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# Dibenzo[*a*,*e*]pentacyclo[12.2.1.1$^{6,9}$.0$^{2,13}$.0$^{5,10}$]octadeca-2(13),5(10)-diene

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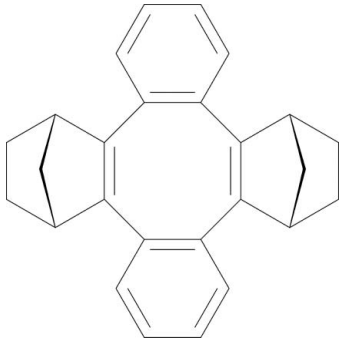
Key indicators: single-crystal X-ray study; $T$ = 90 K, $P$ = 0.0 kPa; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.045; $wR$ factor = 0.121; data-to-parameter ratio = 21.3.

In the title compound, $C_{26}H_{24}$, the central cyclooctatetraene ring has a boat conformation, and the molecule is saddle shaped. The seat is defined by the mean plane of the four-atom attachment points (r.m.s. deviation = 0.014 Å) of the two bicycloheptane substituents. These substituents comprise the pommel and cantle, with each mean plane defined by four atoms proximate to the seat (r.m.s. deviations = 0.001 and 0.000 Å). Relative to the seat, the pommel and cantle bend up 33.36 (5) and 34.22 (4)°, while the benzo units (flaps, r.m.s. deviations = 0.008 and 0.013 Å) bend down 33.48 (4) and 36.58 (4)°.

## Related literature

For related structures, see: Cambridge Structural Database(Allen, 2002) reference codes BUPDOF and BUPDUL (Durr *et al.*, 1983) and RIBCAH (Sygula *et al.*, 2007). For the synthesis of the title compound, see: Schaller (1994).



## Experimental

### Crystal data

$C_{26}H_{24}$
$M_r$ = 336.45
Triclinic, $P\overline{1}$
$a$ = 9.6962 (4) Å
$b$ = 9.7754 (4) Å
$c$ = 10.3676 (4) Å
$\alpha$ = 77.896 (2)°
$\beta$ = 63.781 (2)°
$\gamma$ = 85.497 (2)°
$V$ = 861.87 (6) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 90 K
0.48 × 0.48 × 0.22 mm

### Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
$T_{min}$ = 0.966, $T_{max}$ = 0.984
8966 measured reflections
5019 independent reflections
4347 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.024

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.121
$S$ = 1.05
5019 reflections
236 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS86* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The purchase of the diffractometer was made possible by Grant No. LEQSF(1999–2000)-ENH-TR-13, administered by the Louisiana Board of Regents.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: MW2032).

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# supporting information

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## Dibenzo[*a*,*e*]pentacyclo[12.2.1.1$^{6,9}$.0$^{2,13}$.0$^{5,10}$]octadeca-2(13),5(10)-diene

**Dixie Gautreaux, Tamara R. Schaller Nauman, Frank R. Fronczek and Steven F. Watkins**

### S1. Comment

The central 8-ring of the title compound adopts the boat configuration, and the overall shape of the molecule is that of a saddle. Relative to the mean plane of the saddle seat (C07, C08, C15, C16, $\delta_{r.m.s.}$ = 0.014 Å), the two bicycloheptane moieties (mean planes C07, C08, C22, C24, $\delta_{r.m.s.}$ = 0.001 Å, and C15, C16, C17, C19, $\delta_{r.m.s.}$ = 0.000 Å) bend up 33.36 (5)° and 34.22 (4)°, while the mean planes of the benzo moieties (C01 – C06, $\delta_{r.m.s.}$ = 0.008. and C09 – C14, $\delta_{r.m.s.}$ = 0.013 Å) bend down 33.48 (4)° and 36.58 (4)°.

### S2. Experimental

The preparation is described by Schaller (1994). Suitable crystals were obtained by recrystallization from benzene.

### S3. Refinement

All H atoms were placed in calculated positions, guided by difference maps, with C—H bond distances 0.95 (aromatic C) and 0.99 (alkyl C) Å, and $U_{iso}$=1.2$U_{eq}$, thereafter refined as riding.

