

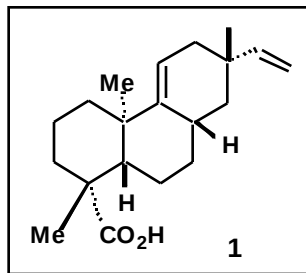
Stereoselective Synthesis of (-) Acanthoic Acid

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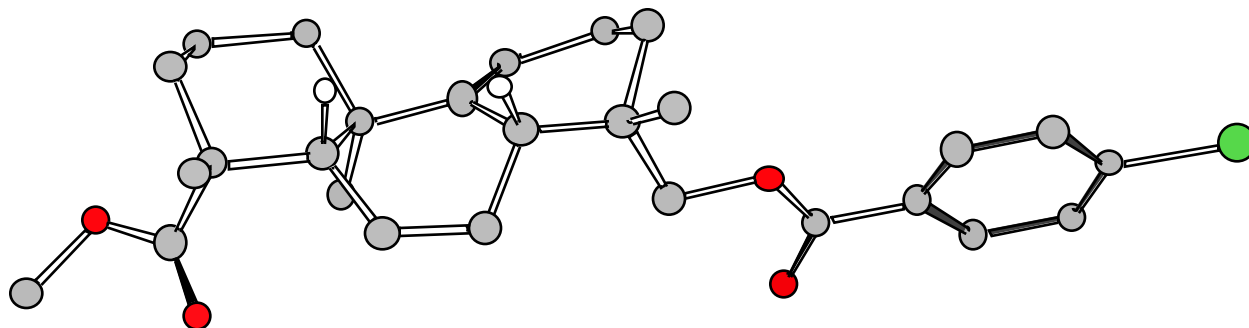
Supporting Information

General techniques. Organic solutions were concentrated by rotary evaporation below 45 °C at about 20 mmHg. All nonaqueous reactions were carried out using flame-dried glassware, under an argon atmosphere in dry, freshly distilled solvents under anhydrous conditions, unless otherwise noted. THF and Et₂O were distilled from sodium/benzophenone; CH₂Cl₂ and toluene from calcium hydride; and benzene from potassium. Pyridine, triethylamine and boron trifluoride etherate were distilled from calcium hydride prior to use. Yields refer to chromatographically and spectroscopically (¹H NMR) homogeneous materials, unless otherwise stated. Reactions were monitored by thin-layer chromatography carried out on 0.25 mm E. Merck silica gel plates (60F-254) using UV light as visualizing agent and *p*-anisaldehyde solution and heat as developing agents. E. Merck silica gel (60, particle size 0.040-0.063 mm) was used for flash chromatography. Preparative thin-layer chromatography separations were carried out on 0.25 or 0.50 mm E. Merck silica gel plates (60F-254). NMR spectra were recorded on a Varian 400 MHz instrument and calibrated using residual undeuterated solvent as an internal reference. IR spectra were recorded on a Nicolet Avatar 320 FT-IR spectrometer. Optical rotations were recorded on a Perkin-Elmer 241 polarimeter. High resolution mass spectra (HRMS) were recorded on a VG 7070 HS mass spectrometer under chemical ionization (CI) conditions or on a VG ZAB-ZSE mass spectrometer under fast atom bombardment (FAB) conditions.



Acanthoic acid (1). To a solution of alkene **21** (16.8 mg, 0.05 mmol) in N, N-dimethylformamide (2 ml) added lithium bromide (5.0 mg, 0.06 mmol) and the mixture was refluxed at 160 °C for 1 hr. The reaction mixture was then cooled to 25 °C, diluted with H₂O (5 ml) and extracted with ethyl acetate (3 x 10 ml). The organic layer was

collected, dried (MgSO₄) and concentrated and residue was chromatographed (silica, 15-20 % ethyl ether in hexane) to afford acanthoic acid (**1**) (14.9 mg, 0.05 mmol, 93%). **1**: white solid; R_f = 0.20 (silica, 30% ethyl ether in hexanes); $[\alpha]^{25}_D$: -26.0 (c= 0.33, benzene); IR (film) $\nu_{\max}$ 3080.6, 2928.9, 2857.6, 1693.6, 1638.2, 1464.7, 1413.8, 1376.4, 1263.1, 1179.3, 1095.9, 1027.5, 999.2, 909.2, 801.7; ¹H NMR (500 MHz, CDCl₃) d 5.82 (dd, 1H, J= 10.5, 17.5 Hz), 5.40 (m, 1H), 4.92 (d, 1H, J= 17.5 Hz), 4.86 (d, 1H, J= 10.5 Hz), 2.30 (bs, 1H), 2.16-1.2 (m, 14H), 1.24 (s, 3H), 1.00-1.10 (m, 2H), 0.99 (s, 3H), 0.95 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) d 185.0, 150.3, 149.9, 116.7, 109.2, 47.9, 41.8, 41.7, 38.3, 38.2, 37.4, 34.8, 31.8, 28.6, 28.5, 27.7, 22.4, 22.1, 20.3, 18.9; HRMS, calcd for C₂₀H₃₀O₂ (M+Cs⁺) 435.1298, found 435.1302.

X-Ray data of compound **16****Table 1.** Crystal data and structure refinement for TAOT

Empirical formula	C ₂₇ H ₃₄ BrO ₄
Formula weight	502.45
Temperature	23 °C
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2 ₁
Unit cell dimensions	a = 11.00(2) Å alpha = 90° b = 19.19(2) Å beta = 109.82(9)° c = 12.459(13) Å gamma = 90°
Crystal size	0.50 x 0.50 x 0.15 mm
Density (calculated)	1.349 Mg/m ³
Absorption coefficient	1.691 mm ⁻¹
Volume, Z, F(000)	2474(5) Å ³ , 4, 1052
q range for data collection	1.74 to 22.50°
Limiting indices	0 ≤ h ≤ 11, 0 ≤ k ≤ 20, -13 ≤ l ≤ 12
Reflections collected	3502, 1796 observed [I > 2σ(I)]
Independent reflections	3318 (R _{int} = 0.1414)
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.9479 and 0.7019
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3318 / 1 / 257
Goodness-of-fit on F ²	1.034
Final R indices [I > 2σ(I)]	R1 = 0.1129, wR2 = 0.2667
R indices (all data)	R1 = 0.1942, wR2 = 0.3406
Absolute structure parameter	-0.08(4)
Largest diff. peak and hole	0.738 and -1.052 eÅ ⁻³
Scan speed, range, type	10°/minute, 0.7°, Wyckoff
Background range, % time	1.0°, 25% each side

