IUCrData

ISSN 2414-3146

7-*tert*-Butyl-1,3-bis(ethoxymethyl)pyrene

Tetsuji Moriguchi,[a]* Misa Sasaki[a] and Noriko Miyoshi[b]

[a]Department of Material Science, Faculty of Engineering, Kyushu Institute of Technology, 1-1 Sensui-cho, Tobata-ku Kitakyushu, Fukuoka, Japan, and [b]Technical Support Department, Management Headquarters, Kyushu Institute of Technology, 1-1 Sensui-cho, Tobata-ku, Kitakyushu 804-8550, Japan. *Correspondence e-mail: moriguchi.tetsuji917@mail.kyutech.jp

Received 6 March 2026
Accepted 20 April 2026

Edited by M. Weil, Vienna University of Technology, Austria

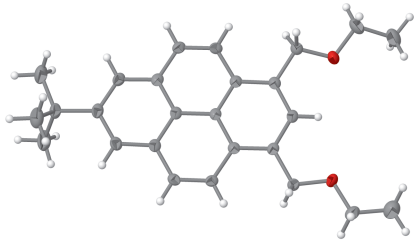
Keywords: crystal structure; substituted pyrene derivative; π–π interactions.

CCDC reference: 2547421

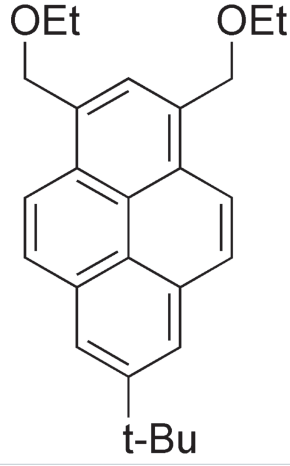
Structural data: full structural data are available from iucrdata.iucr.org

In the molecular structure of the title compound, $C_{26}H_{30}O_2$, the two ethoxymethyl side arms are twisted from the almost planar pyrene system by 29.85 (17) and 15.16 (18)°. In the crystal, adjacent molecules are arranged in pairs that mainly interact through π–π interactions.

3D view



Chemical scheme



Structure description

In recent years, polycyclic aromatic hydrocarbons (PAHs) have been attracting great interest owing to their significant photochemical and electrical properties (Dötz *et al.*, 2000). In the PAHs, pyrene and its derivatives are probably the most studied compounds. They constitute an important class of PAHs found in charcoal and are valuable as intermediates. Moreover, the PAHs comprising the pyrene moiety exhibit *p*-type semiconductor properties (Moriguchi *et al.*, 2017). In the context of our previous studies with respect to substituted pyrene derivatives (Moriguchi *et al.*, 2015; Moriguchi *et al.*, 2018) or a lanthanum complex with four pyrene moieties (Moriguchi *et al.*, 2014), in order to evaluate its fluorescence properties, we report here the result of the crystal structure analysis of 7-*tert*-butyl-1,3-bis(ethoxymethyl)pyrene.

The molecular structure is shown in Fig. 1. The pyrene ring system is almost planar, with an r.m.s. deviation of the non-H atoms of 0.011 Å. The dihedral angles between the planes of the pyrene system and the ethoxymethyl groups are 29.85 (17) (C21/O1/C23/C24) and 15.16 (18)° (C22/O2/C25/C26).

The packing of the molecules within the unit cell is shown in Fig. 2. A particular arrangement results from π–π interactions between molecules arranged in pairs (Fig. 3), with centroid-to-centroid distances of *Cg*1···*Cg*3′ of 3.6216 (8) Å (slippage 1.115 Å), *Cg*1···*Cg*2′ of 3.9104 (8) Å (slippage 1.840 Å), *Cg*1···*Cg*4′ of 3.7156 (8) Å (slippage 1.408 Å) and *Cg*3···*Cg*2′ of 3.7092 (8) Å (slippage 1.403 Å) [*Cg*1 is the centroid of ring C1–C4/C14/C15 (plane 1), *Cg*2 is the centroid of ring C11–C16 (plane 2), *Cg*3 is the centroid of ring C4–C7/C15/C16 (plane 3) and *Cg*4 is the centroid of ring C7–C11/C16

