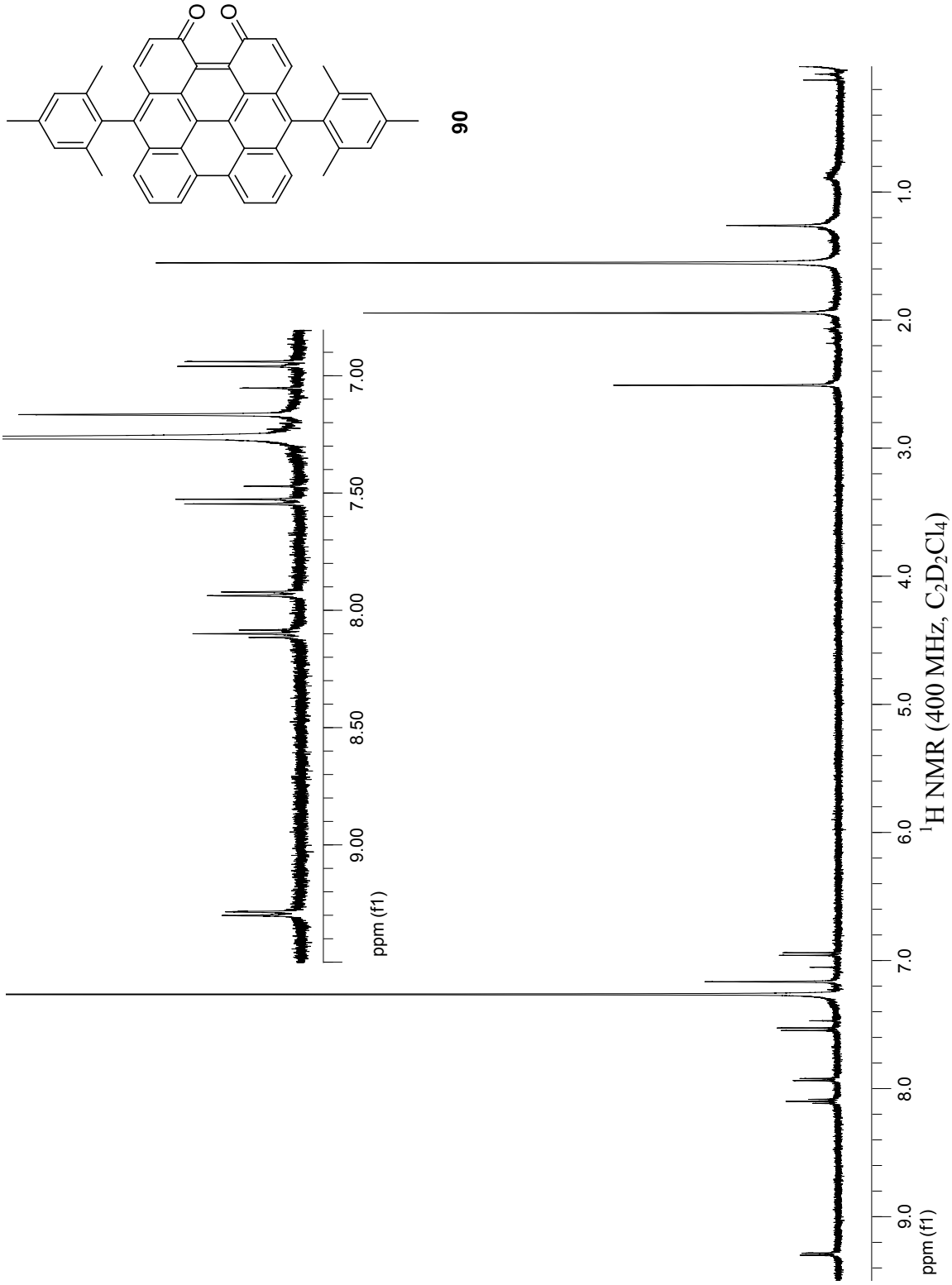
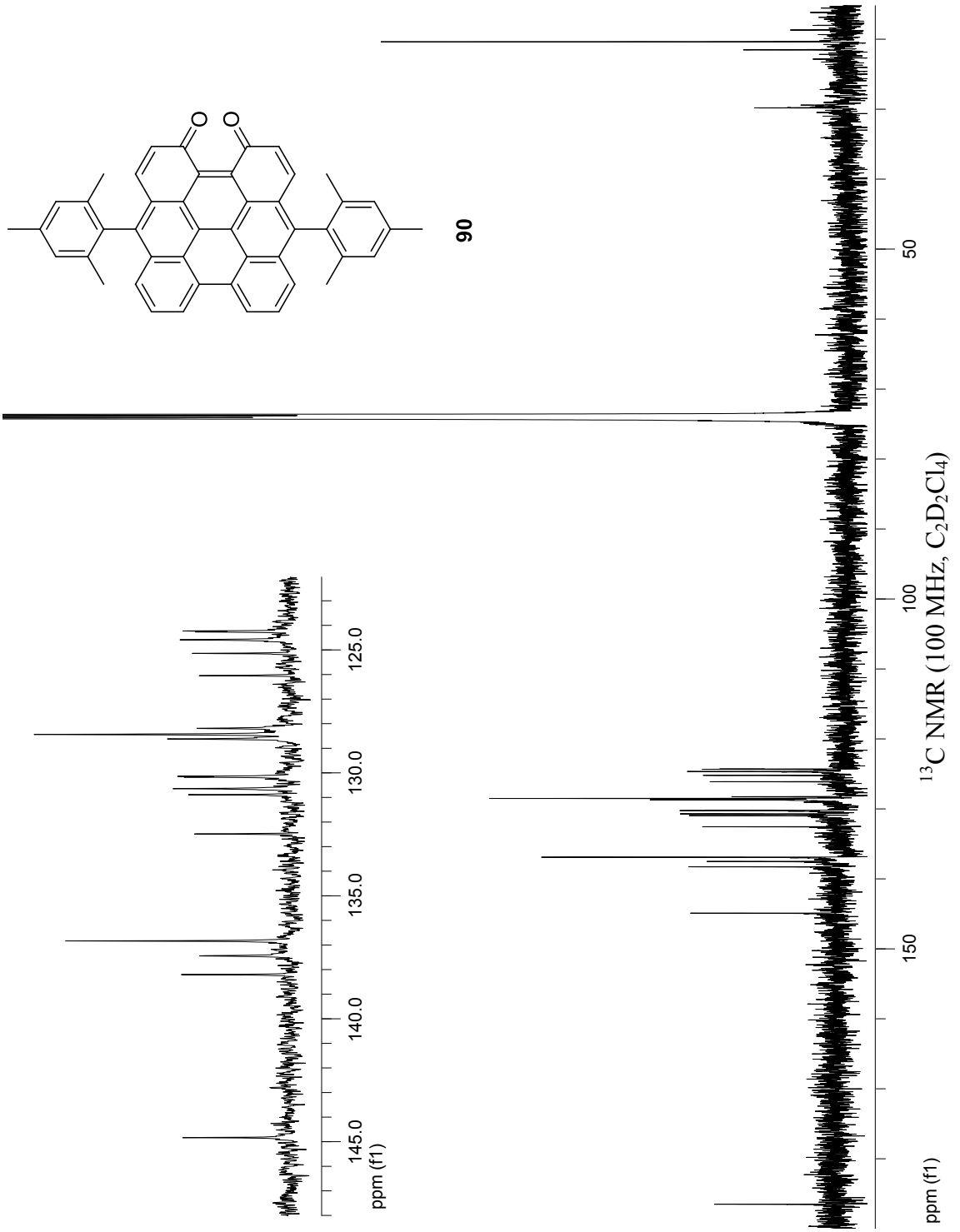
Facile Air-Oxidation of Large Aromatic Hydrocarbon Bay Regions to Bay Region Quinones. Predicted Oxygen-Sensitivity of Hydrogen-Terminated Carbon Nanotubes