Table 2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for TAOT U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	8405(13)	2734(6)	816(8)	74(9)
C(2)	8509(14)	3436(7)	1125(10)	53(6)
C(3)	8062(14)	3949(5)	289(13)	58(7)
C(4)	7512(15)	3759(6)	-855(11)	49(6)
C(5)	7408(12)	3057(6)	-1164(8)	58(7)
C(6)	7855(9)	2545(5)	-328(9)	47(6)
C(7)	7787(15)	1807(5)	-654(13)	35(5)
O(1)	7574(16)	1615(9)	-1648(14)	68(5)
O(2)	8029(15)	1378(9)	171(13)	57(4)
O(3)	8620(25)	-2925(12)	-1086(23)	122(9)
O(4)	7014(17)	-3555(10)	-1053(15)	71(5)
Br(1)	8205(3)	4885(1)	676(3)	83(1)
C(8)	8056(27)	632(13)	-75(22)	64(7)
C(9)	7978(23)	256(13)	936(19)	48(6)
C(10)	9131(27)	475(16)	2022(23)	79(8)
C(11)	6785(24)	503(15)	1267(22)	67(7)
C(12)	5619(32)	329(18)	293(28)	97(10)
C(13)	5581(25)	-427(13)	-155(21)	58(7)
C(14)	6614(23)	-821(13)	186(20)	55(6)
C(15)	7983(22)	-513(12)	858(20)	43(6)
C(16)	8907(20)	-826(11)	292(17)	39(5)
C(17)	9013(26)	-1614(15)	370(24)	72(8)
C(18)	7825(19)	-1976(11)	511(18)	37(5)
C(19)	6543(22)	-1576(13)	-165(19)	51(6)
C(20)	6270(26)	-1626(15)	-1451(21)	75(8)
C(21)	5405(25)	-1914(14)	129(24)	69(7)
C(22)	5349(23)	-2740(14)	-38(22)	69(7)
C(23)	6644(24)	-3062(16)	734(23)	72(8)
C(24)	7818(22)	-2806(13)	419(19)	51(6)
C(25)	8980(25)	-3051(16)	1302(23)	74(8)
C(26)	7873(23)	-3080(13)	-650(20)	47(6)
C(27)	7065(31)	-3908(21)	-2076(28)	102(11)
C(1')	7019(14)	3324(7)	4237(10)	75(9)
C(2')	6872(16)	2627(8)	3895(10)	80(9)
C(3')	7284(16)	2098(6)	4706(14)	62(7)
C(4')	7844(15)	2265(6)	5859(13)	51(6)
C(5')	7992(13)	2961(7)	6201(9)	72(8)
C(6')	7579(11)	3491(6)	5391(11)	49(6)
C(7')	7773(19)	4223(6)	5745(17)	73(8)
O(1')	8054(19)	4397(11)	6737(17)	85(6)
O(2')	7517(17)	4655(9)	4905(15)	69(5)
O(3')	8879(31)	8804(13)	6739(24)	165(14)
O(4')	7655(19)	9646(10)	5912(17)	79(6)
Br(2)	7085(4)	1170(1)	4275(3)	103(1)
C(8')	7776(30)	5400(15)	5187(25)	78(8)
C(9')	7786(28)	5743(16)	4082(24)	74(8)
C(10')	8943(29)	5517(17)	3808(26)	92(10)
C(11')	6569(31)	5576(20)	3156(29)	103(11)
C(12')	5407(34)	5792(19)	3318(31)	108(12)
C(13')	5492(31)	6514(17)	3927(26)	88(9)
C(14')	6641(24)	6877(14)	4277(20)	59(7)
C(15')	7783(29)	6565(17)	4337(27)	85(9)

C(16')	8908(29)	6792(16)	5391(25)	85(9)
C(17')	9066(31)	7615(18)	5372(26)	91(9)
C(18')	7929(22)	7946(12)	4603(21)	50(6)
C(19')	6632(24)	7669(14)	4632(21)	58(7)
C(20')	6519(27)	7689(15)	5817(22)	78(8)
C(21')	5492(28)	8042(15)	3764(25)	82(9)
C(22')	5500(33)	8865(19)	3898(32)	106(11)
C(23')	6827(28)	9093(18)	3837(27)	86(9)
C(24')	7959(29)	8787(17)	4673(26)	82(9)
C(25')	9205(23)	8992(14)	4436(21)	65(7)
C(26')	8155(30)	9058(18)	5868(28)	77(8)
C(27')	7931(27)	9970(20)	7016(25)	87(9)

Table 3. Bond lengths [Å] and angles [°] for TAOT

C(1)-C(6)	1.40
C(1)-C(2)	1.40
C(2)-C(3)	1.40
C(3)-C(4)	1.39
C(3)-Br(1)	1.854(10)
C(4)-C(5)	1.40
C(5)-C(6)	1.40
C(6)-C(7)	1.47
C(7)-O(1)	1.24(2)
C(7)-O(2)	1.27(2)
O(2)-C(8)	1.47(3)
O(3)-C(26)	1.17(3)
O(4)-C(26)	1.29(3)
O(4)-C(27)	1.46(4)
C(8)-C(9)	1.48(3)
C(9)-C(15)	1.48(3)
C(9)-C(10)	1.57(3)
C(9)-C(11)	1.58(4)
C(11)-C(12)	1.47(4)
C(12)-C(13)	1.55(4)
C(13)-C(14)	1.31(3)
C(14)-C(19)	1.51(3)
C(14)-C(15)	1.57(3)
C(15)-C(16)	1.54(3)
C(16)-C(17)	1.52(3)
C(17)-C(18)	1.54(3)
C(18)-C(19)	1.58(3)
C(18)-C(24)	1.60(3)
C(19)-C(20)	1.53(3)
C(19)-C(21)	1.56(3)
C(21)-C(22)	1.60(4)
C(22)-C(23)	1.55(3)
C(23)-C(24)	1.55(4)
C(24)-C(25)	1.45(3)
C(24)-C(26)	1.45(3)
C(1')-C(2')	1.40
C(1')-C(6')	1.40
C(2')-C(3')	1.40
C(3')-C(4')	1.39

