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9,9-Bis[4-(2-chloroethoxy)phenyl]-9H-fluorene

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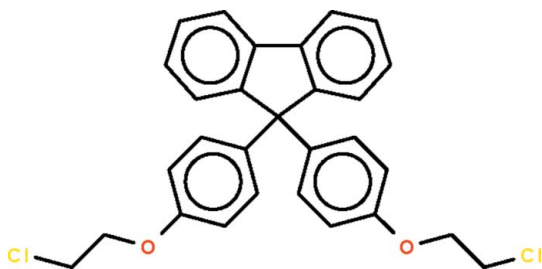
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.061; wR factor = 0.177; data-to-parameter ratio = 14.1.

The title compound, $\text{C}_{29}\text{H}_{24}\text{Cl}_2\text{O}_2$, a fluorene derivative, features a C atom that is connected to four phenylene rings, two of which are almost coplanar (r.m.s. deviation = 0.035 Å) as they belong to the fluorene system. The other two rings are aligned at angles of 67.5 (5) and 85.5 (5)° with respect to the pair. The O and Cl atoms of the $-\text{OCH}_2\text{CH}_2\text{Cl}-$ units adopt a *gauche* conformation [torsion angles = 61.6 (6) and 66.6 (5)°].

Related literature

For related structures, see: Shah *et al.* (2010*a,b*).

Experimental

Crystal data

$\text{C}_{29}\text{H}_{24}\text{Cl}_2\text{O}_2$
 $M_r = 475.38$
 Monoclinic, $P2_1/c$
 $a = 12.2334$ (7) Å
 $b = 10.8063$ (6) Å
 $c = 19.0374$ (12) Å
 $\beta = 108.172$ (2)°

$V = 2391.2$ (2) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.30$ mm⁻¹
 $T = 293$ K
 $0.27 \times 0.15 \times 0.07$ mm

Data collection

Bruker Kappa APEXII diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.783$, $T_{\max} = 0.862$

18388 measured reflections
 4206 independent reflections
 2326 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.062$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.061$
 $wR(F^2) = 0.177$
 $S = 1.01$
 4206 reflections

298 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.53$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.66$ e Å⁻³

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: X-SEED (Barbour, 2001); software used to prepare material for publication: publCIF (Westrip, 2010).

We thank the Higher Education Commission of Pakistan, GC University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NK2052).

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supplementary materials

Acta Cryst. (2010). E66, o2317 [doi:10.1107/S1600536810032046]

9,9-Bis[4-(2-chloroethoxy)phenyl]-9H-fluorene

K. Shah, M. Raza Shah, I. U. Khan and S. W. Ng

Comment

We are interested in *V*-shaped molecules; in the title compound, the kink is provided by the carbon atom of the fluorene system that is also connected to two other aromatic rings having *para* substituents (Scheme I). The compound is synthesized from 9,9-bis[4-(2-hydroxyethoxy)phenyl]fluorene, a commercially available reagent. The compound features a carbon atom that is connected to four phenylene rings, two of which are coplanar as these belong to the fluorene system (Fig. 1). The other two rings are aligned at angles of 67.5 (5) and 85.5 (5) ° with respect to the pair. The oxygen and chlorine atoms of the –OCH₂CH₂Cl– units adopt a *gauche* conformation [torsion angles 61.6 (6), 66.6 (5) °].

Experimental

9,9-Bis[4-(2-hydroxyethoxy)phenyl]fluorene (0.5 g, 3.5 mmol) was dissolved in dichloromethane (20 ml) to give a clear solution. Thionyl chloride (5 ml) along with two drops of *N,N*-dimethylformamide (to serve as catalyst) were added. The mixture was heated for 12 h. Aqueous ammonium hydroxide was added and the precipitated product was extracted with dichloromethane. The compound was recrystallized from dichloromethane/hexane (7:3).

Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.93 to 0.97 Å) and were included in the refinement in the riding model approximation, with $U(\text{H})$ set to $1.2U(\text{C})$.