Eric H. Fort and Lawrence T. Scott*
Merkert Chemistry Center, Boston College
Chestnut Hill, MA 02467-3860 USA

Supplementary Information

7,14-Dimesitylbisanthene-3,4-quinone (2) from Photooxidation of 7,14-dimesitylbisanthene (1). To a 150 mL immersion photolysis vessel equipped with a magnetic stirring bar were added 20 mg (3.4×10^{-2} mmol) of 7,14-*bis*(2,4,6-trimethylphenyl)bisanthene (**1**), 500 μL of a 3.9×10^{-2} M solution of 1,3,5-trimethoxybenzene in 1,1,2,2-tetrachloroethane-d_2 as an NMR internal standard, and 123 mL of dry dichloromethane. Industrial grade oxygen was bubbled through the solution for 30 min prior to photolysis and throughout the irradiation period. A quartz immersion well with a 450 W medium pressure mercury lamp was submerged in the solution, and the lamp was turned on. Aliquots of ~3 mL each were taken at 0 min (before the lamp was turned on) and every five min for 30 min. Each sample was concentrated to dryness under reduced pressure and analyzed by NMR spectroscopy to determine the extent of conversion. Starting material is quickly converted to product; the NMR spectrum shows no signals for starting material after 25 min of irradiation. **^{1}H NMR** (400 MHz, $C_2D_2Cl_4$) δ ppm 9.33 (d, J = 8.0 Hz, 2H), 8.14 (t, J = 8.0 Hz, 2H), 7.96 (d, J = 8.0 Hz, 2H), 7.58 (d, J = 10.0 Hz, 2H), 7.17 (s, 4H), 6.91 (d, J = 10.0 Hz, 2H), 2.51 (s, 6H), 1.94 (s, 12H); **^{13}C NMR** (100 MHz, $C_2D_2Cl_4$) δ ppm 186.5, 144.8, 138.2, 137.4, 136.8, 132.5, 130.9, 130.6, 130.2, 130.1, 128.6, 128.4, 128.2, 126.0, 125.1, 124.6, 124.2, 124.2, 21.3, 20.2; **UV-vis** ($CHCl_3$) λ_{max} (ε, cm^{-1} M^{-1}) 244 (19000), 262 (sh, 9100), 274 (sh, 8500), 298 (sh, 7200), 312 (9400), 352 (sh, 13000), 364 (15000), 394 (sh, 8700), 414 (6600), 460 (1600), 486 (sh, 2300), 496 (2900), 530 (4100); **HRMS** (DART) calc. for $C_{46}H_{33}O_2$ $[M+H]^+$ 617.2481, found 617.2456.