OPEN ACCESS
Published under a CC BY 4.0 licence

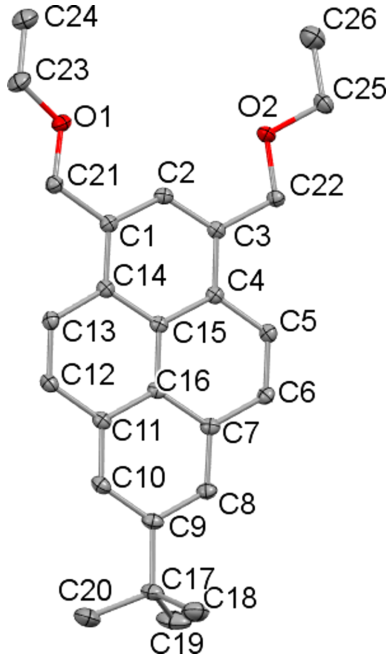


Figure 1
The molecular structure and atom-numbering scheme for the title compound, with displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted for clarity.

(plane 4); symmetry code for primed centroids: $-x+\frac{1}{2}, -y+\frac{1}{2}, -z$]. These values are approximately equal or smaller than the sum of the van der Waals radii of aromatic planes (Rowland & Taylor, 1996).

Synthesis and crystallization

A tetrahydrofuran solution (50 ml) of 4-*tert*-butyl-1,3-bis-(chloromethyl)pyrene (0.10 mmol) was added dropwise to ethanol (1 mmol) in the presence of an excess of sodium (0.5 mmol). The mixed solution was then stirred for 3 h at room temperature before the volatiles were removed under reduced pressure. The crude reaction mixture was subjected to column chromatography using EtOAc/hexane as the mobile phase. The title compound was isolated as a yellow fluorescent solid with 80% yield. Single crystals were obtained by the vapour diffusion method at room temperature by diffusion of hexane into a chloroform solution. MS: M^+, 374.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{26}H_{30}O_2$
M_r	374.50
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	90
a, *b*, *c* (Å)	31.563 (2), 13.4849 (10), 9.4170 (7)
β (°)	92.464 (1)
V (Å^3)	4004.4 (5)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.50 × 0.35 × 0.25
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.666, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	23061, 4876, 3900
R_{int}	0.031
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.676
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.055, 0.173, 1.05
No. of reflections	4876
No. of parameters	258
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.46, −0.47

Computer programs: *SMART* and *SAINT* (Bruker, 2009), *SHELXS* (Sheldrick, 2008), *SHELXL* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

Refinement

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

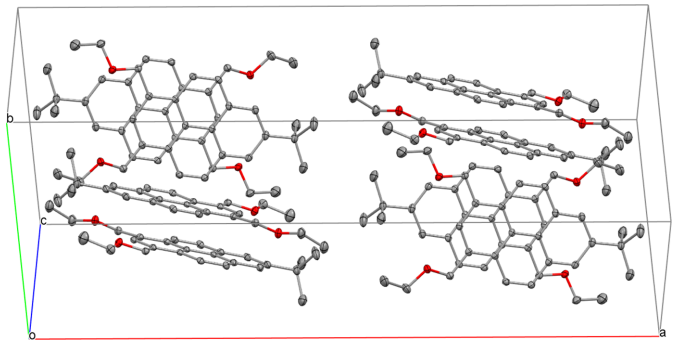


Figure 2
Packing diagram of the title compound, with displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted for clarity.

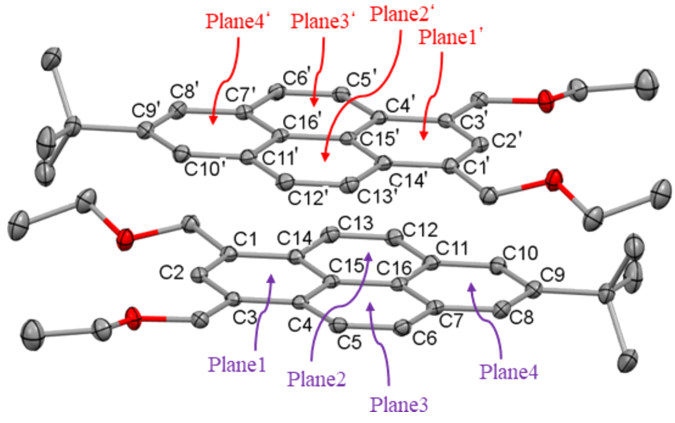


Figure 3
A pair of molecules linked by intermolecular π–π interactions and definitions of the planes. The molecule with primed labels is related by symmetry code $(-x+\frac{1}{2}, -y+\frac{1}{2}, -z)$.