Figures

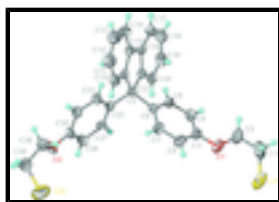


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of C₂₉H₂₄Cl₂O₂ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

9,9-Bis[4-(2-chloroethoxy)phenyl]-9H-fluorene

Crystal data

C₂₉H₂₄Cl₂O₂

$M_r = 475.38$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 12.2334$ (7) Å

$F(000) = 992$

$D_x = 1.321$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2267 reflections

$\theta = 2.3$ – 21.1 °

supplementary materials

$b = 10.8063 (6) \text{ \AA}$
 $c = 19.0374 (12) \text{ \AA}$
 $\beta = 108.172 (2)^\circ$
 $V = 2391.2 (2) \text{ \AA}^3$
 $Z = 4$

$\mu = 0.30 \text{ mm}^{-1}$
 $T = 293 \text{ K}$
Wedge, colourless
 $0.27 \times 0.15 \times 0.07 \text{ mm}$

Data collection

Bruker Kappa APEXII
diffractometer
Radiation source: fine-focus sealed tube
graphite
 φ and ω scans
Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.783$, $T_{\max} = 0.862$
18388 measured reflections

4206 independent reflections
2326 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.062$
 $\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 1.8^\circ$
 $h = -14 \rightarrow 10$
 $k = -12 \rightarrow 11$
 $l = -22 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.061$
 $wR(F^2) = 0.177$
 $S = 1.01$
4206 reflections
298 parameters
0 restraints

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
 $w = 1/[\sigma^2(F_o^2) + (0.0687P)^2 + 1.9561P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.53 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.66 \text{ e \AA}^{-3}$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.99333 (10)	0.53514 (15)	0.63783 (7)	0.0941 (5)
Cl2	0.08864 (16)	-0.1721 (2)	0.48114 (9)	0.1541 (9)
O1	0.7730 (2)	0.4956 (3)	0.50972 (15)	0.0763 (9)
O2	0.1404 (2)	-0.0587 (2)	0.34783 (15)	0.0596 (7)
C1	0.9155 (5)	0.6374 (5)	0.5696 (3)	0.0966 (18)
H1A	0.8605	0.6808	0.5879	0.116*
H1B	0.9681	0.6984	0.5611	0.116*
C2	0.8516 (4)	0.5776 (5)	0.4969 (2)	0.0719 (13)
H2A	0.8121	0.6400	0.4614	0.086*
H2B	0.9049	0.5340	0.4771	0.086*
C3	0.6879 (3)	0.4493 (3)	0.4503 (2)	0.0510 (10)
C4	0.6872 (3)	0.4561 (3)	0.3780 (2)	0.0489 (9)
H4	0.7507	0.4867	0.3667	0.059*

C5	0.5904 (3)	0.4167 (3)	0.32219 (19)	0.0414 (9)
H5	0.5901	0.4216	0.2733	0.050*
C6	0.4953 (3)	0.3708 (3)	0.33692 (18)	0.0372 (8)
C7	0.5013 (3)	0.3592 (4)	0.4106 (2)	0.0570 (11)
H7	0.4396	0.3251	0.4226	0.068*
C8	0.5967 (4)	0.3971 (4)	0.4659 (2)	0.0638 (12)
H8	0.5993	0.3870	0.5149	0.077*
C9	0.3808 (3)	0.3497 (3)	0.27615 (17)	0.0355 (8)
C10	0.3941 (3)	0.3372 (3)	0.19901 (18)	0.0373 (8)
C11	0.4475 (3)	0.2442 (3)	0.1722 (2)	0.0506 (10)
H11	0.4818	0.1778	0.2020	0.061*
C12	0.4487 (4)	0.2521 (4)	0.0999 (2)	0.0658 (12)
H12	0.4834	0.1895	0.0808	0.079*
C13	0.3997 (4)	0.3504 (4)	0.0559 (2)	0.0713 (13)
H13	0.4015	0.3535	0.0074	0.086*
C14	0.3478 (4)	0.4450 (4)	0.0825 (2)	0.0609 (11)
H14	0.3150	0.5121	0.0528	0.073*
C15	0.3458 (3)	0.4375 (3)	0.15460 (19)	0.0426 (9)
C16	0.2981 (3)	0.5234 (3)	0.19711 (19)	0.0411 (8)
C17	0.2481 (3)	0.6392 (4)	0.1796 (2)	0.0570 (11)
H17	0.2381	0.6741	0.1334	0.068*
C18	0.2135 (3)	0.7017 (4)	0.2324 (3)	0.0632 (12)
H18	0.1802	0.7795	0.2213	0.076*
C19	0.2272 (3)	0.6516 (3)	0.3004 (3)	0.0585 (11)
H19	0.2022	0.6950	0.3347	0.070*
C20	0.2779 (3)	0.5368 (3)	0.3186 (2)	0.0454 (9)
H20	0.2872	0.5026	0.3650	0.054*
C21	0.3148 (3)	0.4731 (3)	0.26698 (18)	0.0373 (8)
C22	0.3132 (3)	0.2404 (3)	0.29312 (18)	0.0359 (8)
C23	0.1966 (3)	0.2469 (3)	0.2822 (2)	0.0454 (9)
H23	0.1576	0.3194	0.2634	0.054*
C24	0.1356 (3)	0.1487 (3)	0.2986 (2)	0.0494 (10)
H24	0.0568	0.1554	0.2901	0.059*
C25	0.1925 (3)	0.0417 (3)	0.32734 (19)	0.0444 (9)
C26	0.3081 (3)	0.0317 (3)	0.3370 (2)	0.0495 (10)
H26	0.3467	-0.0414	0.3552	0.059*
C27	0.3669 (3)	0.1297 (3)	0.3198 (2)	0.0466 (9)
H27	0.4451	0.1213	0.3262	0.056*
C28	0.0307 (3)	-0.0406 (4)	0.3561 (2)	0.0630 (11)
H28A	-0.0259	-0.0266	0.3081	0.076*
H28B	0.0320	0.0314	0.3868	0.076*
C29	-0.0001 (4)	-0.1531 (4)	0.3912 (2)	0.0735 (13)
H29A	0.0058	-0.2254	0.3624	0.088*
H29B	-0.0793	-0.1464	0.3910	0.088*

Atomic displacement parameters (\AA^2)

U^{11}

U^{22}

U^{33}

U^{12}

U^{13}

U^{23}

supplementary materials

C11	0.0619 (8)	0.1571 (14)	0.0604 (8)	-0.0277 (8)	0.0152 (6)	-0.0223 (8)
C12	0.1338 (15)	0.225 (2)	0.0792 (11)	-0.0733 (14)	-0.0024 (10)	0.0575 (12)
O1	0.067 (2)	0.102 (2)	0.0507 (18)	-0.0338 (18)	0.0035 (16)	-0.0008 (16)
O2	0.0647 (18)	0.0419 (15)	0.082 (2)	-0.0087 (13)	0.0374 (16)	0.0028 (13)
C1	0.128 (5)	0.091 (4)	0.085 (4)	-0.053 (3)	0.053 (4)	-0.026 (3)
C2	0.057 (3)	0.098 (4)	0.061 (3)	-0.029 (3)	0.019 (2)	-0.014 (2)
C3	0.046 (2)	0.057 (2)	0.046 (2)	-0.0065 (19)	0.008 (2)	-0.0004 (19)
C4	0.040 (2)	0.054 (2)	0.056 (2)	-0.0079 (18)	0.019 (2)	-0.0061 (19)
C5	0.041 (2)	0.045 (2)	0.040 (2)	-0.0015 (17)	0.0148 (18)	-0.0036 (16)
C6	0.041 (2)	0.0345 (18)	0.038 (2)	0.0000 (15)	0.0137 (17)	0.0001 (15)
C7	0.054 (3)	0.075 (3)	0.044 (2)	-0.019 (2)	0.017 (2)	0.003 (2)
C8	0.065 (3)	0.087 (3)	0.036 (2)	-0.018 (2)	0.011 (2)	0.004 (2)
C9	0.0362 (19)	0.0375 (18)	0.0336 (19)	0.0002 (15)	0.0121 (16)	0.0006 (15)
C10	0.038 (2)	0.0393 (19)	0.0350 (19)	-0.0052 (15)	0.0116 (16)	-0.0031 (15)
C11	0.057 (3)	0.045 (2)	0.055 (2)	-0.0002 (18)	0.026 (2)	-0.0043 (18)
C12	0.081 (3)	0.066 (3)	0.061 (3)	-0.002 (2)	0.038 (3)	-0.015 (2)
C13	0.094 (4)	0.086 (3)	0.043 (3)	-0.006 (3)	0.034 (3)	-0.010 (2)
C14	0.073 (3)	0.064 (3)	0.045 (2)	0.000 (2)	0.017 (2)	0.009 (2)
C15	0.042 (2)	0.049 (2)	0.036 (2)	-0.0062 (17)	0.0112 (17)	0.0002 (17)
C16	0.038 (2)	0.039 (2)	0.043 (2)	-0.0014 (16)	0.0068 (17)	0.0015 (16)
C17	0.057 (3)	0.047 (2)	0.060 (3)	0.0026 (19)	0.008 (2)	0.010 (2)
C18	0.055 (3)	0.043 (2)	0.086 (3)	0.0076 (19)	0.015 (2)	-0.001 (2)
C19	0.056 (3)	0.044 (2)	0.079 (3)	0.0018 (19)	0.027 (2)	-0.015 (2)
C20	0.044 (2)	0.046 (2)	0.048 (2)	-0.0053 (17)	0.0168 (18)	-0.0093 (17)
C21	0.0326 (19)	0.0363 (18)	0.042 (2)	-0.0032 (15)	0.0107 (16)	-0.0007 (16)
C22	0.036 (2)	0.0369 (19)	0.0349 (19)	-0.0020 (15)	0.0121 (16)	-0.0024 (15)
C23	0.042 (2)	0.040 (2)	0.052 (2)	-0.0007 (17)	0.0110 (18)	0.0040 (17)
C24	0.037 (2)	0.049 (2)	0.060 (2)	-0.0059 (17)	0.0121 (19)	0.0014 (19)
C25	0.049 (2)	0.037 (2)	0.050 (2)	-0.0071 (17)	0.0215 (19)	-0.0018 (17)
C26	0.053 (3)	0.039 (2)	0.060 (3)	0.0064 (18)	0.023 (2)	0.0060 (18)
C27	0.041 (2)	0.046 (2)	0.058 (2)	0.0055 (17)	0.0242 (19)	0.0028 (18)
C28	0.049 (3)	0.066 (3)	0.072 (3)	-0.015 (2)	0.017 (2)	0.008 (2)
C29	0.064 (3)	0.088 (3)	0.066 (3)	-0.025 (2)	0.017 (2)	0.010 (2)

Geometric parameters (Å, °)

C11—C1	1.745 (6)	C13—C14	1.382 (6)
C12—C29	1.730 (5)	C13—H13	0.9300
O1—C3	1.371 (4)	C14—C15	1.382 (5)
O1—C2	1.385 (5)	C14—H14	0.9300
O2—C25	1.374 (4)	C15—C16	1.466 (5)
O2—C28	1.413 (5)	C16—C17	1.387 (5)
C1—C2	1.506 (6)	C16—C21	1.392 (4)
C1—H1A	0.9700	C17—C18	1.381 (6)
C1—H1B	0.9700	C17—H17	0.9300
C2—H2A	0.9700	C18—C19	1.365 (6)
C2—H2B	0.9700	C18—H18	0.9300
C3—C8	1.363 (5)	C19—C20	1.382 (5)
C3—C4	1.376 (5)	C19—H19	0.9300

C4—C5	1.388 (5)	C20—C21	1.386 (5)
C4—H4	0.9300	C20—H20	0.9300
C5—C6	1.372 (5)	C22—C23	1.377 (5)
C5—H5	0.9300	C22—C27	1.383 (5)
C6—C7	1.388 (5)	C23—C24	1.387 (5)
C6—C9	1.531 (5)	C23—H23	0.9300
C7—C8	1.368 (5)	C24—C25	1.373 (5)
C7—H7	0.9300	C24—H24	0.9300
C8—H8	0.9300	C25—C26	1.372 (5)
C9—C10	1.533 (4)	C26—C27	1.377 (5)
C9—C22	1.532 (4)	C26—H26	0.9300
C9—C21	1.541 (4)	C27—H27	0.9300
C10—C11	1.379 (5)	C28—C29	1.492 (5)
C10—C15	1.389 (5)	C28—H28A	0.9700
C11—C12	1.385 (5)	C28—H28B	0.9700
C11—H11	0.9300	C29—H29A	0.9700
C12—C13	1.370 (6)	C29—H29B	0.9700
C12—H12	0.9300		
C3—O1—C2	118.6 (3)	C13—C14—H14	120.9
C25—O2—C28	117.5 (3)	C14—C15—C10	120.9 (3)
C2—C1—C11	114.8 (4)	C14—C15—C16	130.1 (3)
C2—C1—H1A	108.6	C10—C15—C16	109.0 (3)
C11—C1—H1A	108.6	C17—C16—C21	120.2 (3)
C2—C1—H1B	108.6	C17—C16—C15	131.3 (3)
C11—C1—H1B	108.6	C21—C16—C15	108.4 (3)
H1A—C1—H1B	107.5	C18—C17—C16	118.6 (4)
O1—C2—C1	107.5 (4)	C18—C17—H17	120.7
O1—C2—H2A	110.2	C16—C17—H17	120.7
C1—C2—H2A	110.2	C19—C18—C17	121.4 (4)
O1—C2—H2B	110.2	C19—C18—H18	119.3
C1—C2—H2B	110.2	C17—C18—H18	119.3
H2A—C2—H2B	108.5	C18—C19—C20	120.5 (4)
C8—C3—O1	115.7 (3)	C18—C19—H19	119.8
C8—C3—C4	119.3 (4)	C20—C19—H19	119.8
O1—C3—C4	124.9 (3)	C19—C20—C21	119.1 (4)
C3—C4—C5	119.2 (3)	C19—C20—H20	120.4
C3—C4—H4	120.4	C21—C20—H20	120.4
C5—C4—H4	120.4	C20—C21—C16	120.1 (3)
C6—C5—C4	122.0 (3)	C20—C21—C9	128.6 (3)
C6—C5—H5	119.0	C16—C21—C9	111.2 (3)
C4—C5—H5	119.0	C23—C22—C27	116.8 (3)
C5—C6—C7	117.3 (3)	C23—C22—C9	122.1 (3)
C5—C6—C9	122.3 (3)	C27—C22—C9	121.2 (3)
C7—C6—C9	119.9 (3)	C22—C23—C24	122.1 (3)
C8—C7—C6	121.0 (4)	C22—C23—H23	118.9
C8—C7—H7	119.5	C24—C23—H23	118.9
C6—C7—H7	119.5	C25—C24—C23	119.6 (3)
C3—C8—C7	121.0 (4)	C25—C24—H24	120.2
C3—C8—H8	119.5	C23—C24—H24	120.2

supplementary materials

C7—C8—H8	119.5	C26—C25—O2	116.7 (3)
C10—C9—C6	113.0 (3)	C26—C25—C24	119.5 (3)
C10—C9—C22	111.1 (3)	O2—C25—C24	123.8 (3)
C6—C9—C22	112.5 (3)	C25—C26—C27	120.1 (3)
C10—C9—C21	100.2 (3)	C25—C26—H26	120.0
C6—C9—C21	106.3 (3)	C27—C26—H26	120.0
C22—C9—C21	113.1 (3)	C26—C27—C22	121.9 (3)
C11—C10—C15	120.3 (3)	C26—C27—H27	119.0
C11—C10—C9	128.5 (3)	C22—C27—H27	119.0
C15—C10—C9	111.2 (3)	O2—C28—C29	108.6 (3)
C12—C11—C10	118.4 (4)	O2—C28—H28A	110.0
C12—C11—H11	120.8	C29—C28—H28A	110.0
C10—C11—H11	120.8	O2—C28—H28B	110.0
C13—C12—C11	121.2 (4)	C29—C28—H28B	110.0
C13—C12—H12	119.4	H28A—C28—H28B	108.4
C11—C12—H12	119.4	C28—C29—C12	111.8 (3)
C12—C13—C14	120.8 (4)	C28—C29—H29A	109.3
C12—C13—H13	119.6	C12—C29—H29A	109.3
C14—C13—H13	119.6	C28—C29—H29B	109.3
C15—C14—C13	118.3 (4)	C12—C29—H29B	109.3
C15—C14—H14	120.9	H29A—C29—H29B	107.9
C3—O1—C2—C1	166.2 (4)	C14—C15—C16—C21	178.5 (4)
C11—C1—C2—O1	61.3 (5)	C10—C15—C16—C21	-1.7 (4)
C2—O1—C3—C8	-163.0 (4)	C21—C16—C17—C18	-1.3 (5)
C2—O1—C3—C4	14.7 (6)	C15—C16—C17—C18	-178.0 (4)
C8—C3—C4—C5	4.1 (6)	C16—C17—C18—C19	-0.3 (6)
O1—C3—C4—C5	-173.6 (4)	C17—C18—C19—C20	0.9 (6)
C3—C4—C5—C6	-0.2 (5)	C18—C19—C20—C21	0.0 (6)
C4—C5—C6—C7	-3.1 (5)	C19—C20—C21—C16	-1.6 (5)
C4—C5—C6—C9	168.4 (3)	C19—C20—C21—C9	175.2 (3)
C5—C6—C7—C8	2.7 (6)	C17—C16—C21—C20	2.2 (5)
C9—C6—C7—C8	-169.1 (4)	C15—C16—C21—C20	179.6 (3)
O1—C3—C8—C7	173.3 (4)	C17—C16—C21—C9	-175.1 (3)
C4—C3—C8—C7	-4.6 (7)	C15—C16—C21—C9	2.3 (4)
C6—C7—C8—C3	1.1 (7)	C10—C9—C21—C20	-179.0 (3)
C5—C6—C9—C10	21.6 (4)	C6—C9—C21—C20	-61.2 (4)
C7—C6—C9—C10	-167.0 (3)	C22—C9—C21—C20	62.8 (4)
C5—C6—C9—C22	148.4 (3)	C10—C9—C21—C16	-2.0 (3)
C7—C6—C9—C22	-40.2 (4)	C6—C9—C21—C16	115.8 (3)
C5—C6—C9—C21	-87.3 (4)	C22—C9—C21—C16	-120.3 (3)
C7—C6—C9—C21	84.1 (4)	C10—C9—C22—C23	-96.1 (4)
C6—C9—C10—C11	66.9 (4)	C6—C9—C22—C23	136.1 (3)
C22—C9—C10—C11	-60.6 (4)	C21—C9—C22—C23	15.6 (4)
C21—C9—C10—C11	179.6 (3)	C10—C9—C22—C27	83.4 (4)
C6—C9—C10—C15	-111.7 (3)	C6—C9—C22—C27	-44.4 (4)
C22—C9—C10—C15	120.7 (3)	C21—C9—C22—C27	-164.9 (3)
C21—C9—C10—C15	0.9 (3)	C27—C22—C23—C24	1.4 (5)
C15—C10—C11—C12	-1.7 (5)	C9—C22—C23—C24	-179.1 (3)
C9—C10—C11—C12	179.8 (3)	C22—C23—C24—C25	0.8 (6)

supplementary materials

C10—C11—C12—C13	0.9 (6)	C28—O2—C25—C26	164.5 (3)
C11—C12—C13—C14	0.2 (7)	C28—O2—C25—C24	-15.4 (5)
C12—C13—C14—C15	-0.5 (7)	C23—C24—C25—C26	-2.4 (5)
C13—C14—C15—C10	-0.3 (6)	C23—C24—C25—O2	177.5 (3)
C13—C14—C15—C16	179.5 (4)	O2—C25—C26—C27	-178.1 (3)
C11—C10—C15—C14	1.4 (5)	C24—C25—C26—C27	1.8 (6)
C9—C10—C15—C14	-179.8 (3)	C25—C26—C27—C22	0.5 (6)
C11—C10—C15—C16	-178.4 (3)	C23—C22—C27—C26	-2.1 (5)
C9—C10—C15—C16	0.4 (4)	C9—C22—C27—C26	178.4 (3)
C14—C15—C16—C17	-4.5 (6)	C25—O2—C28—C29	-169.9 (3)
C10—C15—C16—C17	175.3 (4)	O2—C28—C29—C12	66.6 (4)

Fig. 1