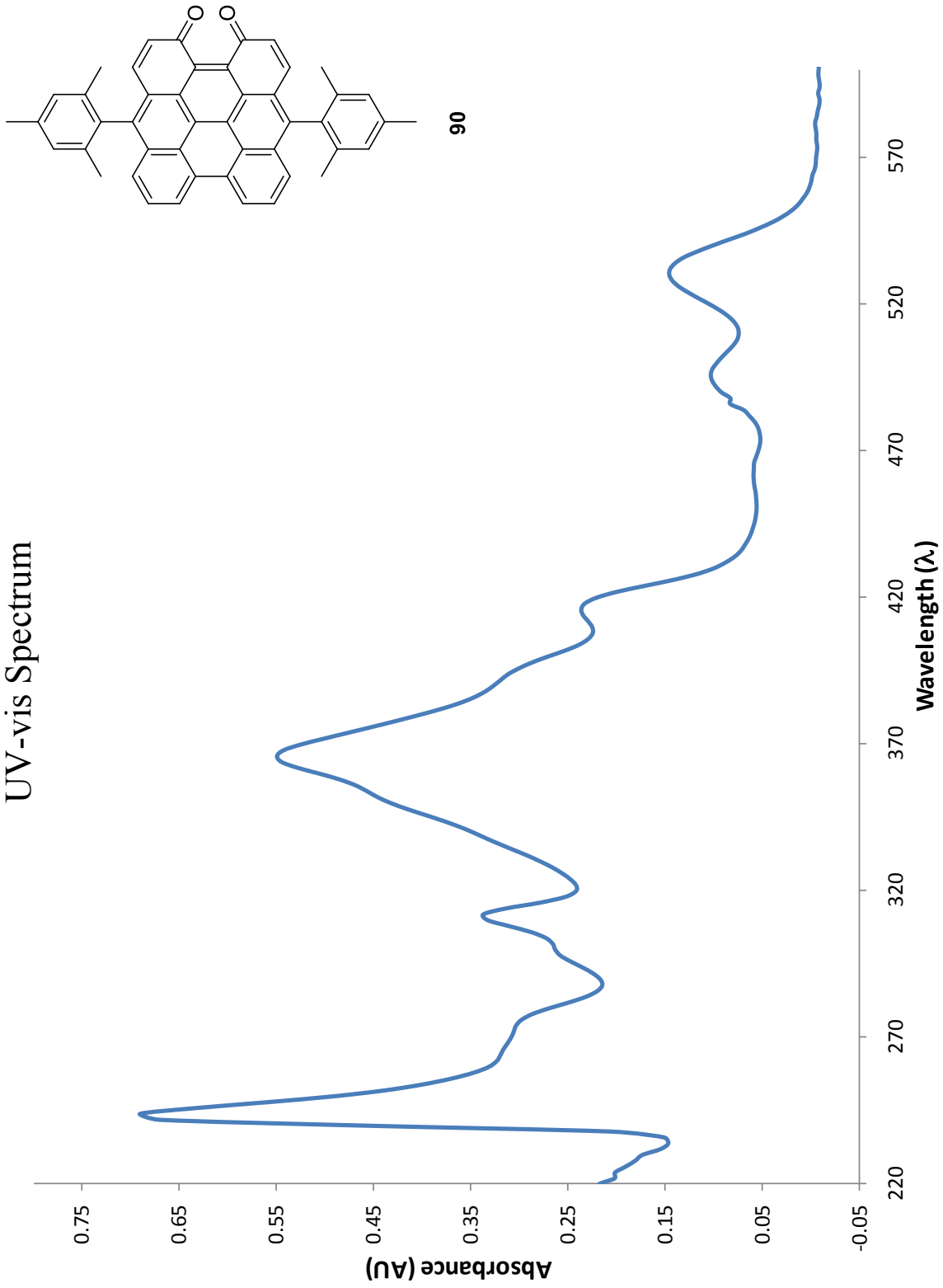


Table 1. Crystal data and structure refinement for $C_{46}H_{32}O_2$ (**CCDC 865170**)

Identification code	$C_{46}H_{32}O_2$	
Empirical formula	$C_{46}H_{32}O_2$	
Formula weight	616.72	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Trigonal	
Space group	R3c	
Unit cell dimensions	a = 36.714(4) Å	α= 90°.
	b = 36.714(4) Å	β= 90°.
	c = 15.1151(15) Å	γ = 120°.
Volume	17645(3) $Å^3$	
Z	18	
Density (calculated)	1.045 Mg/m^3	
Absorption coefficient	0.063 mm^{-1}	
F(000)	5832	
Crystal size	0.14 x 0.08 x 0.06 mm^3	
Theta range for data collection	1.92 to 24.99°.	
Index ranges	-37<=h<=0, 0<=k<=43, -17<=l<=17	
Reflections collected	6887	
Independent reflections	6887 [R(int) = 0.0631]	
Completeness to theta = 24.99°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9963 and 0.9913	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6887 / 492 / 433	
Goodness-of-fit on F^2	1.069	
Final R indices [I>2sigma(I)]	R1 = 0.0628, wR2 = 0.1718	
R indices (all data)	R1 = 0.0874, wR2 = 0.1886	
Absolute structure parameter	2(2)	
Largest diff. peak and hole	0.358 and -0.203 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $C_{46}H_{32}O_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	7049(1)	7420(1)	-1140(2)	89(1)
O(2)	7311(1)	7499(1)	547(2)	72(1)
C(1)	6736(1)	7414(1)	-854(3)	59(1)
C(2)	6345(1)	7138(1)	-1279(3)	63(1)
C(3)	6025(1)	7221(1)	-1255(3)	54(1)
C(4)	6058(1)	7578(1)	-824(2)	49(1)
C(5)	5728(1)	7664(1)	-836(2)	44(1)
C(6)	5768(1)	8020(1)	-399(2)	45(1)
C(7)	5429(1)	8110(1)	-372(3)	54(1)
C(8)	5475(1)	8462(1)	27(3)	65(1)
C(9)	5856(2)	8740(2)	440(4)	93(2)
C(10)	6198(1)	8661(1)	497(2)	49(1)
C(11)	6143(1)	8294(1)	59(2)	44(1)
C(12)	6479(1)	8206(1)	83(2)	41(1)
C(13)	6434(1)	7846(1)	-360(2)	41(1)
C(14)	6764(1)	7746(1)	-351(3)	49(1)