C(3')-Br(2)	1.853(12)
C(4')-C(5')	1.39
C(5')-C(6')	1.40
C(6')-C(7')	1.47
C(7')-O(1')	1.21(2)
C(7')-O(2')	1.29(2)
O(2')-C(8')	1.48(3)
O(3')-C(26')	1.21(3)
O(4')-C(26')	1.26(4)
O(4')-C(27')	1.44(3)
C(8')-C(9')	1.53(4)
C(9')-C(11')	1.48(4)
C(9')-C(10')	1.49(4)
C(9')-C(15')	1.61(4)
C(11')-C(12')	1.42(4)
C(12')-C(13')	1.57(5)
C(13')-C(14')	1.38(4)
C(14')-C(15')	1.37(4)
C(14')-C(19')	1.58(4)
C(15')-C(16')	1.53(4)
C(16')-C(17')	1.59(4)
C(17')-C(18')	1.44(4)
C(18')-C(19')	1.53(3)
C(18')-C(24')	1.62(4)
C(19')-C(20')	1.52(4)
C(19')-C(21')	1.53(4)
C(21')-C(22')	1.59(5)
C(22')-C(23')	1.55(4)
C(23')-C(24')	1.45(4)
C(24')-C(26')	1.52(4)
C(24')-C(25')	1.55(4)
C(6)-C(1)-C(2)	120.0
C(3)-C(2)-C(1)	120.0
C(4)-C(3)-C(2)	120.0
C(4)-C(3)-Br(1)	119.2(8)
C(2)-C(3)-Br(1)	120.8(8)
C(3)-C(4)-C(5)	120.0
C(6)-C(5)-C(4)	120.0
C(5)-C(6)-C(1)	120.0
C(5)-C(6)-C(7)	120.1
C(1)-C(6)-C(7)	119.9
O(1)-C(7)-O(2)	122.2(14)
O(1)-C(7)-C(6)	122.7(12)
O(2)-C(7)-C(6)	115.0(10)
C(7)-O(2)-C(8)	118(2)
C(26)-O(4)-C(27)	115(2)
O(2)-C(8)-C(9)	107(2)
C(8)-C(9)-C(15)	115(2)
C(8)-C(9)-C(10)	110(2)
C(15)-C(9)-C(10)	108(2)
C(8)-C(9)-C(11)	112(2)
C(15)-C(9)-C(11)	110(2)
C(10)-C(9)-C(11)	101(2)
C(12)-C(11)-C(9)	107(2)
C(11)-C(12)-C(13)	115(3)
C(14)-C(13)-C(12)	121(3)
C(13)-C(14)-C(19)	120(2)
C(13)-C(14)-C(15)	122(2)

C(19)-C(14)-C(15)	118(2)
C(9)-C(15)-C(16)	116(2)
C(9)-C(15)-C(14)	113(2)
C(16)-C(15)-C(14)	106(2)
C(17)-C(16)-C(15)	114(2)
C(16)-C(17)-C(18)	114(2)
C(17)-C(18)-C(19)	111(2)
C(17)-C(18)-C(24)	115(2)
C(19)-C(18)-C(24)	118(2)
C(14)-C(19)-C(20)	110(2)
C(14)-C(19)-C(21)	107(2)
C(20)-C(19)-C(21)	109(2)
C(14)-C(19)-C(18)	111(2)
C(20)-C(19)-C(18)	111(2)
C(21)-C(19)-C(18)	108(2)
C(19)-C(21)-C(22)	112(2)
C(23)-C(22)-C(21)	109(2)
C(24)-C(23)-C(22)	113(2)
C(25)-C(24)-C(26)	106(2)
C(25)-C(24)-C(23)	108(2)
C(26)-C(24)-C(23)	115(2)
C(25)-C(24)-C(18)	107(2)
C(26)-C(24)-C(18)	115(2)
C(23)-C(24)-C(18)	106(2)
O(3)-C(26)-O(4)	123(3)
O(3)-C(26)-C(24)	126(2)
O(4)-C(26)-C(24)	111(2)
C(2')-C(1')-C(6')	120.0
C(1')-C(2')-C(3')	120.0
C(4')-C(3')-C(2')	120.0
C(4')-C(3')-Br(2)	119.2(9)
C(2')-C(3')-Br(2)	120.8(9)
C(3')-C(4')-C(5')	120.0
C(4')-C(5')-C(6')	120.0
C(5')-C(6')-C(1')	120.0
C(5')-C(6')-C(7')	120.1
C(1')-C(6')-C(7')	119.9
O(1')-C(7')-O(2')	124(2)
O(1')-C(7')-C(6')	122.0(14)
O(2')-C(7')-C(6')	113.7(11)
C(7')-O(2')-C(8')	117(2)
C(26')-O(4')-C(27')	118(3)
O(2')-C(8')-C(9')	105(2)
C(11')-C(9')-C(10')	112(3)
C(11')-C(9')-C(8')	109(3)
C(10')-C(9')-C(8')	111(3)
C(11')-C(9')-C(15')	108(3)
C(10')-C(9')-C(15')	113(3)
C(8')-C(9')-C(15')	104(3)
C(12')-C(11')-C(9')	117(3)
C(11')-C(12')-C(13')	115(3)
C(14')-C(13')-C(12')	120(3)
C(15')-C(14')-C(13')	121(3)
C(15')-C(14')-C(19')	120(3)
C(13')-C(14')-C(19')	119(3)
C(14')-C(15')-C(16')	112(3)
C(14')-C(15')-C(9')	119(3)
C(16')-C(15')-C(9')	113(3)

C(15')-C(16')-C(17')	109(3)
C(18')-C(17')-C(16')	112(3)
C(17')-C(18')-C(19')	116(2)
C(17')-C(18')-C(24')	114(2)
C(19')-C(18')-C(24')	110(2)
C(20')-C(19')-C(21')	111(2)
C(20')-C(19')-C(18')	113(2)
C(21')-C(19')-C(18')	112(2)
C(20')-C(19')-C(14')	108(2)
C(21')-C(19')-C(14')	109(2)
C(18')-C(19')-C(14')	103(2)
C(19')-C(21')-C(22')	115(3)
C(23')-C(22')-C(21')	104(3)
C(24')-C(23')-C(22')	116(3)
C(23')-C(24')-C(26')	112(3)
C(23')-C(24')-C(25')	111(3)
C(26')-C(24')-C(25')	105(2)
C(23')-C(24')-C(18')	112(3)
C(26')-C(24')-C(18')	113(3)
C(25')-C(24')-C(18')	104(2)
O(3')-C(26')-O(4')	119(3)
O(3')-C(26')-C(24')	125(3)
O(4')-C(26')-C(24')	115(3)

Table 4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for TAOT&N. The factor exponent takes the form: $-2p^2[(ha^*)^2U_{11} + \dots + 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
O(3)	151(20)	80(16)	179(23)	-42(16)	115(19)	-29(15)
O(4)	80(12)	51(13)	82(12)	-28(10)	29(10)	-17(9)
Br(1)	85(2)	32(2)	132(3)	-13(2)	37(2)	0(2)
O(3')	193(28)	78(17)	143(23)	-35(16)	-49(21)	40(18)
O(4')	99(15)	47(13)	96(15)	7(10)	39(12)	21(10)
Br(2)	132(3)	39(2)	134(3)	-19(2)	39(2)	1(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for TAOT

	x	y	z	U(eq)
H(1)	8713(19)	2382(7)	1391(10)	88
H(2)	8887(20)	3567(9)	1912(10)	64
H(4)	7204(21)	4112(7)	-1431(14)	58
H(5)	7030(17)	2927(8)	-1952(8)	69
H(8C)	8850(27)	514(13)	-209(22)	77
H(8D)	7331(27)	510(13)	-747(22)	77
H(10D)	9074(27)	229(16)	2675(23)	119
H(10E)	9093(27)	968(16)	2142(23)	119
H(10F)	9933(27)	363(16)	1916(23)	119
H(11C)	6773(24)	265(15)	1950(22)	80
H(11D)	6829(24)	1001(15)	1409(22)	80
H(12C)	5557(32)	649(18)	-327(28)	116
H(12D)	4866(32)	403(18)	518(28)	116
H(13B)	4818(25)	-602(13)	-670(21)	69

H(15B)	8242(22)	-696(12)	1638(20)	51
H(16C)	9359(20)	-556(11)	-66(17)	46
H(17B)	9772(26)	-1736(15)	1013(24)	87
H(17C)	9138(26)	-1790(15)	-315(24)	87
H(18B)	7925(19)	-1892(11)	1312(18)	44
H(20D)	6224(26)	-2107(15)	-1672(21)	112
H(20E)	6952(26)	-1400(15)	-1637(21)	112
H(20F)	5463(26)	-1401(15)	-1850(21)	112
H(21C)	4597(25)	-1712(14)	-355(24)	83
H(21D)	5502(25)	-1807(14)	915(24)	83
H(22C)	4639(23)	-2930(14)	164(22)	83
H(22D)	5206(23)	-2852(14)	-830(22)	83
H(23C)	6779(24)	-2942(16)	1523(23)	86
H(23D)	6589(24)	-3565(16)	668(23)	86
H(25D)	8990(25)	-2884(16)	2031(23)	110
H(25E)	9727(25)	-2880(16)	1152(23)	110
H(25F)	8991(25)	-3551(16)	1306(23)	110
H(27D)	6392(31)	-4251(21)	-2313(28)	152
H(27E)	7889(31)	-4131(21)	-1911(28)	152
H(27F)	6947(31)	-3573(21)	-2675(28)	152
H(1')	6736(20)	3688(9)	3680(12)	90
H(2')	6486(23)	2512(11)	3102(11)	96
H(4')	8128(22)	1901(8)	6417(16)	61
H(5')	8377(19)	3077(10)	6995(9)	86
H(8A)	8603(30)	5461(15)	5789(25)	93
H(8B)	7105(30)	5601(15)	5434(25)	93
H(10A)	9711(29)	5635(17)	4430(26)	138
H(10B)	8952(29)	5749(17)	3128(26)	138
H(10C)	8911(29)	5022(17)	3690(26)	138
H(11A)	6600(31)	5788(20)	2459(29)	124
H(11B)	6530(31)	5076(20)	3043(29)	124
H(12A)	5160(34)	5441(19)	3765(31)	129
H(12B)	4728(34)	5816(19)	2579(31)	129
H(13A)	4769(31)	6697(17)	4053(26)	106
H(15A)	7988(29)	6777(17)	3704(27)	102
H(16A)	9699(29)	6567(16)	5393(25)	103
H(16B)	8742(29)	6654(16)	6077(25)	103
H(17A)	9804(31)	7854(18)	5806(26)	109
H(18A)	7934(22)	7835(12)	3836(21)	60
H(20A)	7243(27)	7452(15)	6348(22)	117
H(20B)	5733(27)	7463(15)	5798(22)	117
H(20C)	6508(27)	8165(15)	6052(22)	117
H(21A)	4697(28)	7862(15)	3830(25)	98
H(21B)	5489(28)	7931(15)	3003(25)	98
H(22A)	4798(33)	9075(19)	3287(32)	127
H(22B)	5421(33)	8996(19)	4623(32)	127
H(23A)	6844(28)	8980(18)	3083(27)	103
H(23B)	6891(28)	9595(18)	3919(27)	103
H(25A)	9939(23)	8784(14)	5001(21)	97
H(25B)	9298(23)	9489(14)	4466(21)	97
H(25C)	9152(23)	8829(14)	3693(21)	97
H(27A)	7491(27)	10409(20)	6927(25)	130
H(27B)	8845(27)	10043(20)	7355(25)	130
H(27C)	7640(27)	9671(20)	7499(25)	130

Experimental $R1=(\hat{A}||F_o|-|F_c|)/\hat{A}|F_o|)$, $wR2=\hat{A}w(F_o^2-F_c^2)^2/\hat{A}w[(F_o^2)^2]_{1/2}$,

$S=[\hat{A}w(F_o^2-F_c^2)^2/(n-p)]^{1/2}$

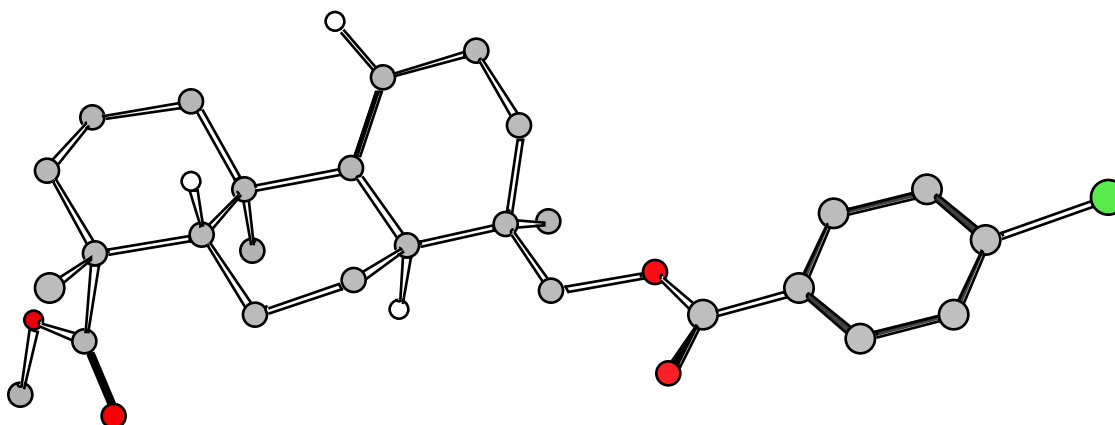
Phenyl rings were treated as regular hexagons of D_{6h} symmetry with C-C =

1.395 Å and C-C-C = 120°. Unit cell dimensions and standard deviations were obtained by least squares fit to 16 reflections ($14 < 2\theta < 26^\circ$).

References

SHELXTL-PC. & G.M.Sheldrick, Siemens Analytical X-ray Instruments Inc. Madison, WI. (1990). H.D.Flack. Acta Crystallographica, A39, 876-881 (1983).

h	k	l	Fo ²	Fc ²	Delta(F ²)/esd	Fc/Fc(max)	Res(A)
-1	0	1	187.31	21.98	4.58	0.014	9.52
1	9	0	11224.33	5492.79	4.42	0.228	2.09
-3	14	5	-93.15	273.07	4.08	0.051	1.18
-2	5	1	649.08	247.09	3.91	0.048	3.14
1	9	1	28888.57	17067.81	3.29	0.401	2.03
-1	9	1	60034.12	36897.02	3.05	0.590	2.08
-2	2	7	331.36	109.37	3.00	0.032	1.75
1	2	11	-204.61	2.23	2.98	0.005	1.02
1	5	0	18363.22	11442.89	2.93	0.328	3.60
-6	10	10	-156.03	101.36	2.93	0.031	1.00
0	12	3	1498.62	855.68	2.91	0.090	1.48
1	0	0	700.98	376.68	2.87	0.060	10.35
3	0	5	-71.53	57.43	2.86	0.023	1.69
2	1	8	90.16	356.22	2.84	0.058	1.30
11	0	0	340.68	27.89	2.83	0.016	0.94
-4	4	10	-149.05	14.52	2.83	0.012	1.20
9	3	4	278.13	16.88	2.81	0.013	0.95
-1	16	3	296.76	714.14	2.81	0.082	1.15
-1	10	2	162.69	11.54	2.77	0.010	1.83
11	3	0	-261.83	1.14	2.77	0.003	0.93
-7	5	5	-76.52	111.15	2.77	0.032	1.40
5	15	4	-148.71	87.60	2.75	0.029	0.97
1	15	3	523.32	215.94	2.75	0.045	1.19
1	1	8	9.98	216.98	2.71	0.045	1.38
0	1	5	52.18	196.97	2.69	0.043	2.33
8	8	1	239.20	21.71	2.69	0.014	1.10
5	13	5	428.84	141.58	2.69	0.037	0.99
2	5	5	-18.30	135.38	2.68	0.036	1.71
-10	3	10	-224.90	9.82	2.68	0.010	0.94
1	4	0	4661.34	2964.77	2.67	0.167	4.35
-5	12	8	-68.53	164.16	2.67	0.039	1.07
1	5	8	-3.66	194.00	2.67	0.043	1.30
-11	1	5	144.39	507.13	2.67	0.069	1.00
8	2	4	-180.65	13.12	2.66	0.011	1.05
2	2	8	-28.94	161.35	2.66	0.039	1.29
-8	8	8	-124.43	95.62	2.61	0.030	1.07
0	8	4	392.67	175.69	2.61	0.041	1.86
-4	10	10	-161.36	24.94	2.59	0.015	1.04
0	14	3	622.70	319.96	2.56	0.055	1.29
4	14	0	1026.68	566.40	2.56	0.073	1.21
5	6	5	-57.89	131.83	2.55	0.035	1.24
-9	8	4	-64.87	135.79	2.55	0.036	1.09
1	14	1	4230.83	2715.46	2.55	0.160	1.34
3	3	6	110.45	351.03	2.54	0.058	1.46
-7	2	10	9.65	236.98	2.54	0.047	1.11
0	12	0	1768.25	1080.90	2.54	0.101	1.60
9	3	2	-168.34	19.40	2.52	0.014	1.05
-2	12	5	1064.94	608.80	2.52	0.076	1.34
-1	16	5	109.46	403.03	2.52	0.062	1.08
-10	9	6	-186.64	32.39	2.51	0.017	0.96

X-Ray data of compound **17****Table 1.** Crystal data and structure refinement for TAOT2

Empirical formula	C ₂₇ H _{34.50} BrO ₄
Formula weight	502.96
Temperature	22 °C
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2 ₁
Unit cell dimensions	a = 10.801(6) Å alpha = 90° b = 22.481(11) Å beta = 109.45(4)° c = 10.819(5) Å gamma = 90°
Crystal size	0.80 x 0.50 x 0.06 mm
Density (calculated)	1.349 Mg/m ³
Absorption coefficient	1.689 mm ⁻¹
Volume, Z, F(000)	2477(2) Å ³ , 4, 1054
q range for data collection	1.81 to 22.50°
Limiting indices	-11 ≤ h ≤ 10, 0 ≤ k < 21, -10 ≤ l ≤ 10
Reflections collected	2728, 1179 observed [I > 2σ(I)]
Independent reflections	2579 (R _{int} = 0.0747)
Absorption correction	None
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2578 / 1 / 257
Goodness-of-fit on F ²	1.035
Final R indices [I > 2σ(I)]	R1 = 0.1126, wR2 = 0.2667
R indices (all data)	R1 = 0.2329, wR2 = 0.3694
Absolute structure parameter	0.00(6)
Largest diff. peak and hole	0.625 and -0.627 eÅ ³
Scan speed, range, type	5°/minute, 0.6°, Wyckoff
Background range, % time	0.6°, 25% each side

Table 2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for TAOT2. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
C(1)	-4359(19)	-2240(9)	-3220(19)	75(12)
C(2)	-3091(20)	-2403(9)	-3148(21)	82(13)
C(3)	-2423(15)	-2074(11)	-3820(21)	41(10)
C(4)	-3023(19)	-1583(11)	-4566(22)	74(12)
C(5)	-4291(19)	-1419(9)	-4638(19)	60(11)
C(6)	-4959(15)	-1748(8)	-3965(16)	35(9)
C(7)	-6309(17)	-1589(13)	-4075(26)	53(11)
Br(1)	-675(5)	-2235(3)	-3662(5)	99(2)
O(1)	-6805(25)	-1163(12)	-4847(24)	64(8)
O(2)	-6846(29)	-1821(14)	-3383(28)	93(10)
O(3)	-14596(22)	-191(16)	-6693(24)	83(9)
O(4)	-15258(20)	631(10)	-7812(21)	55(7)
C(8)	-8113(36)	-947(17)	-4814(36)	56(11)
C(9)	-8475(36)	-399(17)	-5678(34)	51(11)
C(10)	-8369(35)	-484(16)	-6955(32)	54(11)
C(11)	-7453(34)	88(16)	-5041(33)	54(11)
C(12)	-7697(34)	666(16)	-5729(36)	61(11)
C(13)	-9105(35)	830(19)	-6190(35)	67(12)
C(14)	-10088(31)	429(15)	-6317(29)	36(9)
C(15)	-9801(33)	-199(20)	-5809(32)	51(10)
C(16)	-10307(25)	-260(15)	-4665(26)	32(8)
C(17)	-11794(35)	-127(18)	-5067(37)	69(11)
C(18)	-12019(31)	506(15)	-5530(31)	46(9)
C(19)	-11587(30)	663(16)	-6633(30)	36(9)
C(20)	-12310(32)	330(16)	-7958(30)	54(10)
C(21)	-11675(32)	1324(15)	-6890(35)	54(10)
C(22)	-13040(30)	1557(16)	-7173(31)	46(9)
C(23)	-13583(34)	1381(16)	-6137(36)	60(11)
C(24)	-13460(32)	742(16)	-5770(31)	45(9)
C(25)	-13813(40)	665(20)	-4496(39)	87(13)
C(26)	-14501(39)	327(21)	-6854(40)	49(11)
C(27)	-16213(41)	293(20)	-8779(39)	87(14)
C(1')	-10498(21)	2(8)	-11208(21)	60(11)
C(2')	-11807(22)	128(9)	-11368(23)	81(13)
C(3')	-12670(17)	-332(12)	-11360(21)	65(12)
C(4')	-12225(21)	-919(11)	-11192(23)	78(13)
C(5')	-10916(22)	-1045(8)	-11032(22)	69(12)
C(6')	-10053(17)	-585(9)	-11040(16)	65(13)
C(7')	-8687(19)	-719(14)	-10915(28)	62(12)
Br(2)	-14430(4)	-182(3)	-11569(5)	103(2)
O(1')	-8284(25)	-1227(12)	-10352(24)	62(8)
O(2')	-7976(26)	-324(13)	-11199(25)	84(9)
O(3')	-1068(22)	-2486(14)	-10054(23)	80(10)
O(4')	-445(23)	-3407(14)	-9330(21)	72(8)
C(8')	-6860(39)	-1338(20)	-10035(41)	69(13)
C(9')	-6619(33)	-1947(16)	-9411(31)	41(10)
C(10')	-7605(40)	-2403(19)	-10277(39)	81(14)
C(11')	-6778(37)	-1936(17)	-8042(33)	54(11)
C(12')	-6533(42)	-2497(19)	-7386(43)	88(15)
C(13')	-5361(32)	-2842(16)	-7555(32)	54(10)
C(14')	-4756(41)	-2677(19)	-8398(39)	66(13)
C(15')	-5170(35)	-2170(20)	-9266(34)	56(11)

C(16')	-4155(39)	-1651(21)	-8846(43)	89(14)
C(17')	-2814(37)	-1912(17)	-8821(38)	66(11)
C(18')	-2454(35)	-2483(17)	-8035(37)	63(11)
C(19')	-3505(34)	-2953(16)	-8371(32)	44(10)
C(20')	-3739(31)	-3239(16)	-9773(29)	50(10)
C(21')	-3031(33)	-3461(16)	-7390(33)	53(10)
C(22')	-1607(30)	-3724(16)	-7224(34)	49(10)
C(23')	-695(34)	-3245(17)	-6982(32)	55(10)
C(24')	-1012(34)	-2712(16)	-7885(34)	52(10)
C(25')	18(37)	-2203(20)	-7376(37)	80(13)
C(26')	-867(38)	-2861(19)	-9073(41)	55(11)
C(27')	-271(38)	-3534(18)	-10485(38)	78(13)

Table 3. Bond lengths [Å] and angles [°] for TAOT2

C(1)-C(6)	1.39
C(1)-C(2)	1.40
C(2)-C(3)	1.40
C(3)-C(4)	1.39
C(3)-Br(1)	1.87(2)
C(4)-C(5)	1.39
C(5)-C(6)	1.39
C(6)-C(7)	1.47
C(7)-O(2)	1.21(3)
C(7)-O(1)	1.27(3)
O(1)-C(8)	1.51(4)
O(3)-C(26)	1.19(5)
O(4)-C(26)	1.28(4)
O(4)-C(27)	1.42(4)
C(8)-C(9)	1.52(5)
C(9)-C(10)	1.44(5)
C(9)-C(15)	1.46(5)
C(9)-C(11)	1.55(4)
C(11)-C(12)	1.48(5)
C(12)-C(13)	1.48(4)
C(13)-C(14)	1.36(4)
C(14)-C(15)	1.51(5)
C(14)-C(19)	1.63(4)
C(15)-C(16)	1.52(4)
C(16)-C(17)	1.55(4)
C(17)-C(18)	1.50(5)
C(18)-C(19)	1.46(4)
C(18)-C(24)	1.58(4)
C(19)-C(21)	1.51(5)
C(19)-C(20)	1.58(4)
C(21)-C(22)	1.50(4)
C(22)-C(23)	1.48(4)
C(23)-C(24)	1.48(5)
C(24)-C(25)	1.56(5)
C(24)-C(26)	1.62(5)
C(1')-C(2')	1.39
C(1')-C(6')	1.40
C(2')-C(3')	1.40
C(3')-C(4')	1.39

C(3')-Br(2)	1.87(2)
C(4')-C(5')	1.39
C(5')-C(6')	1.39
C(6')-C(7')	1.47
C(7')-O(2')	1.28(4)
C(7')-O(1')	1.30(4)
O(1')-C(8')	1.48(4)
O(3')-C(26')	1.32(4)
O(4')-C(27')	1.35(4)
O(4')-C(26')	1.37(4)
C(8')-C(9')	1.51(5)
C(9')-C(11')	1.55(5)
C(9')-C(10')	1.55(5)
C(9')-C(15')	1.60(5)
C(11')-C(12')	1.43(5)
C(12')-C(13')	1.55(5)
C(13')-C(14')	1.34(5)
C(14')-C(15')	1.45(5)
C(14')-C(19')	1.48(5)
C(15')-C(16')	1.56(5)
C(16')-C(17')	1.55(5)
C(17')-C(18')	1.52(5)
C(18')-C(19')	1.50(5)
C(18')-C(24')	1.60(5)
C(19')-C(21')	1.53(5)
C(19')-C(20')	1.59(4)
C(21')-C(22')	1.60(4)
C(22')-C(23')	1.42(4)
C(23')-C(24')	1.51(5)
C(24')-C(26')	1.39(5)
C(24')-C(25')	1.56(5)
C(6)-C(1)-C(2)	120.0
C(1)-C(2)-C(3)	120.0
C(4)-C(3)-C(2)	120.0
C(4)-C(3)-Br(1)	117.8(13)
C(2)-C(3)-Br(1)	122.1(13)
C(3)-C(4)-C(5)	120.0
C(4)-C(5)-C(6)	120.0
C(5)-C(6)-C(1)	120.0
C(5)-C(6)-C(7)	120.1
C(1)-C(6)-C(7)	119.9
O(2)-C(7)-O(1)	123(2)
O(2)-C(7)-C(6)	121(2)
O(1)-C(7)-C(6)	115(2)
C(7)-O(1)-C(8)	115(2)
C(26)-O(4)-C(27)	115(3)
O(1)-C(8)-C(9)	107(3)
C(10)-C(9)-C(15)	110(3)
C(10)-C(9)-C(8)	114(3)
C(15)-C(9)-C(8)	111(3)
C(10)-C(9)-C(11)	104(3)
C(15)-C(9)-C(11)	111(3)
C(8)-C(9)-C(11)	108(3)
C(12)-C(11)-C(9)	115(3)
C(11)-C(12)-C(13)	112(3)
C(14)-C(13)-C(12)	123(4)
C(13)-C(14)-C(15)	122(3)
C(13)-C(14)-C(19)	120(3)

C(15)-C(14)-C(19)	117(3)
C(9)-C(15)-C(14)	114(3)
C(9)-C(15)-C(16)	120(3)
C(14)-C(15)-C(16)	107(3)
C(15)-C(16)-C(17)	112(3)
C(18)-C(17)-C(16)	108(3)
C(19)-C(18)-C(17)	116(3)
C(19)-C(18)-C(24)	110(3)
C(17)-C(18)-C(24)	115(3)
C(18)-C(19)-C(21)	112(3)
C(18)-C(19)-C(20)	116(3)
C(21)-C(19)-C(20)	109(3)
C(18)-C(19)-C(14)	108(3)
C(21)-C(19)-C(14)	111(3)
C(20)-C(19)-C(14)	101(2)
C(22)-C(21)-C(19)	112(3)
C(23)-C(22)-C(21)	111(3)
C(22)-C(23)-C(24)	116(3)
C(23)-C(24)-C(25)	109(3)
C(23)-C(24)-C(18)	111(3)
C(25)-C(24)-C(18)	110(3)
C(23)-C(24)-C(26)	113(3)
C(25)-C(24)-C(26)	105(3)
C(18)-C(24)-C(26)	109(3)
O(3)-C(26)-O(4)	125(4)
O(3)-C(26)-C(24)	122(4)
O(4)-C(26)-C(24)	112(3)
C(2')-C(1')-C(6')	120.0
C(1')-C(2')-C(3')	120.0
C(4')-C(3')-C(2')	120.0
C(4')-C(3')-Br(2)	118.7(14)
C(2')-C(3')-Br(2)	121.3(14)
C(3')-C(4')-C(5')	120.0
C(6')-C(5')-C(4')	120.0
C(5')-C(6')-C(1')	120.0
C(5')-C(6')-C(7')	120.1
C(1')-C(6')-C(7')	119.9
O(2')-C(7')-O(1')	126(2)
O(2')-C(7')-C(6')	120(2)
O(1')-C(7')-C(6')	113(2)
C(7')-O(1')-C(8')	115(3)
C(27')-O(4')-C(26')	122(3)
O(1')-C(8')-C(9')	105(3)
C(8')-C(9')-C(11')	111(3)
C(8')-C(9')-C(10')	110(3)
C(11')-C(9')-C(10')	109(3)
C(8')-C(9')-C(15')	110(3)
C(11')-C(9')-C(15')	109(3)
C(10')-C(9')-C(15')	108(3)
C(12')-C(11')-C(9')	114(3)
C(11')-C(12')-C(13')	114(4)
C(14')-C(13')-C(12')	123(4)
C(13')-C(14')-C(15')	123(4)
C(13')-C(14')-C(19')	121(4)
C(15')-C(14')-C(19')	115(4)
C(14')-C(15')-C(16')	111(3)
C(14')-C(15')-C(9')	113(3)
C(16')-C(15')-C(9')	111(3)

C(17')-C(16')-C(15')	106(3)
C(18')-C(17')-C(16')	113(3)
C(19')-C(18')-C(17')	115(3)
C(19')-C(18')-C(24')	116(3)
C(17')-C(18')-C(24')	113(3)
C(14')-C(19')-C(18')	109(3)
C(14')-C(19')-C(21')	115(3)
C(18')-C(19')-C(21')	108(3)
C(14')-C(19')-C(20')	107(3)
C(18')-C(19')-C(20')	113(3)
C(21')-C(19')-C(20')	106(3)
C(19')-C(21')-C(22')	116(3)
C(23')-C(22')-C(21')	109(3)
C(22')-C(23')-C(24')	119(3)
C(26')-C(24')-C(23')	110(3)
C(26')-C(24')-C(25')	103(3)
C(23')-C(24')-C(25')	112(3)
C(26')-C(24')-C(18')	113(3)
C(23')-C(24')-C(18')	109(3)
C(25')-C(24')-C(18')	111(3)
O(3')-C(26')-O(4')	113(3)
O(3')-C(26')-C(24')	124(4)
O(4')-C(26')-C(24')	124(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for TAOT2. The factor exponent takes the form: $-2p^2 [(ha^*)^2 U_{11} + \dots + 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
Br(1)	69(3)	140(5)	90(4)	5(4)	29(3)	33(4)
O(3)	42(15)	106(27)	77(18)	33(19)	-12(13)	13(17)
O(4)	37(14)	58(17)	47(15)	14(14)	-17(12)	3(14)
Br(2)	50(3)	174(6)	83(3)	18(4)	18(2)	44(4)
O(3')	46(15)	150(29)	44(16)	-5(18)	15(13)	-13(17)
O(4')	70(17)	127(26)	35(14)	3(16)	37(13)	23(17)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for TAOT2

	x	y	z	U(eq)
H(1)	-4818(26)	-2466(12)	-2757(28)	90
H(2)	-2678(27)	-2742(12)	-2635(30)	98
H(4)	-2563(26)	-1356(14)	-5029(31)	88
H(5)	-4704(27)	-1080(11)	-5151(28)	73
H(8A)	-8054(36)	-848(17)	-3923(36)	67
H(8B)	-8774(36)	-1253(17)	-5138(36)	67
H(10A)	-7496(35)	-612(16)	-6866(32)	81
H(10B)	-8553(35)	-116(16)	-7431(32)	81
H(10C)	-8988(35)	-781(16)	-7422(32)	81
H(11A)	-7435(34)	149(16)	-4148(33)	65
H(11B)	-6592(34)	-54(16)	-5001(33)	65
H(12A)	-7389(34)	647(16)	-6474(36)	74
H(12B)	-7199(34)	973(16)	-5141(36)	74
H(13A)	-9330(35)	1225(19)	-6405(35)	81
H(15A)	-10384(33)	-449(20)	-6501(32)	62

H(16A)	-9832(25)	13(15)	-3975(26)	38
H(16B)	-10142(25)	-661(15)	-4318(26)	38
H(17A)	-12281(35)	-394(18)	-5764(37)	83
H(17B)	-12094(35)	-185(18)	-4325(37)	83
H(18A)	-11462(31)	743(15)	-4794(31)	55
H(20A)	-11960(32)	460(16)	-8619(30)	81
H(20B)	-13232(32)	417(16)	-8232(30)	81
H(20C)	-12179(32)	-91(16)	-7830(30)	81
H(21A)	-11088(32)	1529(15)	-6131(35)	64
H(21B)	-11386(32)	1409(15)	-7630(35)	64
H(22A)	-13030(30)	1988(16)	-7231(31)	55
H(22B)	-13600(30)	1404(16)	-8011(31)	55
H(23A)	-14507(34)	1486(16)	-6426(36)	72
H(23B)	-13147(34)	1613(16)	-5357(36)	72
H(25A)	-13734(40)	253(20)	-4245(39)	130
H(25B)	-14699(40)	795(20)	-4653(39)	130
H(25C)	-13225(40)	899(20)	-3806(39)	130
H(27A)	-16733(41)	554(20)	-9457(39)	130
H(27B)	-16771(41)	92(20)	-8384(39)	130
H(27C)	-15781(41)	5(20)	-9150(39)	130
H(1A)	-9904(27)	318(9)	-11213(33)	72
H(2A)	-12113(30)	532(10)	-11484(35)	97
H(4A)	-12819(27)	-1236(13)	-11186(35)	94
H(5A)	-10610(30)	-1449(8)	-10916(33)	83
H(8C)	-6351(39)	-1039(20)	-9432(41)	83
H(8D)	-6622(39)	-1330(20)	-10824(41)	83
H(10D)	-7442(40)	-2787(19)	-9868(39)	121
H(10E)	-7499(40)	-2424(19)	-11122(39)	121
H(10F)	-8484(40)	-2280(19)	-10377(39)	121
H(11C)	-6178(37)	-1644(17)	-7503(33)	64
H(11D)	-7664(37)	-1810(17)	-8138(33)	64
H(12C)	-7316(42)	-2740(19)	-7715(43)	105
H(12D)	-6367(42)	-2431(19)	-6458(43)	105
H(13B)	-5063(32)	-3180(16)	-7048(32)	65
H(16C)	-4414(39)	-1325(21)	-9467(43)	107
H(16D)	-4096(39)	-1504(21)	-7985(43)	107
H(17C)	-2847(37)	-1989(17)	-9714(38)	79
H(17D)	-2132(37)	-1619(17)	-8449(38)	79
H(18B)	-2385(35)	-2362(17)	-7144(37)	76
H(20D)	-2941(31)	-3423(16)	-9790(29)	75
H(20E)	-3997(31)	-2934(16)	-10431(29)	75
H(20F)	-4419(31)	-3534(16)	-9946(29)	75
H(21C)	-3663(33)	-3783(16)	-7654(33)	64
H(21D)	-3029(33)	-3322(16)	-6540(33)	64
H(22C)	-1344(30)	-4003(16)	-6498(34)	59
H(22D)	-1628(30)	-3934(16)	-8014(34)	59
H(23C)	86(34)	-3260(17)	-6278(32)	66
H(25D)	4(37)	-2066(20)	-6540(37)	120
H(25E)	-196(37)	-1879(20)	-7989(37)	120
H(25F)	877(37)	-2350(20)	-7286(37)	120
H(26A)	-1783(38)	-2993(19)	-9417(41)	66
H(27D)	37(38)	-3936(18)	-10467(38)	117
H(27E)	364(38)	-3266(18)	-10620(38)	117
H(27F)	-1091(38)	-3491(18)	-11186(38)	117

Experimental

$$R1=(\hat{A}||F_o|-|F_c||/\hat{A}|F_o|), \text{ } wR2=\hat{A}w(F_o^2-F_c^2)^2/\hat{A}w[(F_o^2)^2]^{1/2}, \text{ } S=[\hat{A}w(F_o^2-F_c^2)^2/(n-p)]^{1/2}$$

Phenyl rings were treated as regular hexagons of D_{6h} symmetry with C-C = 1.395 Å and C-C-C = 120°. Unit cell dimensions and standard deviations were obtained by least squares fit to 14 reflections ($14 < 2\theta < 22^\circ$).

References SHELXTL-PC. & G.M.Sheldrick, Siemens Analytical X-ray Instr. Inc. Madison, WI. (1990). H.D.Flack. Acta Crystallographica, A39, 876-881(1983).

	h	k	l	Fo ²	Fc ²	Delta(F ²)/esd	Fc/Fc(max)	Res(A)
*	5	12	0	-452.12	47.83	3.54	0.031	1.38
	3	5	6	160.38	879.26	3.29	0.131	1.29
	6	10	2	4304.55	2244.03	3.27	0.209	1.23
	-1	20	3	563.02	4.83	3.14	0.010	1.07
	4	1	6	486.25	1385.35	3.03	0.165	1.23
	3	6	1	3304.76	1854.08	2.99	0.190	2.31
	-10	8	5	-493.07	2.62	2.96	0.007	0.99
	2	14	1	-172.32	189.38	2.95	0.061	1.49
	-3	19	2	-32.42	521.83	2.91	0.101	1.12
	4	17	0	102.37	759.92	2.90	0.122	1.17
	-1	16	2	-394.11	12.04	2.88	0.015	1.36
	2	2	6	168.91	696.11	2.87	0.117	1.46
	-7	13	3	499.89	38.35	2.86	0.027	1.15
	3	4	6	902.54	332.32	2.85	0.081	1.31
	-2	18	5	-479.42	1.34	2.84	0.005	1.08
	2	1	6	-114.31	269.56	2.81	0.073	1.47
	3	8	6	547.67	68.00	2.80	0.036	1.22
	2	5	3	607.38	1277.47	2.79	0.158	2.17
	5	7	5	650.03	143.59	2.76	0.053	1.16
	5	4	0	494.78	147.83	2.76	0.054	1.91
	1	9	6	131.37	625.21	2.73	0.111	1.34
	-6	1	2	235.45	662.42	2.67	0.114	1.79
	5	0	3	5551.73	3335.92	2.67	0.255	1.54
	2	15	5	506.72	53.90	2.66	0.032	1.13
	5	7	1	2366.40	1372.84	2.62	0.164	1.62
	-4	12	4	-332.69	9.64	2.62	0.014	1.43
	-2	7	3	472.60	191.80	2.60	0.061	2.33
	1	5	8	545.96	111.16	2.58	0.047	1.17
	5	1	5	-218.38	170.55	2.57	0.058	1.25
	3	11	3	1409.26	2636.11	2.56	0.227	1.46
	5	15	0	-29.00	435.15	2.55	0.092	1.21
	1	11	1	632.97	1241.97	2.54	0.156	1.94
	-8	3	5	320.75	911.52	2.52	0.133	1.27
	4	4	6	-272.98	158.75	2.52	0.056	1.21
	-4	19	3	-162.08	333.71	2.51	0.081	1.07
	-4	9	2	-6.82	294.67	2.50	0.076	1.82
	-10	10	4	-300.28	129.68	2.50	0.050	0.97
	1	16	4	498.19	86.97	2.49	0.041	1.20
	-8	12	1	999.79	420.93	2.47	0.091	1.08
	8	3	3	421.41	0.14	2.44	0.002	1.07
	-2	14	1	151.85	538.96	2.44	0.103	1.54
	1	10	4	-220.09	50.49	2.43	0.031	1.61
	-4	5	4	-141.61	88.85	2.42	0.042	1.98
	1	12	6	-64.83	331.86	2.38	0.081	1.21
	-2	19	1	-184.26	234.99	2.38	0.068	1.15
	4	17	2	440.18	41.94	2.36	0.029	1.11
	2	0	7	-276.39	72.57	2.36	0.038	1.29
	3	5	1	946.90	543.30	2.34	0.103	2.46
	3	10	6	-141.61	280.87	2.34	0.074	1.16
	2	7	8	-334.40	41.94	2.34	0.029	1.08