Acknowledgements

The authors are grateful to the Center for Instrumental Analysis, Kyushu Institute of Technology (KITCIA), for the X-ray analysis.

References

Bruker (2009). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.

Dötz, F., Brand, J. D., Ito, S., Gherghel, L. & Müllen, K. (2000). *J. Am. Chem. Soc.* **122**, 7707–7717.

Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.

Moriguchi, T., Higashi, M., Yakeya, D., Venkataprasad, J., Tsuge, A., Okauchi, T., Nagamatsu, S. & Takashima, W. (2017). *J. Mol. Struct.* **1127**, 413–418.

Moriguchi, T., Kitou, N., Iwamoto, T., Yoza, K. & Tsuge, A. (2015). *J. Chem. Res.* **39**, 351–356.

Moriguchi, T., Yakeya, D., Tsuge, A. & Venkataprasad, J. (2018). *J. Mol. Struct.* **1157**, 348–354.

Moriguchi, T., Yoza, K. & Tsuge, A. (2014). *J. Crystallogr.* Article ID 271238.

Rowland, R. S. & Taylor, R. (1996). *J. Phys. Chem.* **100**, 7384–7391.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.

Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

full crystallographic data

IUCrData (2026). **11**, x260413 [https://doi.org/10.1107/S241431462600413X]