C(15)	7139(1)	8012(1)	184(2)	47(1)
C(16)	7183(1)	8377(1)	571(2)	43(1)
C(17)	6855(1)	8475(1)	537(2)	40(1)
C(18)	6902(1)	8847(1)	966(2)	44(1)
C(19)	6569(1)	8923(1)	937(2)	44(1)
C(20)	6633(2)	9295(1)	1449(3)	66(1)
C(21)	7016(1)	9568(1)	1824(3)	63(1)
C(22)	7334(1)	9484(1)	1835(3)	56(1)
C(23)	7293(1)	9120(1)	1420(2)	43(1)
C(24)	7625(1)	9026(1)	1427(2)	43(1)
C(25)	7574(1)	8664(1)	1007(2)	45(1)
C(26)	7898(1)	8566(1)	1007(2)	48(1)
C(27)	7844(1)	8208(1)	669(3)	57(1)
C(28)	7444(1)	7893(1)	388(3)	69(1)
C(29)	5319(1)	7373(1)	-1285(2)	47(1)
C(30)	4985(1)	7043(1)	-843(2)	51(1)
C(31)	4609(1)	6809(1)	-1270(3)	58(1)
C(32)	4547(1)	6878(1)	-2139(3)	60(1)
C(33)	4887(2)	7200(1)	-2571(3)	66(1)
C(34)	5262(1)	7445(1)	-2180(2)	51(1)
C(35)	5031(2)	6953(2)	101(3)	74(1)
C(36)	4118(2)	6618(2)	-2567(4)	101(2)
C(37)	5633(2)	7795(2)	-2681(3)	77(1)
C(38)	8027(1)	9304(1)	1915(2)	45(1)
C(39)	8355(1)	9633(1)	1450(3)	55(1)
C(40)	8737(1)	9876(1)	1886(3)	58(1)
C(41)	8806(2)	9795(1)	2727(3)	65(1)
C(42)	8472(1)	9477(1)	3181(3)	60(1)
C(43)	8066(1)	9222(1)	2788(3)	57(1)
C(44)	8310(2)	9732(2)	510(3)	90(2)
C(45)	9219(2)	10059(2)	3168(4)	97(2)
C(46)	7731(2)	8882(2)	3311(3)	78(1)

Table 3. Bond lengths [Å] and angles [°] for $C_{46}H_{32}O_2$.

O(1)-C(1)	1.219(4)	C(8)-H(8A)	0.9500
O(2)-C(28)	1.298(5)	C(9)-C(10)	1.424(6)
C(1)-C(14)	1.394(5)	C(9)-H(9A)	0.9500
C(1)-C(2)	1.430(6)	C(10)-C(19)	1.383(5)
C(2)-C(3)	1.350(5)	C(10)-C(11)	1.423(5)
C(2)-H(2A)	0.9500	C(11)-C(12)	1.423(5)
C(3)-C(4)	1.413(5)	C(12)-C(17)	1.409(3)
C(3)-H(3A)	0.9500	C(12)-C(13)	1.413(5)
C(4)-C(5)	1.397(5)	C(13)-C(14)	1.432(5)
C(4)-C(13)	1.418(5)	C(14)-C(15)	1.469(5)
C(5)-C(6)	1.406(5)	C(15)-C(16)	1.394(5)
C(5)-C(29)	1.500(5)	C(15)-C(28)	1.425(5)
C(6)-C(11)	1.415(5)	C(16)-C(17)	1.421(5)
C(6)-C(7)	1.441(5)	C(16)-C(25)	1.447(5)
C(7)-C(8)	1.356(5)	C(17)-C(18)	1.443(5)
C(7)-H(7A)	0.9500	C(18)-C(19)	1.385(5)
C(8)-C(9)	1.399(6)	C(18)-C(23)	1.449(5)
		C(19)-C(20)	1.484(5)
		C(20)-C(21)	1.375(6)
		C(20)-H(20A)	0.9500

