2)	0.007 (2)	−0.021 (2)	−0.0046 (18)
C24	0.051 (2)	0.057 (2)	0.069 (2)	0.009 (2)	−0.0193 (19)	0.002 (2)
C25	0.063 (2)	0.0461 (19)	0.058 (2)	−0.0042 (18)	−0.0235 (19)	0.0049 (18)

Geometric parameters (Å, °)

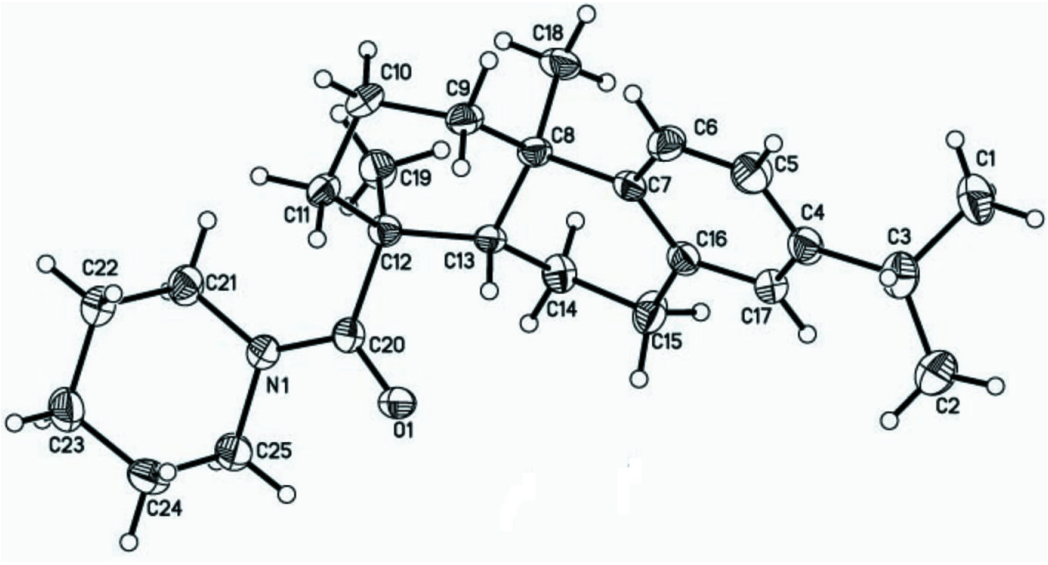
O1—C20	1.226 (4)	C12—C19	1.544 (4)
N1—C20	1.354 (4)	C12—C13	1.552 (4)
N1—C21	1.457 (4)	C12—C20	1.557 (4)
N1—C25	1.461 (4)	C13—C14	1.517 (4)
C1—C3	1.517 (6)	C13—H13A	0.9800
C1—H1A	0.9600	C14—C15	1.507 (4)
C1—H1B	0.9600	C14—H14A	0.9700
C1—H1C	0.9600	C14—H14B	0.9700
C2—C3	1.505 (6)	C15—C16	1.504 (4)
C2—H2A	0.9600	C15—H15A	0.9700
C2—H2B	0.9600	C15—H15B	0.9700
C2—H2C	0.9600	C16—C17	1.410 (4)
C3—C4	1.518 (5)	C17—H17A	0.9300
C3—H3	0.9800	C18—H18A	0.9600
C4—C5	1.375 (5)	C18—H18B	0.9600
C4—C17	1.382 (4)	C18—H18C	0.9600
C5—C6	1.378 (5)	C19—H19A	0.9600
C5—H5	0.9300	C19—H19B	0.9600
C6—C7	1.397 (4)	C19—H19C	0.9600
C6—H6	0.9300	C21—C22	1.521 (5)
C7—C16	1.391 (4)	C21—H21A	0.9700
C7—C8	1.535 (4)	C21—H21B	0.9700
C8—C9	1.544 (4)	C22—C23	1.511 (5)
C8—C18	1.546 (4)	C22—H22A	0.9700
C8—C13	1.554 (4)	C22—H22B	0.9700

C9—C10	1.514 (4)	C23—C24	1.500 (5)
C9—H9A	0.9700	C23—H23A	0.9700
C9—H9B	0.9700	C23—H23B	0.9700
C10—C11	1.514 (4)	C24—C25	1.514 (5)
C10—H10A	0.9700	C24—H24A	0.9700
C10—H10B	0.9700	C24—H24B	0.9700
C11—C12	1.543 (4)	C25—H25A	0.9700
C11—H11A	0.9700	C25—H25B	0.9700
C11—H11B	0.9700		
C20—N1—C21	129.0 (3)	C14—C13—H13A	104.5
C20—N1—C25	118.8 (3)	C12—C13—H13A	104.5
C21—N1—C25	111.5 (3)	C8—C13—H13A	104.5
C3—C1—H1A	109.5	C15—C14—C13	110.7 (2)
C3—C1—H1B	109.5	C15—C14—H14A	109.5
H1A—C1—H1B	109.5	C13—C14—H14A	109.5
C3—C1—H1C	109.5	C15—C14—H14B	109.5
H1A—C1—H1C	109.5	C13—C14—H14B	109.5
H1B—C1—H1C	109.5	H14A—C14—H14B	108.1
C3—C2—H2A	109.5	C16—C15—C14	114.4 (3)
C3—C2—H2B	109.5	C16—C15—H15A	108.6
H2A—C2—H2B	109.5	C14—C15—H15A	108.6
C3—C2—H2C	109.5	C16—C15—H15B	108.6
H2A—C2—H2C	109.5	C14—C15—H15B	108.6
H2B—C2—H2C	109.5	H15A—C15—H15B	107.6
C2—C3—C1	110.4 (3)	C7—C16—C17	119.5 (3)
C2—C3—C4	114.5 (3)	C7—C16—C15	122.7 (3)
C1—C3—C4	110.8 (3)	C17—C16—C15	117.7 (3)
C2—C3—H3	106.9	C4—C17—C16	122.4 (3)
C1—C3—H3	106.9	C4—C17—H17A	118.8
C4—C3—H3	106.9	C16—C17—H17A	118.8
C5—C4—C17	117.1 (3)	C8—C18—H18A	109.5
C5—C4—C3	119.7 (3)	C8—C18—H18B	109.5
C17—C4—C3	123.2 (3)	H18A—C18—H18B	109.5
C4—C5—C6	121.9 (3)	C8—C18—H18C	109.5
C4—C5—H5	119.1	H18A—C18—H18C	109.5
C6—C5—H5	119.1	H18B—C18—H18C	109.5
C5—C6—C7	121.5 (3)	C12—C19—H19A	109.5
C5—C6—H6	119.2	C12—C19—H19B	109.5
C7—C6—H6	119.2	H19A—C19—H19B	109.5
C16—C7—C6	117.6 (3)	C12—C19—H19C	109.5
C16—C7—C8	121.4 (3)	H19A—C19—H19C	109.5
C6—C7—C8	121.0 (3)	H19B—C19—H19C	109.5
C7—C8—C9	110.6 (2)	O1—C20—N1	118.9 (3)
C7—C8—C18	106.1 (2)	O1—C20—C12	119.8 (3)
C9—C8—C18	108.4 (3)	N1—C20—C12	121.3 (3)
C7—C8—C13	106.9 (2)	N1—C21—C22	110.7 (3)
C9—C8—C13	109.1 (2)	N1—C21—H21A	109.5
C18—C8—C13	115.7 (3)	C22—C21—H21A	109.5
C10—C9—C8	111.8 (2)	N1—C21—H21B	109.5

C10—C9—H9A	109.3	C22—C21—H21B	109.5
C8—C9—H9A	109.3	H21A—C21—H21B	108.1
C10—C9—H9B	109.3	C23—C22—C21	111.3 (3)
C8—C9—H9B	109.3	C23—C22—H22A	109.4
H9A—C9—H9B	107.9	C21—C22—H22A	109.4
C9—C10—C11	111.3 (3)	C23—C22—H22B	109.4
C9—C10—H10A	109.4	C21—C22—H22B	109.4
C11—C10—H10A	109.4	H22A—C22—H22B	108.0
C9—C10—H10B	109.4	C24—C23—C22	110.4 (3)
C11—C10—H10B	109.4	C24—C23—H23A	109.6
H10A—C10—H10B	108.0	C22—C23—H23A	109.6
C10—C11—C12	113.5 (3)	C24—C23—H23B	109.6
C10—C11—H11A	108.9	C22—C23—H23B	109.6
C12—C11—H11A	108.9	H23A—C23—H23B	108.1
C10—C11—H11B	108.9	C23—C24—C25	110.7 (3)
C12—C11—H11B	108.9	C23—C24—H24A	109.5
H11A—C11—H11B	107.7	C25—C24—H24A	109.5
C11—C12—C19	112.9 (3)	C23—C24—H24B	109.5
C11—C12—C13	108.7 (2)	C25—C24—H24B	109.5
C19—C12—C13	110.8 (2)	H24A—C24—H24B	108.1
C11—C12—C20	105.9 (2)	N1—C25—C24	110.8 (3)
C19—C12—C20	111.8 (2)	N1—C25—H25A	109.5
C13—C12—C20	106.6 (2)	C24—C25—H25A	109.5
C14—C13—C12	114.1 (2)	N1—C25—H25B	109.5
C14—C13—C8	109.8 (2)	C24—C25—H25B	109.5
C12—C13—C8	117.9 (2)	H25A—C25—H25B	108.1
C2—C3—C4—C5	161.6 (4)	C9—C8—C13—C12	48.4 (3)
C1—C3—C4—C5	−72.8 (4)	C18—C8—C13—C12	−74.0 (3)
C2—C3—C4—C17	−19.8 (5)	C12—C13—C14—C15	−160.0 (3)
C1—C3—C4—C17	105.8 (4)	C8—C13—C14—C15	65.1 (3)
C17—C4—C5—C6	0.7 (5)	C13—C14—C15—C16	−37.4 (4)
C3—C4—C5—C6	179.4 (3)	C6—C7—C16—C17	1.4 (4)
C4—C5—C6—C7	1.1 (5)	C8—C7—C16—C17	179.0 (2)
C5—C6—C7—C16	−2.1 (5)	C6—C7—C16—C15	177.4 (3)
C5—C6—C7—C8	−179.7 (3)	C8—C7—C16—C15	−4.9 (5)
C16—C7—C8—C9	148.5 (3)	C14—C15—C16—C7	7.9 (5)
C6—C7—C8—C9	−34.0 (4)	C14—C15—C16—C17	−176.0 (3)
C16—C7—C8—C18	−94.2 (3)	C5—C4—C17—C16	−1.4 (5)
C6—C7—C8—C18	83.4 (3)	C3—C4—C17—C16	180.0 (3)
C16—C7—C8—C13	29.9 (4)	C7—C16—C17—C4	0.3 (5)
C6—C7—C8—C13	−152.6 (3)	C15—C16—C17—C4	−175.9 (3)
C7—C8—C9—C10	−170.1 (2)	C21—N1—C20—O1	167.1 (3)
C18—C8—C9—C10	73.9 (3)	C25—N1—C20—O1	−2.1 (4)
C13—C8—C9—C10	−52.8 (3)	C21—N1—C20—C12	−11.6 (5)
C8—C9—C10—C11	59.8 (3)	C25—N1—C20—C12	179.3 (3)
C9—C10—C11—C12	−58.9 (3)	C11—C12—C20—O1	−104.9 (3)
C10—C11—C12—C19	−73.1 (3)	C19—C12—C20—O1	131.8 (3)
C10—C11—C12—C13	50.1 (3)	C13—C12—C20—O1	10.7 (4)
C10—C11—C12—C20	164.3 (2)	C11—C12—C20—N1	73.8 (3)

C11—C12—C13—C14	−177.6 (2)	C19—C12—C20—N1	−49.5 (4)
C19—C12—C13—C14	−53.1 (3)	C13—C12—C20—N1	−170.6 (2)
C20—C12—C13—C14	68.7 (3)	C20—N1—C21—C22	−111.6 (4)
C11—C12—C13—C8	−46.6 (3)	C25—N1—C21—C22	58.3 (4)
C19—C12—C13—C8	77.9 (3)	N1—C21—C22—C23	−55.3 (4)
C20—C12—C13—C8	−160.3 (2)	C21—C22—C23—C24	53.5 (4)
C7—C8—C13—C14	−59.0 (3)	C22—C23—C24—C25	−54.2 (4)
C9—C8—C13—C14	−178.6 (2)	C20—N1—C25—C24	111.5 (3)
C18—C8—C13—C14	58.9 (3)	C21—N1—C25—C24	−59.5 (4)
C7—C8—C13—C12	168.0 (2)	C23—C24—C25—N1	57.3 (4)

Fig. 1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