Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

PCCP

"Bottom-up" Self-assembly and "Cold Crystallization" of Butterfly Shaped Tetrabenzofluorene Molecules**

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Crystallographic Details

Supplementary Information

Table 1. Crystal data and structure refinement for **1**.

S.No		
1	CCDC No.	1408969
2	Formula	$C_{45}H_{45}O$
3	Fw	601.81
4	Temperature	296(2) K
5	Wavelength	0.71073 Å
6	Crystal System	Triclinic
7	Crystal size	0.250 x 0.160 x 0.120 mm
8	Crystal colour	Colourless
9	θ range for data collection/°	1.124-27.031
10	Space group	P -1
11	a/Å	9.6555(4)
12	b/Å	10.5975(5)
13	c/Å	18.1996(8)
14	α (°)	86.088(2)
15	β (°)	85.130(2)
16	γ (°)	68.108(2)
17	V ($Å^3$)	1720.38(13)
18	Z	2
19	Density (g cm^{-3})	1.162
20	Absorption coefficient (mm^{-1})	0.067
21	F(000)	646
22	Limiting indices	-12<=h<=11, -13<=k<=13, -23<=l<=23
23	Reflections collected / unique	27453 / 7415
24	R_{int}	0.0432
25	Completeness to theta	25.242 (98.7 %)
26	Absorption correction	None
27	Refinement method	Full-matrix least-squares on F^2
28	Data / restraints / parameters	7415 / 0 / 416
29	Goodness-of-fit on F^2	1.043
30	Final R indices [I>2sigma(I)]	R1 = 0.0706, wR2 = 0.1714
31	R indices (all data)	R1 = 0.1393, wR2 = 0.2082
32	Largest diff. peak and hole/e $Å^{-3}$	0.698, -0.294

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **1**.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	5417(3)	12747(3)	6375(1)	48(1)
C(2)	5253(3)	13012(3)	7110(2)	61(1)
C(3)	5843(4)	13907(3)	7358(2)	66(1)
C(4)	6567(3)	14532(3)	6877(2)	54(1)
C(5)	6755(3)	14295(2)	6116(1)	41(1)
C(6)	7425(2)	15022(2)	5580(1)	39(1)
C(7)	7922(3)	16019(3)	5805(2)	48(1)
C(8)	8396(3)	16815(3)	5300(2)	54(1)
C(9)	8356(3)	16677(3)	4551(2)	54(1)
C(10)	7918(3)	15690(3)	4314(2)	45(1)
C(11)	7511(2)	14795(2)	4820(1)	36(1)
C(12)	7079(2)	13714(2)	4592(1)	35(1)
C(13)	7119(2)	13174(2)	3858(1)	35(1)
C(14)	7934(3)	13225(2)	3158(1)	40(1)
C(15)	9238(3)	13533(3)	3096(2)	51(1)
C(16)	10037(4)	13496(4)	2434(2)	70(1)
C(17)	9556(4)	13160(4)	1803(2)	81(1)
C(18)	8330(4)	12804(4)	1852(2)	70(1)
C(19)	7503(3)	12798(3)	2523(1)	47(1)
C(20)	6313(3)	12258(3)	2587(1)	46(1)
C(21)	5704(4)	11971(3)	1977(2)	66(1)
C(22)	4681(4)	11361(4)	2054(2)	78(1)
C(23)	4225(4)	10991(3)	2748(2)	69(1)

C(24)	4762(3)	11286(3)	3362(2)	53(1)
C(25)	5793(3)	11941(2)	3297(1)	40(1)
C(26)	6256(2)	12392(2)	3923(1)	36(1)
C(27)	5900(2)	12111(2)	4722(1)	37(1)
C(28)	6374(2)	13096(2)	5096(1)	35(1)
C(29)	6167(2)	13370(2)	5863(1)	38(1)
C(30)	6802(3)	10590(2)	4952(1)	42(1)
C(31)	8463(3)	10257(2)	4965(1)	37(1)
C(32)	9048(3)	10411(2)	5608(1)	40(1)
C(33)	9448(3)	9825(2)	4350(1)	37(1)
C(34)	9819(4)	9089(3)	3104(2)	70(1)
C(35)	8944(4)	8675(4)	2571(2)	97(1)
C(36)	9826(5)	8116(5)	1904(2)	118(2)
C(37)	9037(5)	7638(5)	1361(3)	119(2)
C(38)	10025(5)	7105(5)	676(2)	115(2)
C(39)	11328(5)	5813(4)	792(2)	99(1)
C(40)	12228(5)	5201(4)	99(2)	96(1)
C(41)	13474(5)	3892(4)	211(3)	108(1)
C(42)	14373(6)	3241(5)	-461(3)	119(2)
C(43)	15663(7)	1882(6)	-281(3)	137(2)
C(44)	16465(8)	1209(7)	-890(4)	165(2)
C(45)	17740(7)	-96(6)	-674(4)	171(3)
O(1)	8847(2)	9617(2)	3733(1)	53(1)

Table 3. Bond lengths [Å] and angles [deg] for **1**.

C(1)-C(2)	1.370(4)
C(1)-C(29)	1.409(3)
C(1)-H(1)	0.9300
C(2)-C(3)	1.391(4)
C(2)-H(2)	0.9300
C(3)-C(4)	1.362(4)
C(3)-H(3)	0.9300
C(4)-C(5)	1.409(4)
C(4)-H(4)	0.9300
C(5)-C(29)	1.420(4)
C(5)-C(6)	1.458(3)
C(6)-C(7)	1.409(3)
C(6)-C(11)	1.412(3)
C(7)-C(8)	1.370(4)
C(7)-H(7)	0.9300
C(8)-C(9)	1.386(4)
C(8)-H(8)	0.9300
C(9)-C(10)	1.372(4)
C(9)-H(9)	0.9300
C(10)-C(11)	1.413(3)
C(10)-H(10)	0.9300
C(11)-C(12)	1.452(3)
C(12)-C(28)	1.371(3)
C(12)-C(13)	1.481(3)
C(13)-C(26)	1.371(3)

C(13)-C(14)	1.448(3)
C(14)-C(15)	1.408(3)
C(14)-C(19)	1.417(3)
C(15)-C(16)	1.368(4)
C(15)-H(15)	0.9300
C(16)-C(17)	1.390(4)
C(16)-H(16)	0.9300
C(17)-C(18)	1.364(4)
C(17)-H(17)	0.9300
C(18)-C(19)	1.401(4)
C(18)-H(18)	0.9300
C(19)-C(20)	1.456(4)
C(20)-C(21)	1.400(4)
C(20)-C(25)	1.412(3)
C(21)-C(22)	1.361(4)
C(21)-H(21)	0.9300
C(22)-C(23)	1.383(4)
C(22)-H(22)	0.9300
C(23)-C(24)	1.372(4)
C(23)-H(23)	0.9300
C(24)-C(25)	1.404(3)
C(24)-H(24)	0.9300
C(25)-C(26)	1.429(3)
C(26)-C(27)	1.502(3)
C(27)-C(28)	1.505(3)
C(27)-C(30)	1.568(3)
C(27)-H(27)	0.9800

C(28)-C(29)	1.429(3)
C(30)-C(31)	1.510(3)
C(30)-H(30A)	0.9700
C(30)-H(30B)	0.9700
C(31)-C(32)	1.386(3)
C(31)-C(33)	1.389(3)
C(32)-C(33)#1	1.387(3)
C(32)-H(32)	0.9300
C(33)-O(1)	1.374(3)
C(33)-C(32)#1	1.387(3)
C(34)-O(1)	1.420(3)
C(34)-C(35)	1.523(4)
C(34)-H(34A)	0.9700
C(34)-H(34B)	0.9700
C(35)-C(36)	1.447(5)
C(35)-H(35A)	0.9700
C(35)-H(35B)	0.9700
C(36)-C(37)	1.517(5)
C(36)-H(36A)	0.9700
C(36)-H(36B)	0.9700
C(37)-C(38)	1.507(6)
C(37)-H(37A)	0.9700
C(37)-H(37B)	0.9700
C(38)-C(39)	1.492(6)
C(38)-H(38A)	0.9700
C(38)-H(38B)	0.9700
C(39)-C(40)	1.508(5)

C(39)-H(39A)	0.9700
C(39)-H(39B)	0.9700
C(40)-C(41)	1.474(5)
C(40)-H(40A)	0.9700
C(40)-H(40B)	0.9700
C(41)-C(42)	1.488(5)
C(41)-H(41A)	0.9700
C(41)-H(41B)	0.9700
C(42)-C(43)	1.549(7)
C(42)-H(42A)	0.9700
C(42)-H(42B)	0.9700
C(43)-C(44)	1.374(6)
C(43)-H(43A)	0.9700
C(43)-H(43B)	0.9700
C(44)-C(45)	1.524(8)
C(44)-H(44A)	0.9700
C(44)-H(44B)	0.9700
C(45)-H(45A)	0.9600
C(45)-H(45B)	0.9600
C(45)-H(45C)	0.9600

C(2)-C(1)-C(29)	121.3(3)
C(2)-C(1)-H(1)	119.4
C(29)-C(1)-H(1)	119.4
C(1)-C(2)-C(3)	119.5(3)
C(1)-C(2)-H(2)	120.3
C(3)-C(2)-H(2)	120.3

C(4)-C(3)-C(2)	120.7(3)
C(4)-C(3)-H(3)	119.6
C(2)-C(3)-H(3)	119.6
C(3)-C(4)-C(5)	121.7(3)
C(3)-C(4)-H(4)	119.1
C(5)-C(4)-H(4)	119.1
C(4)-C(5)-C(29)	117.6(2)
C(4)-C(5)-C(6)	123.0(2)
C(29)-C(5)-C(6)	119.2(2)
C(7)-C(6)-C(11)	118.5(2)
C(7)-C(6)-C(5)	120.9(2)
C(11)-C(6)-C(5)	120.5(2)
C(8)-C(7)-C(6)	121.4(3)
C(8)-C(7)-H(7)	119.3
C(6)-C(7)-H(7)	119.3
C(7)-C(8)-C(9)	120.1(3)
C(7)-C(8)-H(8)	119.9
C(9)-C(8)-H(8)	119.9
C(10)-C(9)-C(8)	119.9(3)
C(10)-C(9)-H(9)	120.1
C(8)-C(9)-H(9)	120.1
C(9)-C(10)-C(11)	121.3(3)
C(9)-C(10)-H(10)	119.3
C(11)-C(10)-H(10)	119.3
C(6)-C(11)-C(10)	118.3(2)
C(6)-C(11)-C(12)	118.5(2)
C(10)-C(11)-C(12)	123.1(2)

C(28)-C(12)-C(11)	119.7(2)
C(28)-C(12)-C(13)	108.3(2)
C(11)-C(12)-C(13)	131.7(2)
C(26)-C(13)-C(14)	118.3(2)
C(26)-C(13)-C(12)	107.6(2)
C(14)-C(13)-C(12)	133.9(2)
C(15)-C(14)-C(19)	118.3(2)
C(15)-C(14)-C(13)	122.7(2)
C(19)-C(14)-C(13)	118.6(2)
C(16)-C(15)-C(14)	121.5(3)
C(16)-C(15)-H(15)	119.2
C(14)-C(15)-H(15)	119.2
C(15)-C(16)-C(17)	119.9(3)
C(15)-C(16)-H(16)	120.0
C(17)-C(16)-H(16)	120.0
C(18)-C(17)-C(16)	119.8(3)
C(18)-C(17)-H(17)	120.1
C(16)-C(17)-H(17)	120.1
C(17)-C(18)-C(19)	122.0(3)
C(17)-C(18)-H(18)	119.0
C(19)-C(18)-H(18)	119.0
C(18)-C(19)-C(14)	118.3(3)
C(18)-C(19)-C(20)	121.3(2)
C(14)-C(19)-C(20)	120.1(2)
C(21)-C(20)-C(25)	118.0(2)
C(21)-C(20)-C(19)	123.3(3)
C(25)-C(20)-C(19)	118.6(2)

C(22)-C(21)-C(20)	121.9(3)
C(22)-C(21)-H(21)	119.1
C(20)-C(21)-H(21)	119.1
C(21)-C(22)-C(23)	120.2(3)
C(21)-C(22)-H(22)	119.9
C(23)-C(22)-H(22)	119.9
C(24)-C(23)-C(22)	119.8(3)
C(24)-C(23)-H(23)	120.1
C(22)-C(23)-H(23)	120.1
C(23)-C(24)-C(25)	121.0(3)
C(23)-C(24)-H(24)	119.5
C(25)-C(24)-H(24)	119.5
C(24)-C(25)-C(20)	119.0(2)
C(24)-C(25)-C(26)	122.4(2)
C(20)-C(25)-C(26)	118.4(2)
C(13)-C(26)-C(25)	122.6(2)
C(13)-C(26)-C(27)	110.3(2)
C(25)-C(26)-C(27)	127.1(2)
C(26)-C(27)-C(28)	101.81(19)
C(26)-C(27)-C(30)	110.54(19)
C(28)-C(27)-C(30)	112.76(19)
C(26)-C(27)-H(27)	110.5
C(28)-C(27)-H(27)	110.5
C(30)-C(27)-H(27)	110.5
C(12)-C(28)-C(29)	122.8(2)
C(12)-C(28)-C(27)	110.4(2)
C(29)-C(28)-C(27)	126.8(2)

C(1)-C(29)-C(5)	119.2(2)
C(1)-C(29)-C(28)	122.4(2)
C(5)-C(29)-C(28)	118.4(2)
C(31)-C(30)-C(27)	113.49(19)
C(31)-C(30)-H(30A)	108.9
C(27)-C(30)-H(30A)	108.9
C(31)-C(30)-H(30B)	108.9
C(27)-C(30)-H(30B)	108.9
H(30A)-C(30)-H(30B)	107.7
C(32)-C(31)-C(33)	117.7(2)
C(32)-C(31)-C(30)	119.5(2)
C(33)-C(31)-C(30)	122.8(2)
C(31)-C(32)-C(33)#1	122.5(2)
C(31)-C(32)-H(32)	118.8
C(33)#1-C(32)-H(32)	118.8
O(1)-C(33)-C(32)#1	123.9(2)
O(1)-C(33)-C(31)	116.3(2)
C(32)#1-C(33)-C(31)	119.8(2)
O(1)-C(34)-C(35)	107.8(3)
O(1)-C(34)-H(34A)	110.1
C(35)-C(34)-H(34A)	110.1
O(1)-C(34)-H(34B)	110.1
C(35)-C(34)-H(34B)	110.1
H(34A)-C(34)-H(34B)	108.5
C(36)-C(35)-C(34)	112.9(3)
C(36)-C(35)-H(35A)	109.0
C(34)-C(35)-H(35A)	109.0

C(36)-C(35)-H(35B)	109.0
C(34)-C(35)-H(35B)	109.0
H(35A)-C(35)-H(35B)	107.8
C(35)-C(36)-C(37)	115.6(4)
C(35)-C(36)-H(36A)	108.4
C(37)-C(36)-H(36A)	108.4
C(35)-C(36)-H(36B)	108.4
C(37)-C(36)-H(36B)	108.4
H(36A)-C(36)-H(36B)	107.4
C(38)-C(37)-C(36)	111.9(4)
C(38)-C(37)-H(37A)	109.2
C(36)-C(37)-H(37A)	109.2
C(38)-C(37)-H(37B)	109.2
C(36)-C(37)-H(37B)	109.2
H(37A)-C(37)-H(37B)	107.9
C(39)-C(38)-C(37)	115.0(4)
C(39)-C(38)-H(38A)	108.5
C(37)-C(38)-H(38A)	108.5
C(39)-C(38)-H(38B)	108.5
C(37)-C(38)-H(38B)	108.5
H(38A)-C(38)-H(38B)	107.5
C(38)-C(39)-C(40)	115.1(4)
C(38)-C(39)-H(39A)	108.5
C(40)-C(39)-H(39A)	108.5
C(38)-C(39)-H(39B)	108.5
C(40)-C(39)-H(39B)	108.5
H(39A)-C(39)-H(39B)	107.5

C(41)-C(40)-C(39)	115.1(4)
C(41)-C(40)-H(40A)	108.5
C(39)-C(40)-H(40A)	108.5
C(41)-C(40)-H(40B)	108.5
C(39)-C(40)-H(40B)	108.5
H(40A)-C(40)-H(40B)	107.5
C(40)-C(41)-C(42)	116.8(4)
C(40)-C(41)-H(41A)	108.1
C(42)-C(41)-H(41A)	108.1
C(40)-C(41)-H(41B)	108.1
C(42)-C(41)-H(41B)	108.1
H(41A)-C(41)-H(41B)	107.3
C(41)-C(42)-C(43)	112.6(4)
C(41)-C(42)-H(42A)	109.1
C(43)-C(42)-H(42A)	109.1
C(41)-C(42)-H(42B)	109.1
C(43)-C(42)-H(42B)	109.1
H(42A)-C(42)-H(42B)	107.8
C(44)-C(43)-C(42)	114.4(5)
C(44)-C(43)-H(43A)	108.7
C(42)-C(43)-H(43A)	108.7
C(44)-C(43)-H(43B)	108.7
C(42)-C(43)-H(43B)	108.7
H(43A)-C(43)-H(43B)	107.6
C(43)-C(44)-C(45)	111.7(6)
C(43)-C(44)-H(44A)	109.3
C(45)-C(44)-H(44A)	109.3

C(43)-C(44)-H(44B)	109.3
C(45)-C(44)-H(44B)	109.3
H(44A)-C(44)-H(44B)	107.9
C(44)-C(45)-H(45A)	109.5
C(44)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(44)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
C(33)-O(1)-C(34)	118.7(2)

Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y+2,-z+1

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 1.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	44(2)	50(2)	46(2)	1(1)	-2(1)	-13(1)
C(2)	63(2)	68(2)	46(2)	9(2)	4(1)	-19(2)
C(3)	76(2)	70(2)	44(2)	-4(2)	-4(2)	-17(2)
C(4)	60(2)	49(2)	48(2)	-1(1)	-11(1)	-14(1)
C(5)	35(1)	35(1)	43(1)	0(1)	-9(1)	-1(1)
C(6)	32(1)	31(1)	48(2)	-1(1)	-10(1)	-3(1)
C(7)	46(2)	37(1)	59(2)	-5(1)	-18(1)	-10(1)
C(8)	50(2)	40(2)	76(2)	-3(1)	-18(1)	-16(1)
C(9)	51(2)	40(2)	73(2)	8(1)	-10(1)	-21(1)
C(10)	41(1)	38(1)	54(2)	2(1)	-8(1)	-13(1)
C(11)	28(1)	31(1)	45(1)	1(1)	-7(1)	-6(1)
C(12)	28(1)	31(1)	41(1)	3(1)	-7(1)	-4(1)
C(13)	32(1)	31(1)	39(1)	4(1)	-8(1)	-7(1)
C(14)	40(1)	37(1)	40(1)	3(1)	-5(1)	-11(1)
C(15)	48(2)	61(2)	46(2)	-2(1)	-2(1)	-23(1)
C(16)	67(2)	91(3)	62(2)	-4(2)	10(2)	-43(2)
C(17)	89(3)	114(3)	49(2)	-6(2)	15(2)	-53(2)
C(18)	91(3)	86(2)	44(2)	-4(2)	-2(2)	-44(2)
C(19)	56(2)	45(2)	38(2)	2(1)	-7(1)	-16(1)
C(20)	51(2)	42(2)	45(2)	0(1)	-13(1)	-15(1)
C(21)	79(2)	75(2)	50(2)	0(2)	-18(2)	-33(2)
C(22)	92(3)	91(3)	67(2)	-7(2)	-30(2)	-46(2)
C(23)	74(2)	68(2)	82(2)	-6(2)	-22(2)	-40(2)

C(24)	53(2)	51(2)	60(2)	-2(1)	-12(1)	-23(1)
C(25)	38(1)	33(1)	46(2)	0(1)	-12(1)	-9(1)
C(26)	32(1)	29(1)	43(1)	2(1)	-6(1)	-7(1)
C(27)	28(1)	34(1)	46(1)	2(1)	-6(1)	-8(1)
C(28)	28(1)	30(1)	42(1)	2(1)	-6(1)	-4(1)
C(29)	28(1)	36(1)	41(1)	3(1)	-5(1)	-2(1)
C(30)	38(1)	35(1)	53(2)	5(1)	-5(1)	-15(1)
C(31)	37(1)	25(1)	44(1)	5(1)	-7(1)	-7(1)
C(32)	40(1)	29(1)	40(1)	2(1)	0(1)	-3(1)
C(33)	42(1)	26(1)	39(1)	0(1)	-10(1)	-7(1)
C(34)	71(2)	68(2)	52(2)	-16(2)	-16(2)	2(2)
C(35)	85(3)	110(3)	65(2)	-28(2)	-32(2)	11(2)
C(36)	115(4)	143(4)	90(3)	-34(3)	-20(3)	-32(3)
C(37)	114(4)	111(4)	130(4)	-32(3)	-55(3)	-23(3)
C(38)	126(4)	108(4)	103(3)	-35(3)	-25(3)	-25(3)
C(39)	110(3)	80(3)	112(3)	11(2)	-33(3)	-38(3)
C(40)	117(3)	93(3)	82(3)	-9(2)	-14(2)	-40(3)
C(41)	109(4)	89(3)	125(4)	14(3)	-23(3)	-34(3)
C(42)	119(4)	114(4)	124(4)	-23(3)	-1(3)	-40(3)
C(43)	148(5)	131(5)	120(4)	-12(4)	2(4)	-40(4)
C(44)	209(8)	140(6)	150(5)	-17(4)	-7(5)	-68(5)
C(45)	150(5)	109(4)	234(7)	28(4)	-27(5)	-27(4)
O(1)	51(1)	51(1)	48(1)	-11(1)	-14(1)	-6(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **1**.

	x	y	z	U(eq)
H(1)	5026	12145	6210	58
H(2)	4750	12596	7441	74
H(3)	5742	14081	7858	80
H(4)	6947	15130	7056	65
H(7)	7929	16139	6306	58
H(8)	8746	17450	5460	65
H(9)	8625	17253	4210	64
H(10)	7888	15608	3811	54
H(15)	9564	13768	3514	61
H(16)	10900	13696	2407	84
H(17)	10068	13179	1348	97
H(18)	8035	12557	1428	85
H(21)	6007	12204	1505	79
H(22)	4288	11193	1639	94
H(23)	3555	10543	2799	83
H(24)	4439	11048	3829	64
H(27)	4823	12326	4817	45
H(30A)	6422	10391	5439	50
H(30B)	6636	10005	4610	50
H(32)	8407	10682	6027	47
H(34A)	10680	8307	3248	84
H(34B)	10169	9775	2870	84
H(35A)	8585	8004	2817	117
H(35B)	8079	9465	2440	117
H(36A)	10711	7353	2043	142

H(36B)	10157	8803	1656	142
H(37A)	8733	6926	1597	143
H(37B)	8142	8390	1222	143
H(38A)	9421	6962	315	138
H(38B)	10395	7797	470	138
H(39A)	10967	5150	1047	119
H(39B)	11987	5983	1113	119
H(40A)	11560	5071	-232	115
H(40B)	12629	5847	-143	115
H(41A)	13068	3258	465	130
H(41B)	14144	4032	537	130
H(42A)	14789	3863	-720	143
H(42B)	13722	3073	-787	143
H(43A)	16341	2066	22	164
H(43B)	15247	1289	8	164
H(44A)	16871	1801	-1187	198
H(44B)	15803	991	-1187	198
H(45A)	18429	122	-405	257
H(45B)	18249	-559	-1111	257
H(45C)	17343	-674	-369	257

Table 6. Torsion angles [deg] for **1**.

C(29)-C(1)-C(2)-C(3)	-0.3(4)
C(1)-C(2)-C(3)-C(4)	0.7(5)
C(2)-C(3)-C(4)-C(5)	-0.4(4)
C(3)-C(4)-C(5)-C(29)	-0.3(4)
C(3)-C(4)-C(5)-C(6)	175.3(2)
C(4)-C(5)-C(6)-C(7)	-0.1(3)
C(29)-C(5)-C(6)-C(7)	175.4(2)
C(4)-C(5)-C(6)-C(11)	-176.6(2)
C(29)-C(5)-C(6)-C(11)	-1.1(3)
C(11)-C(6)-C(7)-C(8)	4.0(4)
C(5)-C(6)-C(7)-C(8)	-172.5(2)
C(6)-C(7)-C(8)-C(9)	1.8(4)
C(7)-C(8)-C(9)-C(10)	-3.6(4)
C(8)-C(9)-C(10)-C(11)	-0.4(4)
C(7)-C(6)-C(11)-C(10)	-7.7(3)
C(5)-C(6)-C(11)-C(10)	168.8(2)
C(7)-C(6)-C(11)-C(12)	176.5(2)
C(5)-C(6)-C(11)-C(12)	-7.0(3)
C(9)-C(10)-C(11)-C(6)	6.1(3)
C(9)-C(10)-C(11)-C(12)	-178.4(2)
C(6)-C(11)-C(12)-C(28)	10.7(3)
C(10)-C(11)-C(12)-C(28)	-164.9(2)
C(6)-C(11)-C(12)-C(13)	-176.1(2)
C(10)-C(11)-C(12)-C(13)	8.3(4)
C(28)-C(12)-C(13)-C(26)	8.3(2)
C(11)-C(12)-C(13)-C(26)	-165.5(2)
C(28)-C(12)-C(13)-C(14)	-166.0(2)

C(11)-C(12)-C(13)-C(14)	20.2(4)
C(26)-C(13)-C(14)-C(15)	-155.3(2)
C(12)-C(13)-C(14)-C(15)	18.5(4)
C(26)-C(13)-C(14)-C(19)	17.3(3)
C(12)-C(13)-C(14)-C(19)	-168.8(2)
C(19)-C(14)-C(15)-C(16)	3.4(4)
C(13)-C(14)-C(15)-C(16)	176.1(3)
C(14)-C(15)-C(16)-C(17)	0.6(5)
C(15)-C(16)-C(17)-C(18)	-3.2(6)
C(16)-C(17)-C(18)-C(19)	1.8(6)
C(17)-C(18)-C(19)-C(14)	2.3(5)
C(17)-C(18)-C(19)-C(20)	-172.3(3)
C(15)-C(14)-C(19)-C(18)	-4.8(4)
C(13)-C(14)-C(19)-C(18)	-177.7(2)
C(15)-C(14)-C(19)-C(20)	169.9(2)
C(13)-C(14)-C(19)-C(20)	-3.0(4)
C(18)-C(19)-C(20)-C(21)	-13.5(4)
C(14)-C(19)-C(20)-C(21)	172.0(3)
C(18)-C(19)-C(20)-C(25)	163.3(3)
C(14)-C(19)-C(20)-C(25)	-11.2(4)
C(25)-C(20)-C(21)-C(22)	-2.4(5)
C(19)-C(20)-C(21)-C(22)	174.4(3)
C(20)-C(21)-C(22)-C(23)	-0.7(5)
C(21)-C(22)-C(23)-C(24)	2.5(5)
C(22)-C(23)-C(24)-C(25)	-1.1(5)
C(23)-C(24)-C(25)-C(20)	-2.0(4)
C(23)-C(24)-C(25)-C(26)	173.3(3)
C(21)-C(20)-C(25)-C(24)	3.7(4)

C(19)-C(20)-C(25)-C(24)	-173.3(2)
C(21)-C(20)-C(25)-C(26)	-171.8(2)
C(19)-C(20)-C(25)-C(26)	11.2(3)
C(14)-C(13)-C(26)-C(25)	-17.9(3)
C(12)-C(13)-C(26)-C(25)	166.8(2)
C(14)-C(13)-C(26)-C(27)	162.32(19)
C(12)-C(13)-C(26)-C(27)	-13.0(2)
C(24)-C(25)-C(26)-C(13)	-171.9(2)
C(20)-C(25)-C(26)-C(13)	3.4(3)
C(24)-C(25)-C(26)-C(27)	7.9(4)
C(20)-C(25)-C(26)-C(27)	-176.8(2)
C(13)-C(26)-C(27)-C(28)	12.4(2)
C(25)-C(26)-C(27)-C(28)	-167.4(2)
C(13)-C(26)-C(27)-C(30)	-107.7(2)
C(25)-C(26)-C(27)-C(30)	72.5(3)
C(11)-C(12)-C(28)-C(29)	-6.4(3)
C(13)-C(12)-C(28)-C(29)	178.94(19)
C(11)-C(12)-C(28)-C(27)	174.45(19)
C(13)-C(12)-C(28)-C(27)	-0.2(2)
C(26)-C(27)-C(28)-C(12)	-7.0(2)
C(30)-C(27)-C(28)-C(12)	111.5(2)
C(26)-C(27)-C(28)-C(29)	173.9(2)
C(30)-C(27)-C(28)-C(29)	-67.7(3)
C(2)-C(1)-C(29)-C(5)	-0.3(4)
C(2)-C(1)-C(29)-C(28)	179.0(2)
C(4)-C(5)-C(29)-C(1)	0.6(3)
C(6)-C(5)-C(29)-C(1)	-175.1(2)
C(4)-C(5)-C(29)-C(28)	-178.7(2)

C(6)-C(5)-C(29)-C(28)	5.5(3)
C(12)-C(28)-C(29)-C(1)	178.8(2)
C(27)-C(28)-C(29)-C(1)	-2.1(3)
C(12)-C(28)-C(29)-C(5)	-1.8(3)
C(27)-C(28)-C(29)-C(5)	177.2(2)
C(26)-C(27)-C(30)-C(31)	68.9(3)
C(28)-C(27)-C(30)-C(31)	-44.3(3)
C(27)-C(30)-C(31)-C(32)	89.6(3)
C(27)-C(30)-C(31)-C(33)	-88.9(3)
C(33)-C(31)-C(32)-C(33)#1	1.2(4)
C(30)-C(31)-C(32)-C(33)#1	-177.4(2)
C(32)-C(31)-C(33)-O(1)	176.90(19)
C(30)-C(31)-C(33)-O(1)	-4.5(3)
C(32)-C(31)-C(33)-C(32)#1	-1.2(4)
C(30)-C(31)-C(33)-C(32)#1	177.4(2)
O(1)-C(34)-C(35)-C(36)	-179.9(3)
C(34)-C(35)-C(36)-C(37)	178.0(4)
C(35)-C(36)-C(37)-C(38)	178.6(4)
C(36)-C(37)-C(38)-C(39)	67.9(6)
C(37)-C(38)-C(39)-C(40)	174.0(4)
C(38)-C(39)-C(40)-C(41)	-177.3(4)
C(39)-C(40)-C(41)-C(42)	178.9(4)
C(40)-C(41)-C(42)-C(43)	179.3(4)
C(41)-C(42)-C(43)-C(44)	176.4(5)
C(42)-C(43)-C(44)-C(45)	178.5(5)
C(32)#1-C(33)-O(1)-C(34)	2.1(4)
C(31)-C(33)-O(1)-C(34)	-175.9(2)
C(35)-C(34)-O(1)-C(33)	168.0(2)