C(21)-C(22)	1.349(5)	C(3)-C(2)-C(1)	120.4(4)
C(21)-H(21A)	0.9500	C(3)-C(2)-H(2A)	119.8
C(22)-C(23)	1.412(5)	C(1)-C(2)-H(2A)	119.8
C(22)-H(22A)	0.9500	C(2)-C(3)-C(4)	122.7(4)
C(23)-C(24)	1.424(5)	C(2)-C(3)-H(3A)	118.7
C(24)-C(25)	1.399(5)	C(4)-C(3)-H(3A)	118.7
C(24)-C(38)	1.502(5)	C(5)-C(4)-C(3)	121.5(4)
C(25)-C(26)	1.405(5)	C(5)-C(4)-C(13)	120.1(3)
C(26)-C(27)	1.331(5)	C(3)-C(4)-C(13)	118.4(3)
C(26)-H(26A)	0.9500	C(4)-C(5)-C(6)	120.4(4)
C(27)-C(28)	1.406(6)	C(4)-C(5)-C(29)	121.1(3)
C(27)-H(27A)	0.9500	C(6)-C(5)-C(29)	118.5(3)
C(29)-C(30)	1.390(6)	C(5)-C(6)-C(11)	120.2(3)
C(29)-C(34)	1.415(5)	C(5)-C(6)-C(7)	121.8(3)
C(30)-C(31)	1.370(6)	C(11)-C(6)-C(7)	118.0(3)
C(30)-C(35)	1.494(6)	C(8)-C(7)-C(6)	121.3(4)
C(31)-C(32)	1.378(6)	C(8)-C(7)-H(7A)	119.4
C(31)-H(31A)	0.9500	C(6)-C(7)-H(7A)	119.4
C(32)-C(33)	1.380(6)	C(7)-C(8)-C(9)	119.8(4)
C(32)-C(36)	1.521(6)	C(7)-C(8)-H(8A)	120.1
C(33)-C(34)	1.346(5)	C(9)-C(8)-H(8A)	120.1
C(33)-H(33A)	0.9500	C(8)-C(9)-C(10)	122.7(4)
C(34)-C(37)	1.528(6)	C(8)-C(9)-H(9A)	118.7
C(35)-H(35A)	0.9800	C(10)-C(9)-H(9A)	118.7
C(35)-H(35B)	0.9800	C(19)-C(10)-C(11)	120.4(3)
C(35)-H(35C)	0.9800	C(19)-C(10)-C(9)	123.3(4)
C(36)-H(36A)	0.9800	C(11)-C(10)-C(9)	116.3(4)
C(36)-H(36B)	0.9800	C(6)-C(11)-C(10)	121.8(3)
C(36)-H(36C)	0.9800	C(6)-C(11)-C(12)	119.8(3)
C(37)-H(37A)	0.9800	C(10)-C(11)-C(12)	118.4(3)
C(37)-H(37B)	0.9800	C(17)-C(12)-C(13)	120.1(2)
C(37)-H(37C)	0.9800	C(17)-C(12)-C(11)	120.6(3)
C(38)-C(43)	1.375(5)	C(13)-C(12)-C(11)	119.4(3)
C(38)-C(39)	1.398(5)	C(12)-C(13)-C(4)	120.1(3)
C(39)-C(40)	1.394(6)	C(12)-C(13)-C(14)	121.2(3)
C(39)-C(44)	1.495(6)	C(4)-C(13)-C(14)	118.6(3)
C(40)-C(41)	1.358(6)	C(1)-C(14)-C(13)	121.2(3)
C(40)-H(40A)	0.9500	C(1)-C(14)-C(15)	121.2(3)
C(41)-C(42)	1.381(6)	C(13)-C(14)-C(15)	117.6(3)
C(41)-C(45)	1.488(6)	C(16)-C(15)-C(28)	118.0(3)
C(42)-C(43)	1.434(6)	C(16)-C(15)-C(14)	119.5(3)
C(42)-H(42A)	0.9500	C(28)-C(15)-C(14)	122.2(3)
C(43)-C(46)	1.470(6)	C(15)-C(16)-C(17)	121.3(3)
C(44)-H(44A)	0.9800	C(15)-C(16)-C(25)	119.3(3)
C(44)-H(44B)	0.9800	C(17)-C(16)-C(25)	119.4(3)
C(44)-H(44C)	0.9800	C(12)-C(17)-C(16)	119.8(3)
C(45)-H(45A)	0.9800	C(12)-C(17)-C(18)	119.7(2)
C(45)-H(45B)	0.9800	C(16)-C(17)-C(18)	120.5(3)
C(45)-H(45C)	0.9800	C(19)-C(18)-C(17)	118.5(3)
C(46)-H(46A)	0.9800	C(19)-C(18)-C(23)	123.0(3)
C(46)-H(46B)	0.9800	C(17)-C(18)-C(23)	118.6(3)
C(46)-H(46C)	0.9800	C(10)-C(19)-C(18)	122.5(3)
		C(10)-C(19)-C(20)	122.7(3)
O(1)-C(1)-C(14)	121.3(4)	C(18)-C(19)-C(20)	114.8(4)
O(1)-C(1)-C(2)	117.3(4)	C(21)-C(20)-C(19)	121.3(4)
C(14)-C(1)-C(2)	118.2(3)	C(21)-C(20)-H(20A)	119.4

