Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

9,9-Bis(cyanoethanoic)fluorene

Hongxia Liu

School of Environmental Science and Engineering, Huangshi Institute of Technology, Huangshi, 435003, People's Republic of China
Correspondence e-mail: chliuhx@hsit.edu.cn

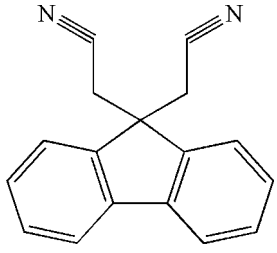
Received 18 July 2007; accepted 6 September 2007

Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.002 Å; R factor = 0.050; wR factor = 0.144; data-to-parameter ratio = 18.1.

The title compound, $C_{19}H_{16}N_2$, crystallizes with two molecules in the asymmetric unit related by a non-crystallographic plane of symmetry. The three fused rings of the fluorene system are almost coplanar. The cyanoethanoic groups display extended conformations and are nearly perpendicular to the fluorene plane. The packing of the molecules in the crystal structure is mainly due to van der Waals forces.

Related literature

For related literature, see: Bazyl (1986); Carroll *et al.* (2006); Hu *et al.* (2005, 2006); Johansson *et al.* (2001); Redecker *et al.* (1999).



Experimental

Crystal data

$C_{19}H_{16}N_2$
M_r = 272.34
Monoclinic, $P2_1/c$
a = 21.8136 (15) Å
b = 8.9446 (6) Å
c = 15.9938 (11) Å
β = 105.087 (1)°
V = 3013.0 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 292 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1000 CCD area detector diffractometer
Absorption correction: none
25122 measured reflections
6870 independent reflections
4957 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.144
S = 1.07
6870 reflections
379 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

The author is grateful to Dr Zhi-Guo Wang for helpful discussions and Dr Xiang-Gao Meng for the X-ray data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZ2095).

References

Bazyl, O. K. (1986). *J. Appl. Spectrosc.* **45**, 1256–1259.
Bruker (2001). *SAINT-Plus* (Version 6.45) and *SMART* (Version 5.628). Bruker AXS Inc., Madison, Wisconsin, USA.
Carroll, F. I., Blough, B. E., Huang, X. D., Nie, Z., Mascarella, S. W., Deschamps, J. & Navarro, H. A. (2006). *J. Med. Chem.* **49**, 4589–4594.
Hu, W.-B., Liu, H.-X., Tian, D.-T., Liu, C.-M. & Liu, Z.-L. (2005). *Acta Cryst.* E**61**, o3346–o3348.
Hu, W.-B., Liu, H.-X., Tian, D.-T., Liu, C.-M. & Liu, Z.-L. (2006). *Acta Cryst.* E**62**, o1105–o1106.
Johansson, D. M., Granlund, T., Theander, M., Inganas, O. & Andersson, M. R. (2001). *Synth. Met.* **121**, 1761–1762.
Redecker, M., Bradley, D. D. C., Inbasekaran, M. & Woo, E. P. (1999). *Appl. Phys. Lett.* **74**, 1400–1402.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

 doi:10.1107/S1600536807043772

supplementary materials

Acta Cryst. (2007). E**63**, o4033 [**doi:10.1107/S1600536807043772**]

9,9-Bis(cyanoethanoic)fluorene

H. Liu

Comment

Fluorene and its polymeric derivatives have been used as laser-generating (Bazyl, 1986) or photo-active fluorescent materials (Johansson *et al.*, 2001). However, insolubility is a common problem for fluorene polymers. Appropriate substitution of the fluorene ring system may modify the solubility of fluorene polymers (Redecker *et al.*, 1999). As a continuation of our interest in this area (Hu *et al.*, 2005; 2006), the structure of the title compound (I) is presented.

The title compound with the atomic labelling scheme is shown in Fig. 1. There are two molecules in the asymmetric unit related by a non-crystallographic plane of symmetry (1/2 − *x*, 3/2 − *y*). The bond lengths and angles of (I) are not unusual for a molecule of this type and are, therefore, not discussed in detail here. The three fused rings of the fluorene system are almost coplanar. The cyanoethanoic groups display extended conformations and are nearly perpendicular to the fluorene plane. The packing of the molecules in the lattice is mainly due to van der Waals forces.

Experimental

Compound (I) was synthesized as reported previously (Carroll *et al.*, 2006). Crystals of (I) appropriate for data collection were obtained from a methanol solution by slow evaporation.

Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93 Å for phenyl H, 0.97 Å for methene H, and with U_{iso}(H) = 1.2U_{eq}(C).

Figures

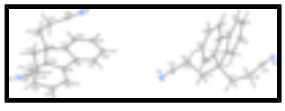


Fig. 1. View of the molecule of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

9,9-Bis(cyanoethanoic)fluorene

Crystal data

$C_{19}H_{16}N_2$	F_{000} = 1152
M_r = 272.34	D_x = 1.201 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 8741 reflections
a = 21.8136 (15) Å	θ = 2.5–26.0º

b = 8.9446 (6) Å	μ = 0.07 mm^{-1}
c = 15.9938 (11) Å	T = 292 (2) K
β = 105.087 (1)º	Block, colorless
V = 3013.0 (4) Å^3	0.30 × 0.20 × 0.20 mm
Z = 8	

Data collection

Bruker SMART 1000 CCD area detector diffractometer	4957 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.027
Monochromator: graphite	θ_{max} = 27.5º
T = 292(2) K	θ_{min} = 1.9º
φ and ω scans	h = −28→27
Absorption correction: none	k = −11→11
25122 measured reflections	l = −20→20
6870 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.050	H-atom parameters constrained
$wR(F^2)$ = 0.144	$w = 1/[\sigma^2(F_o^2) + (0.0789P)^2 + 0.0936P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max}$ = 0.001
6870 reflections	$\Delta\rho_{max}$ = 0.23 e Å^{-3}
379 parameters	$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Primary atom site location: structure-invariant direct methods	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}
C1	0.10546 (6)	0.85273 (14)	0.88581 (8)	0.0444 (3)

C2	0.09406 (7)	0.94873 (17)	0.81597 (9)	0.0558 (4)
H2	0.0684	0.9196	0.7624	0.067*
C3	0.12165 (8)	1.08946 (16)	0.82714 (11)	0.0619 (4)
H3	0.1150	1.1546	0.7803	0.074*
C4	0.15875 (8)	1.13416 (16)	0.90652 (11)	0.0611 (4)
H4	0.1764	1.2295	0.9127	0.073*
C5	0.17025 (7)	1.03923 (15)	0.97731 (10)	0.0527 (3)
H5	0.1949	1.0702	1.0311	0.063*
C6	0.14417 (6)	0.89693 (14)	0.96623 (8)	0.0422 (3)
C7	0.15184 (6)	0.76961 (15)	1.02563 (8)	0.0421 (3)
C8	0.18743 (7)	0.75290 (17)	1.11041 (9)	0.0519 (4)
H8	0.2094	0.8338	1.1406	0.062*
C9	0.18993 (8)	0.61477 (19)	1.14965 (10)	0.0618 (4)
H9	0.2138	0.6028	1.2066	0.074*
C10	0.15748 (8)	0.49425 (18)	1.10545 (10)	0.0617 (4)
H10	0.1603	0.4015	1.1324	0.074*
C11	0.12080 (7)	0.51055 (16)	1.02116 (9)	0.0535 (4)
H11	0.0987	0.4294	0.9914	0.064*
C12	0.11741 (6)	0.64896 (14)	0.98173 (8)	0.0427 (3)
C13	0.08048 (6)	0.69481 (15)	0.89097 (8)	0.0457 (3)
C14	0.09187 (7)	0.58927 (16)	0.82044 (9)	0.0545 (4)
H14A	0.0762	0.4905	0.8290	0.065*
H14B	0.0678	0.6250	0.7642	0.065*
C15	0.16140 (8)	0.57755 (18)	0.82076 (10)	0.0653 (4)
H15A	0.1763	0.6747	0.8075	0.078*
H15B	0.1861	0.5492	0.8782	0.078*
C16	0.17184 (9)	0.46816 (18)	0.75800 (11)	0.0682 (5)
C17	0.00818 (7)	0.69765 (17)	0.88239 (10)	0.0575 (4)
H17A	−0.0134	0.7213	0.8228	0.069*
H17B	−0.0049	0.5979	0.8941	0.069*
C18	−0.01448 (8)	0.80746 (18)	0.94118 (11)	0.0640 (4)
H18A	0.0033	0.9050	0.9351	0.077*
H18B	−0.0603	0.8161	0.9208	0.077*
C19	0.00157 (8)	0.76934 (18)	1.03307 (13)	0.0616 (4)
C20	0.39206 (6)	0.64880 (14)	0.30907 (8)	0.0459 (3)
C21	0.40496 (8)	0.54718 (17)	0.25103 (10)	0.0600 (4)
H21	0.4339	0.5701	0.2193	0.072*
C22	0.37408 (9)	0.41066 (18)	0.24076 (11)	0.0700 (5)
H22	0.3820	0.3419	0.2012	0.084*
C23	0.33174 (9)	0.37530 (17)	0.28856 (11)	0.0688 (5)
H23	0.3117	0.2826	0.2811	0.083*
C24	0.31872 (7)	0.47538 (16)	0.34719 (10)	0.0562 (4)
H24	0.2906	0.4505	0.3798	0.067*
C25	0.34839 (6)	0.61394 (14)	0.35662 (8)	0.0445 (3)
C26	0.34160 (6)	0.74440 (14)	0.40902 (8)	0.0427 (3)
C27	0.30395 (7)	0.76840 (17)	0.46582 (9)	0.0528 (4)
H27	0.2785	0.6923	0.4779	0.063*
C28	0.30498 (8)	0.90669 (18)	0.50391 (10)	0.0618 (4)
H28	0.2803	0.9234	0.5425	0.074*

C29	0.34202 (8)	1.02088 (18)	0.48574 (10)	0.0614 (4)
H29	0.3412	1.1143	0.5110	0.074*
C30	0.38051 (7)	0.99751 (16)	0.43000 (9)	0.0518 (3)
H30	0.4056	1.0744	0.4178	0.062*
C31	0.38089 (6)	0.85826 (14)	0.39313 (8)	0.0417 (3)
C32	0.42012 (6)	0.80382 (14)	0.33293 (8)	0.0438 (3)
C33	0.41473 (7)	0.90703 (16)	0.25476 (8)	0.0498 (3)
H33A	0.4300	1.0058	0.2752	0.060*
H33B	0.4418	0.8691	0.2201	0.060*
C34	0.34714 (8)	0.91985 (18)	0.19820 (10)	0.0633 (4)
H34A	0.3327	0.8224	0.1745	0.076*
H34B	0.3195	0.9524	0.2334	0.076*
C35	0.34275 (8)	1.02567 (18)	0.12727 (10)	0.0611 (4)
C36	0.49145 (7)	0.79347 (17)	0.38082 (9)	0.0531 (4)
H36A	0.5146	0.7637	0.3394	0.064*
H36B	0.5061	0.8925	0.4014	0.064*
C37	0.50846 (8)	0.68589 (18)	0.45729 (10)	0.0610 (4)
H37A	0.4876	0.5911	0.4391	0.073*
H37B	0.5539	0.6682	0.4717	0.073*
C38	0.49164 (8)	0.73456 (18)	0.53538 (11)	0.0591 (4)
N1	0.17890 (10)	0.38247 (17)	0.70915 (11)	0.0961 (6)
N2	0.01173 (8)	0.7400 (2)	1.10417 (11)	0.0851 (5)
N3	0.34077 (8)	1.10905 (17)	0.07340 (10)	0.0861 (5)
N4	0.48175 (8)	0.7716 (2)	0.59840 (10)	0.0837 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0488 (7)	0.0424 (7)	0.0418 (7)	0.0001 (6)	0.0114 (6)	−0.0013 (5)
C2	0.0652 (9)	0.0544 (8)	0.0462 (8)	0.0005 (7)	0.0117 (7)	0.0062 (7)
C3	0.0733 (10)	0.0494 (9)	0.0656 (10)	0.0047 (7)	0.0225 (8)	0.0159 (7)
C4	0.0661 (10)	0.0382 (7)	0.0829 (11)	−0.0031 (7)	0.0268 (9)	0.0019 (7)
C5	0.0531 (8)	0.0453 (7)	0.0598 (9)	−0.0025 (6)	0.0148 (7)	−0.0100 (7)
C6	0.0422 (7)	0.0409 (7)	0.0443 (7)	0.0015 (5)	0.0129 (6)	−0.0037 (5)
C7	0.0416 (7)	0.0478 (7)	0.0381 (7)	0.0022 (5)	0.0127 (5)	−0.0031 (5)
C8	0.0506 (8)	0.0635 (9)	0.0403 (7)	0.0030 (6)	0.0096 (6)	−0.0074 (6)
C9	0.0636 (10)	0.0813 (11)	0.0401 (8)	0.0139 (8)	0.0128 (7)	0.0112 (8)
C10	0.0743 (11)	0.0608 (10)	0.0548 (9)	0.0086 (8)	0.0254 (8)	0.0185 (7)
C11	0.0638 (9)	0.0482 (8)	0.0514 (8)	−0.0047 (6)	0.0204 (7)	0.0040 (6)
C12	0.0476 (7)	0.0439 (7)	0.0383 (7)	−0.0009 (5)	0.0142 (6)	−0.0005 (5)
C13	0.0540 (8)	0.0434 (7)	0.0377 (7)	−0.0051 (6)	0.0085 (6)	−0.0006 (6)
C14	0.0730 (10)	0.0485 (8)	0.0391 (7)	−0.0085 (7)	0.0095 (7)	−0.0062 (6)
C15	0.0850 (12)	0.0583 (9)	0.0591 (9)	−0.0107 (8)	0.0305 (8)	−0.0138 (7)
C16	0.1051 (14)	0.0473 (9)	0.0627 (10)	−0.0049 (8)	0.0404 (9)	0.0014 (8)
C17	0.0541 (9)	0.0593 (9)	0.0534 (9)	−0.0091 (7)	0.0040 (7)	0.0003 (7)
C18	0.0543 (9)	0.0594 (9)	0.0796 (11)	0.0019 (7)	0.0198 (8)	0.0046 (8)
C19	0.0565 (9)	0.0592 (9)	0.0715 (11)	−0.0036 (7)	0.0210 (8)	−0.0110 (8)
C20	0.0549 (8)	0.0430 (7)	0.0421 (7)	−0.0035 (6)	0.0167 (6)	−0.0005 (5)

C21	0.0746 (10)	0.0540 (9)	0.0576 (9)	−0.0035 (7)	0.0286 (8)	−0.0078 (7)
C22	0.0929 (13)	0.0495 (9)	0.0707 (11)	−0.0038 (8)	0.0266 (10)	−0.0165 (8)
C23	0.0838 (12)	0.0426 (8)	0.0772 (11)	−0.0130 (8)	0.0161 (9)	−0.0052 (8)
C24	0.0616 (9)	0.0486 (8)	0.0595 (9)	−0.0109 (7)	0.0177 (7)	0.0059 (7)
C25	0.0490 (8)	0.0433 (7)	0.0411 (7)	−0.0039 (6)	0.0113 (6)	0.0035 (6)
C26	0.0424 (7)	0.0477 (7)	0.0383 (7)	−0.0016 (5)	0.0114 (5)	0.0033 (5)
C27	0.0498 (8)	0.0609 (9)	0.0526 (8)	−0.0031 (6)	0.0222 (7)	0.0041 (7)
C28	0.0611 (9)	0.0763 (11)	0.0560 (9)	0.0051 (8)	0.0294 (7)	−0.0060 (8)
C29	0.0693 (10)	0.0603 (9)	0.0584 (9)	0.0021 (8)	0.0232 (8)	−0.0154 (7)
C30	0.0587 (8)	0.0479 (8)	0.0516 (8)	−0.0068 (6)	0.0191 (7)	−0.0072 (6)
C31	0.0438 (7)	0.0452 (7)	0.0370 (6)	−0.0032 (5)	0.0123 (5)	−0.0006 (5)
C32	0.0508 (8)	0.0435 (7)	0.0416 (7)	−0.0061 (6)	0.0201 (6)	−0.0027 (5)
C33	0.0579 (8)	0.0508 (8)	0.0447 (7)	−0.0110 (6)	0.0209 (6)	−0.0004 (6)
C34	0.0679 (10)	0.0646 (10)	0.0552 (9)	−0.0160 (8)	0.0123 (8)	0.0081 (7)
C35	0.0741 (11)	0.0527 (9)	0.0516 (9)	−0.0127 (7)	0.0078 (8)	0.0003 (7)
C36	0.0515 (8)	0.0586 (8)	0.0545 (8)	−0.0052 (7)	0.0232 (7)	−0.0010 (7)
C37	0.0597 (9)	0.0594 (9)	0.0627 (9)	0.0065 (7)	0.0138 (7)	0.0017 (8)
C38	0.0607 (9)	0.0605 (9)	0.0554 (9)	−0.0049 (7)	0.0142 (8)	0.0115 (7)
N1	0.1630 (18)	0.0570 (9)	0.0876 (11)	0.0009 (10)	0.0670 (12)	−0.0096 (8)
N2	0.0834 (11)	0.1038 (13)	0.0725 (11)	0.0041 (9)	0.0282 (9)	−0.0134 (9)
N3	0.1111 (13)	0.0705 (10)	0.0674 (10)	−0.0158 (9)	0.0067 (9)	0.0162 (8)
N4	0.0923 (11)	0.1028 (12)	0.0607 (9)	0.0005 (9)	0.0280 (8)	0.0120 (8)

Geometric parameters (Å, °)

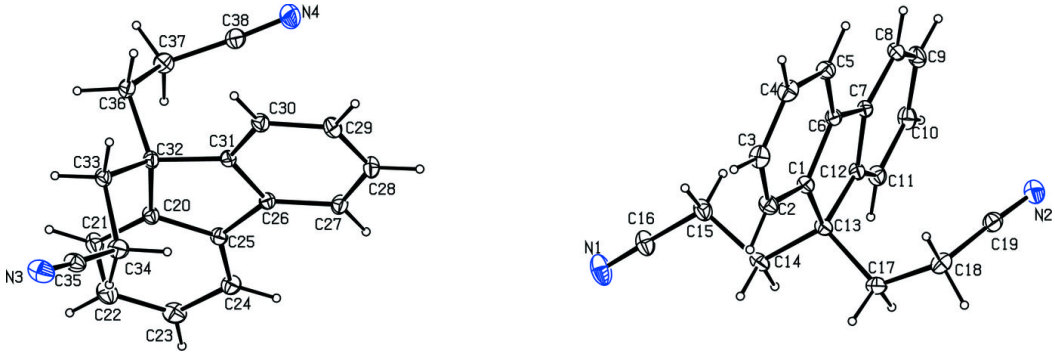
C1—C2	1.3793 (18)	C20—C21	1.3795 (19)
C1—C6	1.3993 (18)	C20—C25	1.4001 (18)
C1—C13	1.5239 (18)	C20—C32	1.5236 (18)
C2—C3	1.387 (2)	C21—C22	1.383 (2)
C2—H2	0.9300	C21—H21	0.9300
C3—C4	1.375 (2)	C22—C23	1.380 (2)
C3—H3	0.9300	C22—H22	0.9300
C4—C5	1.385 (2)	C23—C24	1.378 (2)
C4—H4	0.9300	C23—H23	0.9300
C5—C6	1.3867 (18)	C24—C25	1.3881 (18)
C5—H5	0.9300	C24—H24	0.9300
C6—C7	1.4645 (18)	C25—C26	1.4665 (18)
C7—C8	1.3840 (19)	C26—C27	1.3908 (19)
C7—C12	1.3954 (18)	C26—C31	1.3962 (17)
C8—C9	1.380 (2)	C27—C28	1.376 (2)
C8—H8	0.9300	C27—H27	0.9300
C9—C10	1.379 (2)	C28—C29	1.379 (2)
C9—H9	0.9300	C28—H28	0.9300
C10—C11	1.385 (2)	C29—C30	1.390 (2)
C10—H10	0.9300	C29—H29	0.9300
C11—C12	1.3826 (18)	C30—C31	1.3789 (18)
C11—H11	0.9300	C30—H30	0.9300
C12—C13	1.5216 (18)	C31—C32	1.5250 (17)
C13—C14	1.5400 (18)	C32—C33	1.5339 (18)

C13—C17	1.547 (2)	C32—C36	1.548 (2)
C14—C15	1.519 (2)	C33—C34	1.520 (2)
C14—H14A	0.9700	C33—H33A	0.9700
C14—H14B	0.9700	C33—H33B	0.9700
C15—C16	1.462 (2)	C34—C35	1.461 (2)
C15—H15A	0.9700	C34—H34A	0.9700
C15—H15B	0.9700	C34—H34B	0.9700
C16—N1	1.133 (2)	C35—N3	1.1318 (19)
C17—C18	1.528 (2)	C36—C37	1.524 (2)
C17—H17A	0.9700	C36—H36A	0.9700
C17—H17B	0.9700	C36—H36B	0.9700
C18—C19	1.460 (3)	C37—C38	1.457 (2)
C18—H18A	0.9700	C37—H37A	0.9700
C18—H18B	0.9700	C37—H37B	0.9700
C19—N2	1.131 (2)	C38—N4	1.134 (2)
C2—C1—C6	120.46 (12)	C21—C20—C25	120.37 (12)
C2—C1—C13	128.99 (12)	C21—C20—C32	128.99 (12)
C6—C1—C13	110.54 (11)	C25—C20—C32	110.64 (11)
C1—C2—C3	118.69 (14)	C20—C21—C22	118.90 (14)
C1—C2—H2	120.7	C20—C21—H21	120.6
C3—C2—H2	120.7	C22—C21—H21	120.6
C4—C3—C2	120.95 (14)	C23—C22—C21	120.78 (15)
C4—C3—H3	119.5	C23—C22—H22	119.6
C2—C3—H3	119.5	C21—C22—H22	119.6
C3—C4—C5	120.95 (14)	C24—C23—C22	120.93 (14)
C3—C4—H4	119.5	C24—C23—H23	119.5
C5—C4—H4	119.5	C22—C23—H23	119.5
C4—C5—C6	118.51 (14)	C23—C24—C25	118.75 (14)
C4—C5—H5	120.7	C23—C24—H24	120.6
C6—C5—H5	120.7	C25—C24—H24	120.6
C5—C6—C1	120.41 (12)	C24—C25—C20	120.25 (13)
C5—C6—C7	131.07 (12)	C24—C25—C26	131.22 (12)
C1—C6—C7	108.44 (11)	C20—C25—C26	108.50 (11)
C8—C7—C12	120.05 (13)	C27—C26—C31	120.07 (12)
C8—C7—C6	131.28 (13)	C27—C26—C25	131.35 (12)
C12—C7—C6	108.61 (11)	C31—C26—C25	108.56 (11)
C9—C8—C7	119.19 (14)	C28—C27—C26	118.91 (13)
C9—C8—H8	120.4	C28—C27—H27	120.5
C7—C8—H8	120.4	C26—C27—H27	120.5
C10—C9—C8	120.82 (14)	C27—C28—C29	121.00 (13)
C10—C9—H9	119.6	C27—C28—H28	119.5
C8—C9—H9	119.6	C29—C28—H28	119.5
C9—C10—C11	120.40 (14)	C28—C29—C30	120.56 (14)
C9—C10—H10	119.8	C28—C29—H29	119.7
C11—C10—H10	119.8	C30—C29—H29	119.7
C12—C11—C10	119.15 (14)	C31—C30—C29	118.80 (13)
C12—C11—H11	120.4	C31—C30—H30	120.6
C10—C11—H11	120.4	C29—C30—H30	120.6
C11—C12—C7	120.33 (12)	C30—C31—C26	120.59 (12)

C11—C12—C13	128.95 (12)	C30—C31—C32	128.69 (12)
C7—C12—C13	110.71 (11)	C26—C31—C32	110.72 (11)
C12—C13—C1	101.15 (10)	C20—C32—C31	101.18 (10)
C12—C13—C14	112.78 (11)	C20—C32—C33	113.77 (11)
C1—C13—C14	113.60 (11)	C31—C32—C33	112.70 (11)
C12—C13—C17	111.31 (11)	C20—C32—C36	110.86 (11)
C1—C13—C17	110.52 (11)	C31—C32—C36	111.33 (10)
C14—C13—C17	107.47 (11)	C33—C32—C36	107.05 (10)
C15—C14—C13	113.03 (12)	C34—C33—C32	112.78 (11)
C15—C14—H14A	109.0	C34—C33—H33A	109.0
C13—C14—H14A	109.0	C32—C33—H33A	109.0
C15—C14—H14B	109.0	C34—C33—H33B	109.0
C13—C14—H14B	109.0	C32—C33—H33B	109.0
H14A—C14—H14B	107.8	H33A—C33—H33B	107.8
C16—C15—C14	112.20 (14)	C35—C34—C33	111.60 (13)
C16—C15—H15A	109.2	C35—C34—H34A	109.3
C14—C15—H15A	109.2	C33—C34—H34A	109.3
C16—C15—H15B	109.2	C35—C34—H34B	109.3
C14—C15—H15B	109.2	C33—C34—H34B	109.3
H15A—C15—H15B	107.9	H34A—C34—H34B	108.0
N1—C16—C15	178.8 (2)	N3—C35—C34	178.30 (18)
C18—C17—C13	116.19 (12)	C37—C36—C32	115.99 (12)
C18—C17—H17A	108.2	C37—C36—H36A	108.3
C13—C17—H17A	108.2	C32—C36—H36A	108.3
C18—C17—H17B	108.2	C37—C36—H36B	108.3
C13—C17—H17B	108.2	C32—C36—H36B	108.3
H17A—C17—H17B	107.4	H36A—C36—H36B	107.4
C19—C18—C17	115.99 (13)	C38—C37—C36	115.86 (13)
C19—C18—H18A	108.3	C38—C37—H37A	108.3
C17—C18—H18A	108.3	C36—C37—H37A	108.3
C19—C18—H18B	108.3	C38—C37—H37B	108.3
C17—C18—H18B	108.3	C36—C37—H37B	108.3
H18A—C18—H18B	107.4	H37A—C37—H37B	107.4
N2—C19—C18	177.50 (18)	N4—C38—C37	176.46 (18)
C6—C1—C2—C3	0.0 (2)	C25—C20—C21—C22	0.0 (2)
C13—C1—C2—C3	179.12 (14)	C32—C20—C21—C22	178.98 (15)
C1—C2—C3—C4	−1.2 (2)	C20—C21—C22—C23	−0.9 (3)
C2—C3—C4—C5	0.8 (2)	C21—C22—C23—C24	0.5 (3)
C3—C4—C5—C6	0.8 (2)	C22—C23—C24—C25	0.9 (2)
C4—C5—C6—C1	−2.0 (2)	C23—C24—C25—C20	−1.8 (2)
C4—C5—C6—C7	174.43 (13)	C23—C24—C25—C26	176.13 (15)
C2—C1—C6—C5	1.7 (2)	C21—C20—C25—C24	1.5 (2)
C13—C1—C6—C5	−177.64 (12)	C32—C20—C25—C24	−177.74 (12)
C2—C1—C6—C7	−175.53 (12)	C21—C20—C25—C26	−176.94 (13)
C13—C1—C6—C7	5.17 (14)	C32—C20—C25—C26	3.86 (15)
C5—C6—C7—C8	−0.1 (2)	C24—C25—C26—C27	0.8 (2)
C1—C6—C7—C8	176.64 (13)	C20—C25—C26—C27	178.93 (14)
C5—C6—C7—C12	−177.37 (13)	C24—C25—C26—C31	−177.97 (14)
C1—C6—C7—C12	−0.59 (14)	C20—C25—C26—C31	0.19 (15)

C12—C7—C8—C9	2.0 (2)	C31—C26—C27—C28	1.7 (2)
C6—C7—C8—C9	−174.93 (13)	C25—C26—C27—C28	−176.97 (14)
C7—C8—C9—C10	0.0 (2)	C26—C27—C28—C29	0.7 (2)
C8—C9—C10—C11	−1.2 (2)	C27—C28—C29—C30	−1.6 (3)
C9—C10—C11—C12	0.4 (2)	C28—C29—C30—C31	0.1 (2)
C10—C11—C12—C7	1.6 (2)	C29—C30—C31—C26	2.3 (2)
C10—C11—C12—C13	−179.60 (13)	C29—C30—C31—C32	−177.87 (13)
C8—C7—C12—C11	−2.85 (19)	C27—C26—C31—C30	−3.2 (2)
C6—C7—C12—C11	174.74 (12)	C25—C26—C31—C30	175.70 (12)
C8—C7—C12—C13	178.17 (11)	C27—C26—C31—C32	176.92 (12)
C6—C7—C12—C13	−4.23 (14)	C25—C26—C31—C32	−4.16 (14)
C11—C12—C13—C1	−172.01 (14)	C21—C20—C32—C31	174.96 (15)
C7—C12—C13—C1	6.85 (14)	C25—C20—C32—C31	−5.94 (14)
C11—C12—C13—C14	−50.32 (19)	C21—C20—C32—C33	53.8 (2)
C7—C12—C13—C14	128.55 (12)	C25—C20—C32—C33	−127.05 (12)
C11—C12—C13—C17	70.57 (18)	C21—C20—C32—C36	−66.87 (18)
C7—C12—C13—C17	−110.57 (13)	C25—C20—C32—C36	112.24 (12)
C2—C1—C13—C12	173.57 (14)	C30—C31—C32—C20	−173.79 (14)
C6—C1—C13—C12	−7.21 (14)	C26—C31—C32—C20	6.06 (14)
C2—C1—C13—C14	52.44 (19)	C30—C31—C32—C33	−51.92 (18)
C6—C1—C13—C14	−128.33 (12)	C26—C31—C32—C33	127.93 (12)
C2—C1—C13—C17	−68.44 (18)	C30—C31—C32—C36	68.38 (18)
C6—C1—C13—C17	110.78 (12)	C26—C31—C32—C36	−111.77 (12)
C12—C13—C14—C15	−57.68 (16)	C20—C32—C33—C34	53.61 (16)
C1—C13—C14—C15	56.68 (16)	C31—C32—C33—C34	−60.84 (15)
C17—C13—C14—C15	179.27 (13)	C36—C32—C33—C34	176.43 (12)
C13—C14—C15—C16	175.51 (12)	C32—C33—C34—C35	176.56 (12)
C14—C15—C16—N1	−12 (10)	C33—C34—C35—N3	−17 (7)
C12—C13—C17—C18	61.54 (16)	C20—C32—C36—C37	−50.74 (15)
C1—C13—C17—C18	−50.04 (16)	C31—C32—C36—C37	61.07 (15)
C14—C13—C17—C18	−174.51 (12)	C33—C32—C36—C37	−175.35 (12)
C13—C17—C18—C19	−71.32 (18)	C32—C36—C37—C38	−73.49 (18)
C17—C18—C19—N2	−124 (4)	C36—C37—C38—N4	−123 (3)

Fig. 1


N4
C38
C37
C36
C30
C29
C31
C32
C33
C28
C20
C26
C27
C21
C25
C34
N3
C35
C24
C22
C23
C8
C9
C5
C4
C7
C6
C10
C3
C1
C12
C11
N2
C16
C2
C15
C13
N1
C19
C14
C17
C18