7-*tert*-Butyl-1,3-bis(ethoxymethyl)pyrene

Tetsuji Moriguchi, Misa Sasaki and Noriko Miyoshi

7-*tert*-Butyl-1,3-bis(ethoxymethyl)pyrene

Crystal data

$C_{26}H_{30}O_2$
M_r = 374.50
Monoclinic, $C2/c$
a = 31.563 (2) Å
b = 13.4849 (10) Å
c = 9.4170 (7) Å
β = 92.464 (1)°
V = 4004.4 (5) Å^3
Z = 8
$F(000)$ = 1616
D_x = 1.242 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7217 reflections
θ = 2.5–28.5°
μ = 0.08 mm^{-1}
T = 90 K
Prism, clear light colourless
0.50 × 0.35 × 0.25 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
Detector resolution: 8 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.666, T_{max} = 0.746
23061 measured reflections
4876 independent reflections
3900 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 28.7°, θ_{min} = 1.6°
h = −40→41
k = −17→18
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.173
S = 1.05
4876 reflections
258 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0977P)^2 + 3.0623P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.12093 (3)	0.49719 (8)	0.09130 (12)	0.0282 (3)
O2	0.14358 (3)	0.23373 (8)	0.39513 (11)	0.0264 (3)
C1	0.18957 (4)	0.41990 (10)	0.09130 (14)	0.0202 (3)
C2	0.17553 (4)	0.35367 (10)	0.19234 (14)	0.0200 (3)
H2	0.147300	0.356026	0.216684	0.024*
C3	0.20235 (4)	0.28392 (10)	0.25827 (13)	0.0189 (3)
C4	0.24518 (4)	0.27928 (10)	0.22227 (13)	0.0184 (3)
C5	0.27447 (4)	0.20736 (10)	0.28424 (14)	0.0207 (3)
H5	0.264937	0.162385	0.350582	0.025*
C6	0.31544 (4)	0.20404 (11)	0.24785 (14)	0.0221 (3)
H6	0.333469	0.156872	0.289762	0.026*
C7	0.33165 (4)	0.27162 (10)	0.14618 (14)	0.0208 (3)
C8	0.37391 (4)	0.26903 (11)	0.10699 (15)	0.0242 (3)
H8	0.392067	0.222113	0.148895	0.029*
C9	0.38982 (4)	0.33436 (11)	0.00726 (15)	0.0249 (3)
C10	0.36178 (4)	0.40291 (11)	−0.05576 (15)	0.0237 (3)
H10	0.371724	0.446394	−0.123375	0.028*
C11	0.31912 (4)	0.40857 (10)	−0.02072 (14)	0.0208 (3)
C12	0.29017 (4)	0.47819 (11)	−0.08668 (15)	0.0230 (3)
H12	0.299875	0.521467	−0.154981	0.028*
C13	0.24900 (4)	0.48248 (10)	−0.05191 (15)	0.0220 (3)
H13	0.231062	0.528372	−0.097248	0.026*
C14	0.23239 (4)	0.41764 (10)	0.05358 (14)	0.0197 (3)
C15	0.26024 (4)	0.34700 (10)	0.12030 (13)	0.0180 (3)
C16	0.30358 (4)	0.34268 (10)	0.08249 (14)	0.0190 (3)
C17	0.43655 (5)	0.32752 (13)	−0.02992 (17)	0.0297 (3)
C18	0.44405 (6)	0.22943 (15)	−0.1055 (2)	0.0440 (5)
H18A	0.436099	0.175498	−0.045671	0.066*
H18B	0.473517	0.223630	−0.125507	0.066*
H18C	0.427258	0.227436	−0.192908	0.066*
C19	0.46469 (6)	0.3341 (2)	0.1055 (2)	0.0526 (6)
H19A	0.458905	0.394888	0.154212	0.079*
H19B	0.493939	0.332769	0.081555	0.079*
H19C	0.458934	0.278932	0.166122	0.079*
C20	0.44954 (6)	0.41281 (16)	−0.1274 (2)	0.0488 (5)
H20A	0.432821	0.410135	−0.214909	0.073*
H20B	0.479018	0.406459	−0.146977	0.073*
H20C	0.444898	0.475073	−0.081145	0.073*
C21	0.15861 (4)	0.48931 (11)	0.01536 (15)	0.0236 (3)
H21A	0.171421	0.554309	0.006909	0.028*
H21B	0.151861	0.464552	−0.079645	0.028*
C22	0.18585 (4)	0.21118 (10)	0.36365 (14)	0.0211 (3)
H22A	0.187148	0.144655	0.324899	0.025*
H22B	0.203585	0.213168	0.450330	0.025*
C23	0.08765 (5)	0.54219 (14)	0.0076 (2)	0.0377 (4)

H23A	0.079379	0.499682	−0.071942	0.045*
H23B	0.097029	0.605225	−0.029458	0.045*
C24	0.05040 (6)	0.55790 (16)	0.1017 (2)	0.0463 (5)
H24A	0.027562	0.588779	0.047480	0.069*
H24B	0.058927	0.599810	0.180190	0.069*
H24C	0.041134	0.495061	0.136829	0.069*
C25	0.12618 (5)	0.15790 (12)	0.47949 (17)	0.0310 (3)
H25A	0.144671	0.146157	0.562741	0.037*
H25B	0.124111	0.096805	0.425257	0.037*
C26	0.08382 (6)	0.18715 (17)	0.5240 (2)	0.0510 (5)
H26A	0.065729	0.199860	0.441426	0.076*
H26B	0.086119	0.246069	0.581013	0.076*
H26C	0.071990	0.134609	0.578500	0.076*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0200 (5)	0.0328 (6)	0.0319 (6)	0.0042 (4)	0.0009 (4)	0.0053 (4)
O2	0.0232 (5)	0.0280 (5)	0.0286 (5)	0.0012 (4)	0.0092 (4)	0.0056 (4)
C1	0.0207 (6)	0.0205 (6)	0.0191 (6)	−0.0004 (5)	−0.0011 (5)	−0.0030 (5)
C2	0.0186 (6)	0.0229 (7)	0.0186 (6)	−0.0017 (5)	0.0005 (5)	−0.0035 (5)
C3	0.0210 (6)	0.0207 (6)	0.0150 (6)	−0.0024 (5)	0.0010 (5)	−0.0035 (5)
C4	0.0204 (6)	0.0195 (6)	0.0152 (6)	−0.0018 (5)	−0.0014 (5)	−0.0036 (5)
C5	0.0231 (7)	0.0229 (6)	0.0160 (6)	−0.0017 (5)	−0.0012 (5)	−0.0002 (5)
C6	0.0213 (6)	0.0245 (7)	0.0199 (6)	0.0011 (5)	−0.0034 (5)	0.0002 (5)
C7	0.0194 (6)	0.0254 (7)	0.0174 (6)	−0.0019 (5)	−0.0017 (5)	−0.0036 (5)
C8	0.0193 (7)	0.0293 (7)	0.0238 (7)	−0.0002 (5)	−0.0022 (5)	−0.0016 (6)
C9	0.0195 (6)	0.0314 (7)	0.0238 (7)	−0.0043 (6)	0.0010 (5)	−0.0044 (6)
C10	0.0219 (7)	0.0280 (7)	0.0213 (7)	−0.0066 (5)	0.0012 (5)	−0.0003 (5)
C11	0.0215 (7)	0.0234 (7)	0.0173 (6)	−0.0047 (5)	−0.0007 (5)	−0.0030 (5)
C12	0.0239 (7)	0.0250 (7)	0.0199 (6)	−0.0054 (5)	−0.0002 (5)	0.0020 (5)
C13	0.0235 (7)	0.0219 (6)	0.0202 (6)	−0.0014 (5)	−0.0022 (5)	0.0012 (5)
C14	0.0211 (6)	0.0205 (6)	0.0173 (6)	−0.0026 (5)	−0.0012 (5)	−0.0027 (5)
C15	0.0189 (6)	0.0201 (6)	0.0148 (6)	−0.0032 (5)	−0.0012 (5)	−0.0043 (5)
C16	0.0186 (6)	0.0217 (6)	0.0166 (6)	−0.0034 (5)	−0.0014 (5)	−0.0047 (5)
C17	0.0181 (7)	0.0408 (9)	0.0304 (8)	−0.0033 (6)	0.0023 (6)	0.0003 (7)
C18	0.0296 (9)	0.0502 (11)	0.0529 (11)	0.0012 (8)	0.0112 (8)	−0.0052 (9)
C19	0.0233 (8)	0.0935 (17)	0.0408 (10)	−0.0099 (9)	−0.0019 (7)	−0.0037 (10)
C20	0.0279 (9)	0.0553 (12)	0.0643 (13)	−0.0033 (8)	0.0137 (8)	0.0125 (10)
C21	0.0222 (7)	0.0249 (7)	0.0238 (7)	0.0007 (5)	0.0006 (5)	0.0009 (5)
C22	0.0212 (7)	0.0233 (6)	0.0190 (6)	0.0005 (5)	0.0017 (5)	−0.0007 (5)
C23	0.0278 (8)	0.0406 (9)	0.0440 (10)	0.0084 (7)	−0.0060 (7)	0.0047 (7)
C24	0.0290 (9)	0.0485 (11)	0.0613 (13)	0.0075 (8)	−0.0006 (8)	0.0051 (9)
C25	0.0322 (8)	0.0314 (8)	0.0297 (8)	−0.0051 (6)	0.0063 (6)	0.0058 (6)
C26	0.0440 (11)	0.0556 (12)	0.0543 (12)	0.0011 (9)	0.0127 (9)	0.0115 (10)

Geometric parameters (Å, º)

O1—C21	1.4177 (17)	C14—C15	1.4239 (19)
O1—C23	1.4219 (18)	C15—C16	1.4295 (18)
O2—C22	1.4123 (16)	C17—C18	1.525 (3)
O2—C25	1.4198 (18)	C17—C19	1.525 (2)
C1—C2	1.3912 (19)	C17—C20	1.538 (2)
C1—C14	1.4126 (19)	C18—H18A	0.9600
C1—C21	1.5107 (19)	C18—H18B	0.9600
C2—H2	0.9300	C18—H18C	0.9600
C2—C3	1.3935 (19)	C19—H19A	0.9600
C3—C4	1.4089 (18)	C19—H19B	0.9600
C3—C22	1.5042 (18)	C19—H19C	0.9600
C4—C5	1.4455 (19)	C20—H20A	0.9600
C4—C15	1.4217 (18)	C20—H20B	0.9600
C5—H5	0.9300	C20—H20C	0.9600
C5—C6	1.3527 (19)	C21—H21A	0.9700
C6—H6	0.9300	C21—H21B	0.9700
C6—C7	1.4321 (19)	C22—H22A	0.9700
C7—C8	1.3998 (19)	C22—H22B	0.9700
C7—C16	1.4201 (19)	C23—H23A	0.9700
C8—H8	0.9300	C23—H23B	0.9700
C8—C9	1.397 (2)	C23—C24	1.517 (3)
C9—C10	1.395 (2)	C24—H24A	0.9600
C9—C17	1.533 (2)	C24—H24B	0.9600
C10—H10	0.9300	C24—H24C	0.9600
C10—C11	1.4021 (19)	C25—H25A	0.9700
C11—C12	1.433 (2)	C25—H25B	0.9700
C11—C16	1.4196 (19)	C25—C26	1.472 (2)
C12—H12	0.9300	C26—H26A	0.9600
C12—C13	1.3550 (19)	C26—H26B	0.9600
C13—H13	0.9300	C26—H26C	0.9600
C13—C14	1.4390 (19)		
C21—O1—C23	111.60 (12)	C19—C17—C20	107.14 (15)
C22—O2—C25	110.73 (11)	C17—C18—H18A	109.5
C2—C1—C14	119.64 (12)	C17—C18—H18B	109.5
C2—C1—C21	120.19 (12)	C17—C18—H18C	109.5
C14—C1—C21	120.05 (12)	H18A—C18—H18B	109.5
C1—C2—H2	118.9	H18A—C18—H18C	109.5
C1—C2—C3	122.19 (13)	H18B—C18—H18C	109.5
C3—C2—H2	118.9	C17—C19—H19A	109.5
C2—C3—C4	119.57 (12)	C17—C19—H19B	109.5
C2—C3—C22	120.87 (12)	C17—C19—H19C	109.5
C4—C3—C22	119.52 (12)	H19A—C19—H19B	109.5
C3—C4—C5	122.42 (12)	H19A—C19—H19C	109.5
C3—C4—C15	119.09 (12)	H19B—C19—H19C	109.5
C15—C4—C5	118.48 (12)	C17—C20—H20A	109.5

C4—C5—H5	119.3	C17—C20—H20B	109.5
C6—C5—C4	121.45 (13)	C17—C20—H20C	109.5
C6—C5—H5	119.3	H20A—C20—H20B	109.5
C5—C6—H6	119.3	H20A—C20—H20C	109.5
C5—C6—C7	121.41 (13)	H20B—C20—H20C	109.5
C7—C6—H6	119.3	O1—C21—C1	110.31 (11)
C8—C7—C6	122.16 (13)	O1—C21—H21A	109.6
C8—C7—C16	119.31 (13)	O1—C21—H21B	109.6
C16—C7—C6	118.52 (12)	C1—C21—H21A	109.6
C7—C8—H8	118.8	C1—C21—H21B	109.6
C9—C8—C7	122.39 (13)	H21A—C21—H21B	108.1
C9—C8—H8	118.8	O2—C22—C3	110.80 (11)
C8—C9—C17	119.52 (13)	O2—C22—H22A	109.5
C10—C9—C8	117.68 (13)	O2—C22—H22B	109.5
C10—C9—C17	122.80 (13)	C3—C22—H22A	109.5
C9—C10—H10	118.9	C3—C22—H22B	109.5
C9—C10—C11	122.28 (13)	H22A—C22—H22B	108.1
C11—C10—H10	118.9	O1—C23—H23A	110.1
C10—C11—C12	122.31 (12)	O1—C23—H23B	110.1
C10—C11—C16	119.37 (13)	O1—C23—C24	107.98 (15)
C16—C11—C12	118.32 (12)	H23A—C23—H23B	108.4
C11—C12—H12	119.2	C24—C23—H23A	110.1
C13—C12—C11	121.56 (13)	C24—C23—H23B	110.1
C13—C12—H12	119.2	C23—C24—H24A	109.5
C12—C13—H13	119.3	C23—C24—H24B	109.5
C12—C13—C14	121.50 (13)	C23—C24—H24C	109.5
C14—C13—H13	119.3	H24A—C24—H24B	109.5
C1—C14—C13	122.78 (12)	H24A—C24—H24C	109.5
C1—C14—C15	118.86 (12)	H24B—C24—H24C	109.5
C15—C14—C13	118.35 (12)	O2—C25—H25A	109.6
C4—C15—C14	120.64 (12)	O2—C25—H25B	109.6
C4—C15—C16	119.57 (12)	O2—C25—C26	110.12 (14)
C14—C15—C16	119.77 (12)	H25A—C25—H25B	108.1
C7—C16—C15	120.56 (12)	C26—C25—H25A	109.6
C11—C16—C7	118.94 (12)	C26—C25—H25B	109.6
C11—C16—C15	120.49 (12)	C25—C26—H26A	109.5
C9—C17—C20	112.03 (14)	C25—C26—H26B	109.5
C18—C17—C9	109.20 (13)	C25—C26—H26C	109.5
C18—C17—C20	108.61 (15)	H26A—C26—H26B	109.5
C19—C17—C9	109.68 (13)	H26A—C26—H26C	109.5
C19—C17—C18	110.15 (16)	H26B—C26—H26C	109.5

C1—C2—C3—C4	−0.15 (19)	C9—C10—C11—C12	−179.23 (13)
C1—C2—C3—C22	−178.02 (12)	C9—C10—C11—C16	0.1 (2)
C1—C14—C15—C4	0.52 (19)	C10—C9—C17—C18	−112.72 (17)
C1—C14—C15—C16	179.28 (11)	C10—C9—C17—C19	126.49 (18)
C2—C1—C14—C13	178.77 (12)	C10—C9—C17—C20	7.6 (2)
C2—C1—C14—C15	0.11 (19)	C10—C11—C12—C13	179.79 (13)

C2—C1—C21—O1	18.16 (18)	C10—C11—C16—C7	−0.90 (19)
C2—C3—C4—C5	−178.61 (12)	C10—C11—C16—C15	179.90 (11)
C2—C3—C4—C15	0.78 (18)	C11—C12—C13—C14	0.3 (2)
C2—C3—C22—O2	−7.55 (17)	C12—C11—C16—C7	178.45 (12)
C3—C4—C5—C6	179.82 (12)	C12—C11—C16—C15	−0.76 (19)
C3—C4—C15—C14	−0.97 (18)	C12—C13—C14—C1	−179.53 (13)
C3—C4—C15—C16	−179.72 (11)	C12—C13—C14—C15	−0.9 (2)
C4—C3—C22—O2	174.58 (11)	C13—C14—C15—C4	−178.20 (12)
C4—C5—C6—C7	0.0 (2)	C13—C14—C15—C16	0.55 (18)
C4—C15—C16—C7	−0.18 (18)	C14—C1—C2—C3	−0.3 (2)
C4—C15—C16—C11	179.01 (11)	C14—C1—C21—O1	−165.83 (12)
C5—C4—C15—C14	178.44 (12)	C14—C15—C16—C7	−178.95 (12)
C5—C4—C15—C16	−0.31 (18)	C14—C15—C16—C11	0.24 (19)
C5—C6—C7—C8	−179.81 (13)	C15—C4—C5—C6	0.43 (19)
C5—C6—C7—C16	−0.5 (2)	C16—C7—C8—C9	0.3 (2)
C6—C7—C8—C9	179.60 (13)	C16—C11—C12—C13	0.5 (2)
C6—C7—C16—C11	−178.64 (12)	C17—C9—C10—C11	−179.90 (13)
C6—C7—C16—C15	0.57 (19)	C21—O1—C23—C24	−173.86 (14)
C7—C8—C9—C10	−1.0 (2)	C21—C1—C2—C3	175.73 (12)
C7—C8—C9—C17	179.70 (13)	C21—C1—C14—C13	2.7 (2)
C8—C7—C16—C11	0.73 (19)	C21—C1—C14—C15	−175.92 (12)
C8—C7—C16—C15	179.94 (12)	C22—O2—C25—C26	174.09 (14)
C8—C9—C10—C11	0.9 (2)	C22—C3—C4—C5	−0.71 (19)
C8—C9—C17—C18	66.50 (18)	C22—C3—C4—C15	178.67 (11)
C8—C9—C17—C19	−54.3 (2)	C23—O1—C21—C1	−166.10 (12)
C8—C9—C17—C20	−173.13 (15)	C25—O2—C22—C3	172.25 (11)