C(19)-C(20)-H(20A)	119.4
C(22)-C(21)-C(20)	121.7(4)
C(22)-C(21)-H(21A)	119.1
C(20)-C(21)-H(21A)	119.1
C(21)-C(22)-C(23)	121.0(4)
C(21)-C(22)-H(22A)	119.5
C(23)-C(22)-H(22A)	119.5
C(22)-C(23)-C(24)	121.8(3)
C(22)-C(23)-C(18)	117.8(3)
C(24)-C(23)-C(18)	120.4(3)
C(25)-C(24)-C(23)	120.3(3)
C(25)-C(24)-C(38)	119.1(3)
C(23)-C(24)-C(38)	120.5(3)
C(24)-C(25)-C(26)	121.1(3)
C(24)-C(25)-C(16)	120.7(3)
C(26)-C(25)-C(16)	118.2(3)
C(27)-C(26)-C(25)	121.7(4)
C(27)-C(26)-H(26A)	119.1
C(25)-C(26)-H(26A)	119.1
C(26)-C(27)-C(28)	120.4(4)
C(26)-C(27)-H(27A)	119.8
C(28)-C(27)-H(27A)	119.8
O(2)-C(28)-C(27)	121.0(3)
O(2)-C(28)-C(15)	117.8(4)
C(27)-C(28)-C(15)	118.3(3)
C(30)-C(29)-C(34)	118.2(4)
C(30)-C(29)-C(5)	122.5(3)
C(34)-C(29)-C(5)	119.3(3)
C(31)-C(30)-C(29)	119.7(4)
C(31)-C(30)-C(35)	120.1(4)
C(29)-C(30)-C(35)	120.2(4)
C(30)-C(31)-C(32)	122.6(4)
C(30)-C(31)-H(31A)	118.7
C(32)-C(31)-H(31A)	118.7
C(31)-C(32)-C(33)	116.6(4)
C(31)-C(32)-C(36)	120.2(4)
C(33)-C(32)-C(36)	123.1(4)
C(34)-C(33)-C(32)	123.2(4)
C(34)-C(33)-H(33A)	118.4
C(32)-C(33)-H(33A)	118.4
C(33)-C(34)-C(29)	119.6(4)
C(33)-C(34)-C(37)	121.9(3)
C(29)-C(34)-C(37)	118.5(3)
C(30)-C(35)-H(35A)	109.5
C(30)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(30)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(32)-C(36)-H(36A)	109.5
C(32)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(32)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(34)-C(37)-H(37A)	109.5
C(34)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
C(34)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
C(43)-C(38)-C(39)	122.2(4)
C(43)-C(38)-C(24)	119.8(3)
C(39)-C(38)-C(24)	118.0(3)
C(40)-C(39)-C(38)	118.1(4)
C(40)-C(39)-C(44)	119.4(4)
C(38)-C(39)-C(44)	122.4(4)
C(41)-C(40)-C(39)	122.7(4)
C(41)-C(40)-H(40A)	118.6
C(39)-C(40)-H(40A)	118.6
C(40)-C(41)-C(42)	117.9(4)
C(40)-C(41)-C(45)	121.2(4)
C(42)-C(41)-C(45)	120.8(4)
C(41)-C(42)-C(43)	122.6(4)
C(41)-C(42)-H(42A)	118.7
C(43)-C(42)-H(42A)	118.7
C(38)-C(43)-C(42)	116.3(4)
C(38)-C(43)-C(46)	124.5(4)
C(42)-C(43)-C(46)	119.1(4)
C(39)-C(44)-H(44A)	109.5
C(39)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(39)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(41)-C(45)-H(45A)	109.5
C(41)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(41)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
C(43)-C(46)-H(46A)	109.5
C(43)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	109.5
C(43)-C(46)-H(46C)	109.5
H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3)for $C_{46}H_{32}O_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	95(2)	126(2)	94(2)	-44(2)	-23(2)	91(2)
O(2)	89(2)	77(2)	78(2)	-9(1)	-13(1)	63(2)
C(1)	54(2)	76(3)	67(3)	-25(2)	-8(2)	49(2)
C(2)	62(2)	55(2)	80(3)	-29(2)	-13(2)	35(2)
C(3)	58(2)	56(2)	52(2)	-13(2)	-10(2)	32(2)
C(4)	54(2)	47(2)	58(2)	-5(2)	-4(2)	35(2)
C(5)	52(2)	47(2)	43(2)	0(2)	-2(2)	32(2)
C(6)	55(2)	60(2)	36(2)	6(2)	-2(2)	41(2)
C(7)	53(2)	61(3)	65(3)	-5(2)	-3(2)	40(2)
C(8)	58(3)	63(3)	97(3)	-11(2)	-18(2)	47(2)
C(9)	81(3)	80(3)	149(5)	-46(3)	-41(3)	63(3)
C(10)	64(2)	41(2)	55(2)	1(2)	-5(2)	36(2)
C(11)	50(2)	52(2)	43(2)	4(2)	6(2)	35(2)
C(12)	46(2)	45(2)	41(2)	-2(2)	-3(2)	30(2)
C(13)	44(2)	42(2)	48(2)	2(2)	1(2)	30(2)
C(14)	52(2)	56(2)	52(2)	-5(2)	-2(2)	36(2)
C(15)	50(2)	53(2)	50(2)	-2(2)	-1(2)	35(2)
C(16)	54(2)	38(2)	48(2)	3(2)	-2(2)	32(2)
C(17)	50(2)	39(2)	42(2)	9(2)	9(2)	32(2)
C(18)	61(2)	49(2)	34(2)	-2(2)	3(2)	37(2)
C(19)	52(2)	45(2)	45(2)	6(2)	6(2)	33(2)
C(20)	76(3)	61(3)	85(3)	-21(2)	-9(2)	53(2)
C(21)	76(3)	69(3)	65(3)	-19(2)	1(2)	51(2)
C(22)	65(2)	46(2)	68(3)	-16(2)	-9(2)	36(2)
C(23)	52(2)	44(2)	37(2)	4(2)	4(2)	27(2)
C(24)	53(2)	41(2)	41(2)	3(2)	4(2)	28(2)
C(25)	46(2)	34(2)	57(2)	5(2)	4(2)	22(2)
C(26)	54(2)	49(2)	53(2)	1(2)	-4(2)	34(2)
C(27)	56(2)	64(3)	70(3)	-3(2)	-1(2)	44(2)
C(28)	79(3)	52(2)	108(3)	-30(2)	-39(2)	56(2)
C(29)	56(2)	47(2)	51(2)	2(2)	-2(2)	36(2)
C(30)	53(2)	55(2)	50(2)	-1(2)	-1(2)	29(2)
C(31)	64(3)	40(2)	67(3)	4(2)	6(2)	24(2)
C(32)	59(3)	55(3)	71(3)	-4(2)	-19(2)	31(2)
C(33)	86(3)	63(3)	46(2)	3(2)	-15(2)	36(2)
C(34)	60(2)	58(2)	46(2)	-3(2)	0(2)	39(2)
C(35)	76(3)	80(3)	59(3)	3(2)	6(2)	34(3)
C(36)	93(4)	81(4)	113(4)	-22(3)	-48(3)	31(3)
C(37)	80(3)	92(3)	42(2)	15(2)	-4(2)	29(2)
C(38)	50(2)	50(2)	41(2)	-8(2)	-2(2)	30(2)
C(39)	67(3)	51(2)	55(2)	0(2)	2(2)	35(2)
C(40)	59(3)	55(2)	55(2)	-4(2)	-3(2)	24(2)
C(41)	71(3)	50(2)	63(3)	-17(2)	-5(2)	22(2)
C(42)	69(3)	64(3)	55(2)	-12(2)	-13(2)	40(2)
C(43)	70(3)	52(2)	53(2)	1(2)	-7(2)	33(2)
C(44)	80(3)	85(4)	69(3)	35(3)	-7(3)	14(3)
C(45)	79(3)	74(3)	97(4)	1(3)	-21(3)	9(3)
C(46)	82(3)	82(3)	73(3)	14(3)	8(3)	44(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $C_{46}H_{32}O_2$.