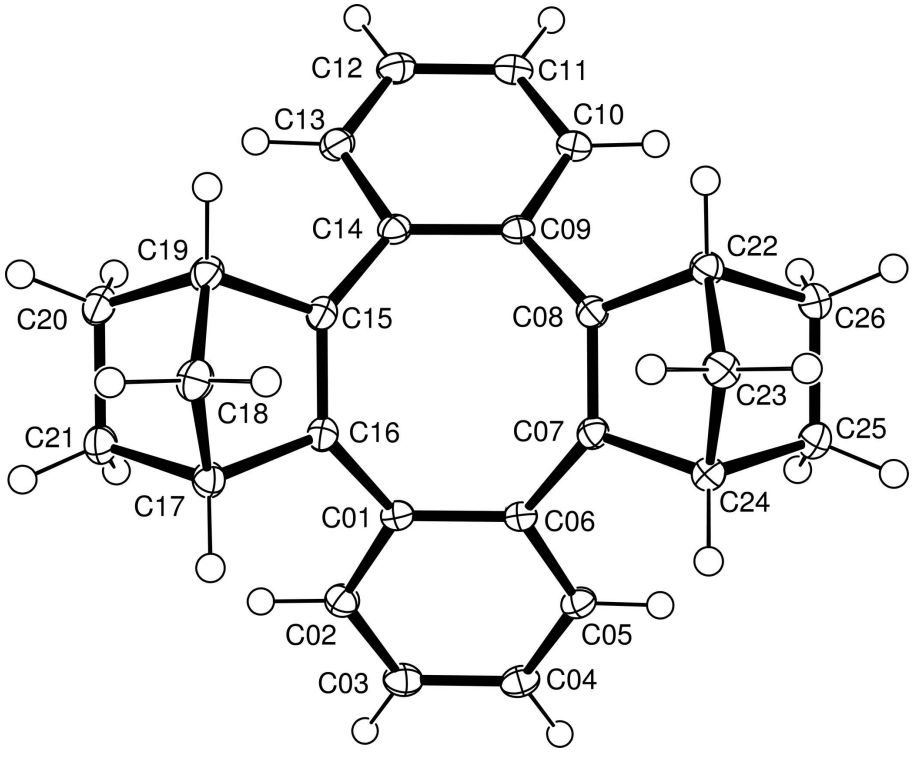

**Figure 1**

View of (I) (50% probability displacement ellipsoids)

**Dibenzo[*a*,*e*]pentacyclo[12.2.1.1$^{6,9}$.0$^{2,13}$.0$^{5,10}$]octadeca- 2(13),5(10)-diene**

*Crystal data*

$C_{26}H_{24}$
$M_r$ = 336.45
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a$ = 9.6962 (4) Å
$b$ = 9.7754 (4) Å
$c$ = 10.3676 (4) Å
$\alpha$ = 77.896 (2)°
$\beta$ = 63.781 (2)°
$\gamma$ = 85.497 (2)°
$V$ = 861.87 (6) Å$^3$
$Z$ = 2
$F(000)$ = 360
$D_x$ = 1.296 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 4596 reflections
$\theta$ = 2.6–30.0°
$\mu$ = 0.07 mm$^{-1}$
$T$ = 90 K
Prism, colorless
0.48 × 0.48 × 0.22 mm

*Data collection*

Nonius KappaCCD diffractometer
Radiation source: sealed tube
Horizonally mounted graphite crystal monochromator
Detector resolution: 9 pixels mm$^{-1}$
CCD rotation images, thick slices scans
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
$T_{min}$ = 0.966, $T_{max}$ = 0.984
8966 measured reflections
5019 independent reflections
4347 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.024
$\theta_{max}$ = 30.0°, $\theta_{min}$ = 2.8°
$h$ = −13→13
$k$ = −13→13
$l$ = −14→14

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.121
$S$ = 1.05
5019 reflections
236 parameters
0 restraints
0 constraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0535P)^2 + 0.4358P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.41 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.015 (4)

*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.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C01 | 0.28621 (12) | 0.39958 (11) | −0.15111 (11) | 0.0134 (2) |

| | | | | |
|---|---|---|---|---|
| C02 | 0.25832 (13) | 0.47525 (12) | −0.26849 (12) | 0.0164 (2) |
| H02 | 0.2906 | 0.4377 | −0.3546 | 0.020* |
| C03 | 0.18494 (13) | 0.60324 (12) | −0.26193 (13) | 0.0182 (2) |
| H03 | 0.1648 | 0.6509 | −0.3415 | 0.022* |
| C04 | 0.14123 (13) | 0.66103 (11) | −0.13797 (13) | 0.0172 (2) |
| H04 | 0.0917 | 0.7489 | −0.1325 | 0.021* |
| C05 | 0.17053 (12) | 0.58930 (11) | −0.02231 (12) | 0.0153 (2) |
| H05 | 0.1424 | 0.6302 | 0.0611 | 0.018* |
| C06 | 0.24068 (12) | 0.45787 (11) | −0.02517 (11) | 0.01283 (19) |
| C07 | 0.27322 (12) | 0.39265 (11) | 0.10023 (11) | 0.01297 (19) |
| C08 | 0.24073 (12) | 0.26227 (11) | 0.18361 (11) | 0.01301 (19) |
| C09 | 0.16507 (12) | 0.14103 (11) | 0.17577 (11) | 0.0130 (2) |
| C10 | 0.04120 (12) | 0.07520 (11) | 0.30452 (12) | 0.0153 (2) |
| H10 | 0.0077 | 0.1117 | 0.3914 | 0.018* |
| C11 | −0.03322 (13) | −0.04209 (12) | 0.30719 (13) | 0.0175 (2) |
| H11 | −0.1194 | −0.0824 | 0.3940 | 0.021* |
| C12 | 0.01873 (14) | −0.10005 (12) | 0.18273 (13) | 0.0187 (2) |
| H12 | −0.0311 | −0.1805 | 0.1840 | 0.022* |
| C13 | 0.14420 (13) | −0.03930 (11) | 0.05642 (12) | 0.0169 (2) |
| H13 | 0.1819 | −0.0814 | −0.0273 | 0.020* |
| C14 | 0.21718 (12) | 0.08297 (11) | 0.04893 (12) | 0.0137 (2) |
| C15 | 0.35046 (12) | 0.14034 (11) | −0.08965 (12) | 0.0137 (2) |
| C16 | 0.37693 (12) | 0.27080 (11) | −0.17235 (11) | 0.0134 (2) |
| C17 | 0.51686 (12) | 0.26307 (11) | −0.31741 (12) | 0.0151 (2) |
| H17 | 0.5725 | 0.3538 | −0.3743 | 0.018* |
| C18 | 0.61003 (13) | 0.15005 (12) | −0.26337 (13) | 0.0171 (2) |
| H18A | 0.6967 | 0.1150 | −0.3443 | 0.021* |
| H18B | 0.6465 | 0.1803 | −0.1982 | 0.021* |
| C19 | 0.47281 (12) | 0.04601 (11) | −0.17980 (12) | 0.0155 (2) |
| H19 | 0.4917 | −0.0432 | −0.1226 | 0.019* |
| C20 | 0.43547 (14) | 0.03038 (12) | −0.30813 (13) | 0.0179 (2) |
| H20A | 0.5039 | −0.0380 | −0.3645 | 0.021* |
| H20B | 0.3271 | 0.0006 | −0.2711 | 0.021* |
| C21 | 0.46571 (14) | 0.18041 (12) | −0.40311 (12) | 0.0183 (2) |
| H21A | 0.3713 | 0.2199 | −0.4096 | 0.022* |
| H21B | 0.5479 | 0.1811 | −0.5033 | 0.022* |
| C22 | 0.27239 (12) | 0.26323 (11) | 0.31521 (12) | 0.0142 (2) |
| H22 | 0.2899 | 0.1695 | 0.3663 | 0.017* |
| C23 | 0.40970 (12) | 0.36642 (12) | 0.24377 (12) | 0.0158 (2) |
| H23A | 0.5024 | 0.3309 | 0.1687 | 0.019* |
| H23B | 0.4350 | 0.3968 | 0.3162 | 0.019* |
| C24 | 0.32682 (12) | 0.47954 (11) | 0.17707 (12) | 0.0146 (2) |
| H24 | 0.3892 | 0.5655 | 0.1138 | 0.018* |
| C25 | 0.18178 (13) | 0.50237 (12) | 0.31881 (12) | 0.0170 (2) |
| H25A | 0.2046 | 0.5684 | 0.3676 | 0.020* |
| H25B | 0.0949 | 0.5382 | 0.2962 | 0.020* |
| C26 | 0.14585 (13) | 0.35287 (12) | 0.41540 (12) | 0.0163 (2) |
| H26A | 0.0416 | 0.3206 | 0.4391 | 0.020* |

| | | | | |
|---|---|---|---|---|
| H26B | 0.1545 | 0.3495 | 0.5077 | 0.020* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C01 | 0.0133 (4) | 0.0118 (4) | 0.0146 (5) | 0.0001 (3) | −0.0060 (4) | −0.0017 (4) |
| C02 | 0.0187 (5) | 0.0156 (5) | 0.0160 (5) | 0.0007 (4) | −0.0090 (4) | −0.0022 (4) |
| C03 | 0.0195 (5) | 0.0166 (5) | 0.0198 (5) | 0.0010 (4) | −0.0116 (4) | 0.0003 (4) |
| C04 | 0.0165 (5) | 0.0129 (5) | 0.0225 (5) | 0.0023 (4) | −0.0099 (4) | −0.0017 (4) |
| C05 | 0.0150 (5) | 0.0124 (5) | 0.0177 (5) | 0.0012 (4) | −0.0065 (4) | −0.0030 (4) |
| C06 | 0.0122 (4) | 0.0114 (4) | 0.0141 (4) | −0.0002 (3) | −0.0055 (4) | −0.0014 (3) |
| C07 | 0.0125 (4) | 0.0125 (5) | 0.0136 (4) | 0.0016 (3) | −0.0053 (4) | −0.0034 (4) |
| C08 | 0.0126 (4) | 0.0134 (5) | 0.0129 (4) | 0.0017 (3) | −0.0054 (4) | −0.0028 (4) |
| C09 | 0.0140 (4) | 0.0112 (4) | 0.0145 (5) | 0.0016 (3) | −0.0076 (4) | −0.0009 (3) |
| C10 | 0.0165 (5) | 0.0141 (5) | 0.0151 (5) | 0.0005 (4) | −0.0075 (4) | −0.0008 (4) |
| C11 | 0.0174 (5) | 0.0149 (5) | 0.0183 (5) | −0.0020 (4) | −0.0077 (4) | 0.0016 (4) |
| C12 | 0.0212 (5) | 0.0137 (5) | 0.0222 (5) | −0.0026 (4) | −0.0111 (4) | −0.0006 (4) |
| C13 | 0.0204 (5) | 0.0136 (5) | 0.0182 (5) | 0.0005 (4) | −0.0098 (4) | −0.0033 (4) |
| C14 | 0.0151 (4) | 0.0117 (4) | 0.0153 (5) | 0.0017 (3) | −0.0080 (4) | −0.0019 (4) |
| C15 | 0.0145 (4) | 0.0134 (5) | 0.0147 (5) | 0.0020 (4) | −0.0073 (4) | −0.0046 (4) |
| C16 | 0.0138 (4) | 0.0142 (5) | 0.0138 (4) | 0.0018 (4) | −0.0068 (4) | −0.0043 (4) |
| C17 | 0.0150 (5) | 0.0157 (5) | 0.0141 (5) | 0.0016 (4) | −0.0055 (4) | −0.0043 (4) |
| C18 | 0.0144 (5) | 0.0185 (5) | 0.0191 (5) | 0.0034 (4) | −0.0071 (4) | −0.0063 (4) |
| C19 | 0.0169 (5) | 0.0138 (5) | 0.0170 (5) | 0.0033 (4) | −0.0081 (4) | −0.0049 (4) |
| C20 | 0.0207 (5) | 0.0164 (5) | 0.0191 (5) | 0.0028 (4) | −0.0096 (4) | −0.0076 (4) |
| C21 | 0.0221 (5) | 0.0189 (5) | 0.0157 (5) | 0.0018 (4) | −0.0089 (4) | −0.0057 (4) |
| C22 | 0.0146 (4) | 0.0142 (5) | 0.0136 (4) | 0.0006 (4) | −0.0063 (4) | −0.0024 (4) |
| C23 | 0.0149 (5) | 0.0174 (5) | 0.0159 (5) | −0.0007 (4) | −0.0074 (4) | −0.0027 (4) |
| C24 | 0.0156 (5) | 0.0136 (5) | 0.0148 (5) | −0.0002 (4) | −0.0067 (4) | −0.0029 (4) |
| C25 | 0.0191 (5) | 0.0154 (5) | 0.0169 (5) | 0.0019 (4) | −0.0075 (4) | −0.0057 (4) |
| C26 | 0.0173 (5) | 0.0169 (5) | 0.0139 (5) | 0.0005 (4) | −0.0058 (4) | −0.0038 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C01—C02 | 1.4082 (14) | C15—C19 | 1.5301 (15) |
| C01—C06 | 1.4099 (15) | C16—C17 | 1.5287 (15) |
| C01—C16 | 1.4758 (14) | C17—C18 | 1.5433 (15) |
| C02—C03 | 1.3891 (15) | C17—C21 | 1.5626 (15) |
| C02—H02 | 0.9500 | C17—H17 | 1.0000 |
| C03—C04 | 1.3914 (16) | C18—C19 | 1.5426 (16) |
| C03—H03 | 0.9500 | C18—H18A | 0.9900 |
| C04—C05 | 1.3883 (15) | C18—H18B | 0.9900 |
| C04—H04 | 0.9500 | C19—C20 | 1.5634 (15) |
| C05—C06 | 1.4054 (14) | C19—H19 | 1.0000 |
| C05—H05 | 0.9500 | C20—C21 | 1.5534 (16) |
| C06—C07 | 1.4763 (14) | C20—H20A | 0.9900 |
| C07—C08 | 1.3532 (14) | C20—H20B | 0.9900 |
| C07—C24 | 1.5314 (15) | C21—H21A | 0.9900 |

| | | | |
|---|---|---|---|
| C08—C09 | 1.4762 (14) | C21—H21B | 0.9900 |
| C08—C22 | 1.5270 (15) | C22—C23 | 1.5378 (15) |
| C09—C10 | 1.4082 (15) | C22—C26 | 1.5617 (15) |
| C09—C14 | 1.4098 (15) | C22—H22 | 1.0000 |
| C10—C11 | 1.3910 (15) | C23—C24 | 1.5420 (15) |
| C10—H10 | 0.9500 | C23—H23A | 0.9900 |
| C11—C12 | 1.3883 (17) | C23—H23B | 0.9900 |
| C11—H11 | 0.9500 | C24—C25 | 1.5650 (15) |
| C12—C13 | 1.3882 (16) | C24—H24 | 1.0000 |
| C12—H12 | 0.9500 | C25—C26 | 1.5550 (15) |
| C13—C14 | 1.4073 (15) | C25—H25A | 0.9900 |
| C13—H13 | 0.9500 | C25—H25B | 0.9900 |
| C14—C15 | 1.4779 (15) | C26—H26A | 0.9900 |
| C15—C16 | 1.3512 (15) | C26—H26B | 0.9900 |

| | | | |
|---|---|---|---|
| C02—C01—C06 | 118.50 (10) | C19—C18—C17 | 93.53 (8) |
| C02—C01—C16 | 118.22 (9) | C19—C18—H18A | 113.0 |
| C06—C01—C16 | 122.92 (9) | C17—C18—H18A | 113.0 |
| C03—C02—C01 | 121.88 (10) | C19—C18—H18B | 113.0 |
| C03—C02—H02 | 119.1 | C17—C18—H18B | 113.0 |
| C01—C02—H02 | 119.1 | H18A—C18—H18B | 110.4 |
| C02—C03—C04 | 119.48 (10) | C15—C19—C18 | 100.09 (8) |
| C02—C03—H03 | 120.3 | C15—C19—C20 | 107.17 (9) |
| C04—C03—H03 | 120.3 | C18—C19—C20 | 100.24 (9) |
| C05—C04—C03 | 119.47 (10) | C15—C19—H19 | 115.7 |
| C05—C04—H04 | 120.3 | C18—C19—H19 | 115.7 |
| C03—C04—H04 | 120.3 | C20—C19—H19 | 115.7 |
| C04—C05—C06 | 121.88 (10) | C21—C20—C19 | 102.90 (9) |
| C04—C05—H05 | 119.1 | C21—C20—H20A | 111.2 |
| C06—C05—H05 | 119.1 | C19—C20—H20A | 111.2 |
| C05—C06—C01 | 118.76 (10) | C21—C20—H20B | 111.2 |
| C05—C06—C07 | 117.87 (9) | C19—C20—H20B | 111.2 |
| C01—C06—C07 | 123.22 (9) | H20A—C20—H20B | 109.1 |
| C08—C07—C06 | 130.51 (10) | C20—C21—C17 | 102.78 (9) |
| C08—C07—C24 | 106.88 (9) | C20—C21—H21A | 111.2 |
| C06—C07—C24 | 121.69 (9) | C17—C21—H21A | 111.2 |
| C07—C08—C09 | 131.06 (10) | C20—C21—H21B | 111.2 |
| C07—C08—C22 | 107.00 (9) | C17—C21—H21B | 111.2 |
| C09—C08—C22 | 121.23 (9) | H21A—C21—H21B | 109.1 |
| C10—C09—C14 | 118.74 (10) | C08—C22—C23 | 100.36 (8) |
| C10—C09—C08 | 117.94 (9) | C08—C22—C26 | 107.65 (8) |
| C14—C09—C08 | 123.18 (9) | C23—C22—C26 | 100.28 (9) |
| C11—C10—C09 | 121.42 (10) | C08—C22—H22 | 115.5 |
| C11—C10—H10 | 119.3 | C23—C22—H22 | 115.5 |
| C09—C10—H10 | 119.3 | C26—C22—H22 | 115.5 |
| C12—C11—C10 | 119.87 (10) | C22—C23—C24 | 93.57 (8) |
| C12—C11—H11 | 120.1 | C22—C23—H23A | 113.0 |
| C10—C11—H11 | 120.1 | C24—C23—H23A | 113.0 |

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| C13—C12—C11 | 119.37 (10) | C22—C23—H23B | 113.0 |
| C13—C12—H12 | 120.3 | C24—C23—H23B | 113.0 |
| C11—C12—H12 | 120.3 | H23A—C23—H23B | 110.4 |
| C12—C13—C14 | 121.84 (10) | C07—C24—C23 | 100.19 (8) |
| C12—C13—H13 | 119.1 | C07—C24—C25 | 106.63 (8) |
| C14—C13—H13 | 119.1 | C23—C24—C25 | 100.53 (8) |
| C13—C14—C09 | 118.66 (10) | C07—C24—H24 | 115.8 |
| C13—C14—C15 | 118.30 (10) | C23—C24—H24 | 115.8 |
| C09—C14—C15 | 122.96 (9) | C25—C24—H24 | 115.8 |
| C16—C15—C14 | 129.94 (10) | C26—C25—C24 | 102.79 (8) |
| C16—C15—C19 | 107.15 (9) | C26—C25—H25A | 111.2 |
| C14—C15—C19 | 122.01 (9) | C24—C25—H25A | 111.2 |
| C15—C16—C01 | 131.40 (10) | C26—C25—H25B | 111.2 |
| C15—C16—C17 | 106.96 (9) | C24—C25—H25B | 111.2 |
| C01—C16—C17 | 121.07 (9) | H25A—C25—H25B | 109.1 |
| C16—C17—C18 | 100.22 (8) | C25—C26—C22 | 102.68 (8) |
| C16—C17—C21 | 107.22 (9) | C25—C26—H26A | 111.2 |
| C18—C17—C21 | 100.36 (9) | C22—C26—H26A | 111.2 |
| C16—C17—H17 | 115.6 | C25—C26—H26B | 111.2 |
| C18—C17—H17 | 115.6 | C22—C26—H26B | 111.2 |
| C21—C17—H17 | 115.6 | H26A—C26—H26B | 109.1 |

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| C06—C01—C02—C03 | −1.34 (16) | C14—C15—C16—C17 | −169.06 (10) |
| C16—C01—C02—C03 | −174.67 (10) | C19—C15—C16—C17 | 0.00 (11) |
| C01—C02—C03—C04 | 1.86 (17) | C02—C01—C16—C15 | −130.46 (12) |
| C02—C03—C04—C05 | −0.52 (17) | C06—C01—C16—C15 | 56.53 (17) |
| C03—C04—C05—C06 | −1.31 (16) | C02—C01—C16—C17 | 39.74 (14) |
| C04—C05—C06—C01 | 1.81 (16) | C06—C01—C16—C17 | −133.27 (11) |
| C04—C05—C06—C07 | 177.38 (10) | C15—C16—C17—C18 | −33.99 (11) |
| C02—C01—C06—C05 | −0.48 (15) | C01—C16—C17—C18 | 153.68 (9) |
| C16—C01—C06—C05 | 172.52 (10) | C15—C16—C17—C21 | 70.33 (11) |
| C02—C01—C06—C07 | −175.80 (10) | C01—C16—C17—C21 | −102.00 (11) |
| C16—C01—C06—C07 | −2.80 (16) | C16—C17—C18—C19 | 51.33 (9) |
| C05—C06—C07—C08 | 130.07 (12) | C21—C17—C18—C19 | −58.47 (9) |
| C01—C06—C07—C08 | −54.57 (16) | C16—C15—C19—C18 | 33.99 (11) |
| C05—C06—C07—C24 | −37.51 (14) | C14—C15—C19—C18 | −155.89 (9) |
| C01—C06—C07—C24 | 137.85 (10) | C16—C15—C19—C20 | −70.13 (11) |
| C06—C07—C08—C09 | 1.38 (19) | C14—C15—C19—C20 | 99.99 (11) |
| C24—C07—C08—C09 | 170.36 (10) | C17—C18—C19—C15 | −51.23 (9) |
| C06—C07—C08—C22 | −168.83 (10) | C17—C18—C19—C20 | 58.45 (9) |
| C24—C07—C08—C22 | 0.14 (11) | C15—C19—C20—C21 | 67.15 (10) |
| C07—C08—C09—C10 | −128.15 (12) | C18—C19—C20—C21 | −36.87 (10) |
| C22—C08—C09—C10 | 40.89 (14) | C19—C20—C21—C17 | 0.10 (11) |
| C07—C08—C09—C14 | 56.15 (16) | C16—C17—C21—C20 | −67.52 (10) |
| C22—C08—C09—C14 | −134.80 (10) | C18—C17—C21—C20 | 36.70 (10) |
| C14—C09—C10—C11 | −2.22 (15) | C07—C08—C22—C23 | −34.13 (10) |
| C08—C09—C10—C11 | −178.12 (10) | C09—C08—C22—C23 | 154.49 (9) |
| C09—C10—C11—C12 | 2.77 (17) | C07—C08—C22—C26 | 70.26 (10) |

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| C10—C11—C12—C13 | −0.42 (17) | C09—C08—C22—C26 | −101.12 (11) |
| C11—C12—C13—C14 | −2.45 (17) | C08—C22—C23—C24 | 51.37 (9) |
| C12—C13—C14—C09 | 2.95 (16) | C26—C22—C23—C24 | −58.90 (9) |
| C12—C13—C14—C15 | 179.75 (10) | C08—C07—C24—C23 | 33.77 (10) |
| C10—C09—C14—C13 | −0.60 (15) | C06—C07—C24—C23 | −156.07 (9) |
| C08—C09—C14—C13 | 175.07 (10) | C08—C07—C24—C25 | −70.56 (10) |
| C10—C09—C14—C15 | −177.24 (10) | C06—C07—C24—C25 | 99.60 (11) |
| C08—C09—C14—C15 | −1.58 (15) | C22—C23—C24—C07 | −51.19 (9) |
| C13—C14—C15—C16 | 127.20 (12) | C22—C23—C24—C25 | 58.03 (9) |
| C09—C14—C15—C16 | −56.14 (16) | C07—C24—C25—C26 | 68.46 (10) |
| C13—C14—C15—C19 | −40.45 (14) | C23—C24—C25—C26 | −35.62 (10) |
| C09—C14—C15—C19 | 136.20 (11) | C24—C25—C26—C22 | −1.28 (10) |
| C14—C15—C16—C01 | 2.17 (19) | C08—C22—C26—C25 | −66.56 (10) |
| C19—C15—C16—C01 | 171.23 (11) | C23—C22—C26—C25 | 37.88 (10) |