	x	y	z	U(eq)
H(2A)	6309	6896	-1580	76
H(3A)	5768	7031	-1539	64
H(7A)	5167	7920	-640	65
H(8A)	5250	8519	27	78
H(9A)	5888	8991	691	112
H(20A)	6405	9347	1519	79
H(21A)	7057	9822	2082	76
H(22A)	7590	9672	2126	67
H(26A)	8163	8761	1256	58
H(27A)	8077	8164	618	68
H(31A)	4381	6589	-954	70
H(33A)	4855	7252	-3174	79
H(35A)	4767	6713	309	111
H(35B)	5100	7200	463	111
H(35C)	5257	6885	151	111
H(36A)	4130	6708	-3182	152
H(36B)	3910	6658	-2242	152
H(36C)	4037	6320	-2554	152
H(37A)	5548	7810	-3287	116
H(37B)	5866	7735	-2694	116
H(37C)	5726	8064	-2382	116
H(40A)	8958	10107	1581	70
H(42A)	8513	9424	3778	72
H(44A)	8574	9975	312	134
H(44B)	8082	9796	466	134
H(44C)	8246	9489	136	134
H(45A)	9417	10266	2748	145
H(45B)	9329	9879	3373	145
H(45C)	9183	10204	3676	145
H(46A)	7474	8738	2955	117
H(46B)	7676	9000	3842	117
H(46C)	7819	8681	3485	117

Table 6. Torsion angles [°] for $C_{46}H_{32}O_2$.

O(1)-C(1)-C(2)-C(3)	-154.4(4)
C(14)-C(1)-C(2)-C(3)	5.7(7)
C(1)-C(2)-C(3)-C(4)	0.4(7)
C(2)-C(3)-C(4)-C(5)	177.6(4)
C(2)-C(3)-C(4)-C(13)	-3.4(6)
C(3)-C(4)-C(5)-C(6)	179.8(4)
C(13)-C(4)-C(5)-C(6)	0.8(5)
C(3)-C(4)-C(5)-C(29)	2.0(6)
C(13)-C(4)-C(5)-C(29)	-177.0(3)
C(4)-C(5)-C(6)-C(11)	-0.2(5)
C(29)-C(5)-C(6)-C(11)	177.7(3)
C(4)-C(5)-C(6)-C(7)	-177.8(4)
C(29)-C(5)-C(6)-C(7)	0.1(5)

C(5)-C(6)-C(7)-C(8)	-177.9(4)
C(11)-C(6)-C(7)-C(8)	4.4(6)
C(6)-C(7)-C(8)-C(9)	-1.4(7)
C(7)-C(8)-C(9)-C(10)	-3.0(8)
C(8)-C(9)-C(10)-C(19)	-177.0(5)
C(8)-C(9)-C(10)-C(11)	4.0(8)
C(5)-C(6)-C(11)-C(10)	179.0(3)
C(7)-C(6)-C(11)-C(10)	-3.3(6)
C(5)-C(6)-C(11)-C(12)	-0.5(5)
C(7)-C(6)-C(11)-C(12)	177.2(3)
C(19)-C(10)-C(11)-C(6)	-179.8(3)
C(9)-C(10)-C(11)-C(6)	-0.8(6)
C(19)-C(10)-C(11)-C(12)	-0.2(5)
C(9)-C(10)-C(11)-C(12)	178.8(4)
C(6)-C(11)-C(12)-C(17)	-180.0(3)
C(10)-C(11)-C(12)-C(17)	0.5(4)
C(6)-C(11)-C(12)-C(13)	0.6(5)
C(10)-C(11)-C(12)-C(13)	-179.0(3)
C(17)-C(12)-C(13)-C(4)	-179.4(3)
C(11)-C(12)-C(13)-C(4)	0.0(5)
C(17)-C(12)-C(13)-C(14)	0.7(5)
C(11)-C(12)-C(13)-C(14)	-179.9(3)
C(5)-C(4)-C(13)-C(12)	-0.7(5)
C(3)-C(4)-C(13)-C(12)	-179.8(3)
C(5)-C(4)-C(13)-C(14)	179.2(3)
C(3)-C(4)-C(13)-C(14)	0.2(5)
O(1)-C(1)-C(14)-C(13)	150.4(4)
C(2)-C(1)-C(14)-C(13)	-9.0(6)
O(1)-C(1)-C(14)-C(15)	-27.6(6)
C(2)-C(1)-C(14)-C(15)	173.0(4)
C(12)-C(13)-C(14)-C(1)	-174.0(4)
C(4)-C(13)-C(14)-C(1)	6.1(6)
C(12)-C(13)-C(14)-C(15)	4.1(5)
C(4)-C(13)-C(14)-C(15)	-175.8(3)
C(1)-C(14)-C(15)-C(16)	170.4(4)
C(13)-C(14)-C(15)-C(16)	-7.7(5)
C(1)-C(14)-C(15)-C(28)	-15.1(6)
C(13)-C(14)-C(15)-C(28)	166.8(4)
C(28)-C(15)-C(16)-C(17)	-168.1(4)
C(14)-C(15)-C(16)-C(17)	6.6(5)
C(28)-C(15)-C(16)-C(25)	12.7(5)
C(14)-C(15)-C(16)-C(25)	-172.6(3)
C(13)-C(12)-C(17)-C(16)	-2.0(4)
C(11)-C(12)-C(17)-C(16)	178.6(4)
C(13)-C(12)-C(17)-C(18)	178.2(4)
C(11)-C(12)-C(17)-C(18)	-1.2(4)
C(15)-C(16)-C(17)-C(12)	-1.8(4)
C(25)-C(16)-C(17)-C(12)	177.4(3)
C(15)-C(16)-C(17)-C(18)	178.0(3)
C(25)-C(16)-C(17)-C(18)	-2.8(5)
C(12)-C(17)-C(18)-C(19)	1.7(4)
C(16)-C(17)-C(18)-C(19)	-178.1(3)
C(12)-C(17)-C(18)-C(23)	-179.4(3)
C(16)-C(17)-C(18)-C(23)	0.8(5)
C(11)-C(10)-C(19)-C(18)	0.8(6)
C(9)-C(10)-C(19)-C(18)	-178.2(4)

C(11)-C(10)-C(19)-C(20)	-176.3(3)
C(9)-C(10)-C(19)-C(20)	4.8(6)
C(17)-C(18)-C(19)-C(10)	-1.5(5)
C(23)-C(18)-C(19)-C(10)	179.7(3)
C(17)-C(18)-C(19)-C(20)	175.8(3)
C(23)-C(18)-C(19)-C(20)	-3.0(5)
C(10)-C(19)-C(20)-C(21)	-175.1(4)
C(18)-C(19)-C(20)-C(21)	7.6(6)
C(19)-C(20)-C(21)-C(22)	-8.0(7)
C(20)-C(21)-C(22)-C(23)	3.2(7)
C(21)-C(22)-C(23)-C(24)	-179.9(4)
C(21)-C(22)-C(23)-C(18)	1.5(6)
C(19)-C(18)-C(23)-C(22)	-1.3(5)
C(17)-C(18)-C(23)-C(22)	179.9(3)
C(19)-C(18)-C(23)-C(24)	-180.0(3)
C(17)-C(18)-C(23)-C(24)	1.2(5)
C(22)-C(23)-C(24)-C(25)	-179.8(3)
C(18)-C(23)-C(24)-C(25)	-1.2(5)
C(22)-C(23)-C(24)-C(38)	2.8(5)
C(18)-C(23)-C(24)-C(38)	-178.6(3)
C(23)-C(24)-C(25)-C(26)	-179.9(3)
C(38)-C(24)-C(25)-C(26)	-2.5(5)
C(23)-C(24)-C(25)-C(16)	-0.9(5)
C(38)-C(24)-C(25)-C(16)	176.6(3)
C(15)-C(16)-C(25)-C(24)	-177.9(3)
C(17)-C(16)-C(25)-C(24)	2.9(5)
C(15)-C(16)-C(25)-C(26)	1.1(5)
C(17)-C(16)-C(25)-C(26)	-178.1(3)
C(24)-C(25)-C(26)-C(27)	174.9(4)
C(16)-C(25)-C(26)-C(27)	-4.2(6)
C(25)-C(26)-C(27)-C(28)	-7.1(6)
C(26)-C(27)-C(28)-O(2)	-139.0(4)
C(26)-C(27)-C(28)-C(15)	21.3(7)
C(16)-C(15)-C(28)-O(2)	137.2(4)
C(14)-C(15)-C(28)-O(2)	-37.4(6)
C(16)-C(15)-C(28)-C(27)	-23.8(6)
C(14)-C(15)-C(28)-C(27)	161.6(4)
C(4)-C(5)-C(29)-C(30)	90.5(5)
C(6)-C(5)-C(29)-C(30)	-87.3(4)
C(4)-C(5)-C(29)-C(34)	-92.3(4)
C(6)-C(5)-C(29)-C(34)	89.8(4)
C(34)-C(29)-C(30)-C(31)	-2.3(5)
C(5)-C(29)-C(30)-C(31)	174.9(3)
C(34)-C(29)-C(30)-C(35)	179.7(4)
C(5)-C(29)-C(30)-C(35)	-3.1(6)
C(29)-C(30)-C(31)-C(32)	1.7(6)
C(35)-C(30)-C(31)-C(32)	179.7(4)
C(30)-C(31)-C(32)-C(33)	0.0(6)
C(30)-C(31)-C(32)-C(36)	-177.8(4)
C(31)-C(32)-C(33)-C(34)	-1.2(6)
C(36)-C(32)-C(33)-C(34)	176.6(4)
C(32)-C(33)-C(34)-C(29)	0.6(6)
C(32)-C(33)-C(34)-C(37)	179.1(4)
C(30)-C(29)-C(34)-C(33)	1.2(5)
C(5)-C(29)-C(34)-C(33)	-176.1(4)
C(30)-C(29)-C(34)-C(37)	-177.4(3)

C(5)-C(29)-C(34)-C(37)	5.3(5)
C(25)-C(24)-C(38)-C(43)	-87.4(4)
C(23)-C(24)-C(38)-C(43)	90.0(4)
C(25)-C(24)-C(38)-C(39)	90.9(4)
C(23)-C(24)-C(38)-C(39)	-91.6(4)
C(43)-C(38)-C(39)-C(40)	2.1(6)
C(24)-C(38)-C(39)-C(40)	-176.2(3)
C(43)-C(38)-C(39)-C(44)	-178.0(4)
C(24)-C(38)-C(39)-C(44)	3.7(6)
C(38)-C(39)-C(40)-C(41)	2.4(6)
C(44)-C(39)-C(40)-C(41)	-177.6(5)
C(39)-C(40)-C(41)-C(42)	-4.4(6)
C(39)-C(40)-C(41)-C(45)	179.4(4)
C(40)-C(41)-C(42)-C(43)	2.2(6)
C(45)-C(41)-C(42)-C(43)	178.4(4)
C(39)-C(38)-C(43)-C(42)	-4.0(6)
C(24)-C(38)-C(43)-C(42)	174.2(3)
C(39)-C(38)-C(43)-C(46)	179.7(4)
C(24)-C(38)-C(43)-C(46)	-2.0(6)
C(41)-C(42)-C(43)-C(38)	1.9(6)
C(41)-C(42)-C(43)-C(46)	178.3(4)

Symmetry transformations used to generate equivalent atoms: