Experimental details for compounds prepared

Calix[4]arene 2. To a solution of 1 g (1.54 mmol) of *p-tert*-butylcalix[4]arene and 1.25 g (12.4 mmol) of triethylamine in anhydrous CH_2Cl_2 (30 mL) was added 3.9 g (12.4 mmol) of O-acetyl gallic acid chloride. The mixture was stirred for 5 h at rt under nitrogen. The reaction mixture was washed with water and dried over $MgSO_4$. After removal of the solvent, the product was purified through SiO_2 column ($CHCl_3$/hexane=10/2) to afford 1.68 g (87%) of product. Recrystallization from $CHCl_3$/hexane and dring under reduced pressure gave 1.2 g of crystals **2** having mp=299-306 °C. IR (KBr) ν 3562, 1782 cm^{-1}. ^1H NMR ($CDCl_3$, 20°C) δ 0.87 (s, 18H, CH_3), 1.30 (s, 18H, CH_3), 2.05 (s, 12H, AcO), 2.30 (s, 6H, AcO), 3.39 (d, 4H, $ArCH_2Ar$), 3.95 (d, 4H, $ArCH_2Ar$), 5.38 (s, 2H, OH), 6.75 (s, 4H, ArH), 7.11 (s, 4H, ArH), 8.29 (s, 4H, ArH). ^{13}C NMR ($CDCl_3$ 20°C) δ 20.2, 30.8, 31.6, 31.8, 34.0, 122.8, 125.4, 125.7, 127.0, 128.4, 131.3, 139.6, 142.2, 143.1, 144.2, 148.9, 149.9, 163.4, 166.4, 167.6. MS (ESI-TOF) calcd for $C_{70}H_{77}O_{18}$ 1205.51, found 1205.58 $[M + H]^+$. Anal. Calcd for $C_{70}H_{76}O_{18}$: C, 69.75; H, 6.36. Found: C, 69.43, H, 6.33.

Calix[4]arene 3a To a solution of 1.0 g (0.80 mmol) of **2** in CH_3CN (60 mL) was added 0.24 g (4.8 mmol) of hydrazine monohydrate. The mixture was stirred for 30 min at rt. Acetic acid (0.27 mL) and water (20 mL) was added to the reaction mixture. The organic potion was extracted with ethyl acetate (50 mL X 2), washed with water (30 mL X 2) and sat. aq. NaCl, and dried over $MgSO_4$. The organic solvent was evaporated and acetone was added to produce precipitates. The precipitates were filtrated and washed with acetone to afford 0.58 g (76%) of white solid. Recrystallization and dring under reduced pressure gave prisms **3a** having mp=225-229 °C. IR (KBr) ν 3535, 3300, 3700-3740 cm^{-1}. ^1H NMR (DMSO-d_6) δ 0.91 (s, 18H, CH_3), 1.19 (s, 18H, CH_3), 3.38 (d, 4H, $ArCH_2Ar$), 3.84 (d, 4H, $ArCH_2Ar$), 5.56 (s, 2H, OH), 6.75 (s, 4H, ArH), 7.11 (s, 4H, ArH), 7.23 (s, 4H, ArH), 9.13 (s, 4H, OH), 9.18 (s, 2H, OH). ^{13}C NMR (DMSO-d_6) δ 30.8, 31.6, 33.7, 110.1, 118.6, 125.1, 125.5, 128.8, 131.7, 139.7, 141.9, 143.3, 145.7, 146.9, 150.0, 165.3. MS (ESI-TOF) calcd for $C_{58}H_{65}O_{12}$ 953.45, found 953.47 $[M + H]^+$. Anal. Calcd for $C_{58}H_{64}O_{12}\cdot 2H_2O$: C, 70.43; H, 6.93. Found: C, 70.23, H, 6.90.

Calix[4]arene 3b. To a solution of 0.3 g (0.24 mmol) of **2** in CH_3CN (15 mL) was added 0.44 g (7.2 mmol) of aq NH_3 (28%). The mixture was stirred for 2 h at rt. Acetic acid (0.5 mL) and water (20 mL) was added to the reaction mixture. The organic potion was extracted with ethyl acetate (50 mL X 2), washed with water (30 mL X 2) and sat. aq. NaCl,

and dried over $MgSO_4$. After evaporating the solvent, the product was purified through SiO_2 column ($CHCl_3$/MeOH =10/1) to afford 77 mg of product (40%). Recrystallization from $CHCl_3$/hexane and dring under reduced pressure gave a 45 mg of fine needles **3b** having mp=183-189 °C. IR (KBr) ν 3512, 3345, 1726, 1695 cm^{-1}. ^1H NMR ($CDCl_3$, 20°C) δ 0.75 (s, 18H, CH_3), 1.36 (s, 9H, CH_3), 1.40 (s, 9H, CH_3), 3.45 (d, 2H, $ArCH_2Ar$), 3.85 (d, 2H, $ArCH_2Ar$), 4.02 (d, 2H, $ArCH_2Ar$), 4.14 (d, 2H, $ArCH_2Ar$), 5.19 (s, 1H, OH), 6.55 (d, 2H, ArH), 6.67 (s, 2H, ArH), 6.81 (d, 2H, ArH), 7.22 (s, 2H, ArH), 7.38 (s, 2H, ArH), 8.92 (s, 1H, OH). ^{13}C NMR ($CDCl_3$, 20°C) δ 30.7, 31.50, 31.54, 32.0, 33.5, 34.3, 34.6, 38.1, 109.0, 119.7, 124.9, 125.5, 125.9, 126.8, 127.5, 129.1, 131.5, 135.8, 144.2, 144.5, 146.5, 148.0, 148.6, 150.0, 162.2. MS (ESI-TOF) calcd for $C_{51}H_{61}O_8$ 801.44, found 801.45 $[M + H]^+$. Anal. Calcd for $C_{51}H_{60}O_8 \cdot 2H_2O$: C, 75.62; H, 7.59. Found: C, 75.36, H, 7.58.

X-ray crystallographic details

A. Crystal Data

Empirical Formula	$C_{73}H_{94}0_{17}$
Formula Weight	1243.54
Crystal Color, Habit	colorless, prism
Crystal Dimensions	0.25 X 0.15 X 0.15 mm
Crystal System	tetragonal
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	106437 (5.0 - 136.4°)
Indexing Images	1 oscillations at 1.0 minutes
Camera Radius	127.40 mm
Lattice Parameters	a = 13.9382(3) Å c = 35.3234(8) Å V = 6862.4(3) $Å^3$
Space Group	$P4_12_12$ (#92)
Z value	4
D_{calc}	1.204 g/cm^3
F_{000}	2672.00
μ(Cu Kα)	6.89 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku RAXIS-RAPID Imaging Plate
Radiation	CuKα (λ= 1.54178 Å) graphite monochromated
Temperature	-100.0 °C
Voltage, Current	300 kV, 50 mA
Collimator Size	0.3 mm
Detector Aperture	450.0 mm x 256.0 mm
Data Images	90 exposures at 1.0 minutes per degree
Oscillation Range (ϕ=0.0°, χ=50.0°)	ω 50.0-230.0° with 10.0° step
Oscillation Range (ϕ=90.0°, χ=50.0°)	ω 50.0-230.0° with 10.0° step

Oscillation Range (ϕ=180.0°, χ=50.0°)	ω 50.0-230.0° with 10.0° step
Oscillation Range (ϕ=270.0°, χ=50.0°)	ω 50.0-230.0° with 10.0° step
Oscillation Range (ϕ=0.0°, χ=0.0°)	ω 50.0-230.0° with 10.0° step
Camera Radius	127.40 mm
Pixel Size	0.100 mm
$2\theta_{max}$	136.5°
No. of Reflections Measured	Total: 69324
	Unique: 1216 (R_{int} = 0.039)
Corrections	Lorentz-polarization
	Absorption (trans. factors:
	0.8430 - 0.9018)
	Secondary Extinction
	(coefficient: 7.70470e-07)

C. Structure Solution and Refinement

Structure Solution	Patterson Methods (SHELXS-97)
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma\omega(\|Fo\| - \|Fc\|)^2$
Least Squares Weights	
	$\omega = \frac{1}{\sigma^2(Fo)} = \left[\sigma_c^2(Fo) + \frac{p^2}{4}Fo^2\right]^{-1}$
p-factor	0.1240
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>2.00σ(I))	2652
No. Variables	408
Reflection/Parameter Ratio	6.50
Residuals: R; Rw	0.069; 0.102
Residuals: R1	0.069
No. of Reflections to calc R1	2652
Goodness of Fit Indicator	1.18
Max Shift/Error in Final Cycle	0.186
Maximum peak in Final Diff. Map	0.42 e^-/ Å^3
Minimum peak in Final Diff. Map	-0.38 e^-/ Å^3

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
O(1)	0.3946(2)	0.3078(3)	0.0393(1)	4.42(8)	1.0000
O(2)	0.2329(2)	0.4273(2)	0.0354(1)	4.09(8)	1.0000
O(3)	0.0929(3)	0.4919(3)	0.0563(1)	5.27(10)	1.0000
O(4)	-0.1311(3)	0.2054(3)	0.0363(2)	6.0(1)	1.0000
O(5)	-0.0114(4)	0.0500(3)	0.0423(2)	6.5(1)	1.0000
O(6)	0.1787(3)	0.0711(3)	0.0484(2)	6.1(1)	1.0000
O(7)	0.6756(7)	0.6756	0.0000	18.3(5)	0.5000
O(8)	0.3731(4)	0.0907(4)	0.0612(2)	7.7(2)	1.0000
O(9)	-0.2371(7)	0.0488(6)	0.0149(3)	11.3(3)	1.0000
C(1)	0.5644(4)	0.2900(4)	0.0524(1)	3.9(1)	1.0000
C(2)	0.6414(4)	0.3184(5)	0.0740(2)	5.2(2)	1.0000
C(3)	0.6334(5)	0.3859(6)	0.1033(2)	6.0(2)	1.0000
C(4)	0.5408(4)	0.4188(5)	0.1112(2)	5.3(2)	1.0000
C(5)	0.4612(4)	0.3931(4)	0.0903(2)	4.2(1)	1.0000
C(6)	0.4744(4)	0.3299(4)	0.0603(2)	3.9(1)	1.0000
C(7)	0.3629(4)	0.4347(4)	0.0985(2)	4.0(1)	1.0000
C(8)	0.3400(4)	0.5204(4)	0.0737(1)	3.7(1)	1.0000
C(9)	0.3827(4)	0.6095(4)	0.0811(2)	4.2(1)	1.0000
C(10)	0.3682(4)	0.6895(4)	0.0586(2)	4.1(1)	1.0000
C(11)	0.3127(4)	0.6776(4)	0.0260(2)	4.2(1)	1.0000
C(12)	0.2693(4)	0.5906(4)	0.0170(2)	3.8(1)	1.0000
C(13)	0.2809(4)	0.5150(4)	0.0425(2)	3.8(1)	1.0000
C(14)	0.2184(4)	0.5789(4)	-0.0206(2)	4.3(1)	1.0000
C(15)	0.1376(4)	0.4213(4)	0.0462(2)	4.0(1)	1.0000
C(16)	0.1019(4)	0.3232(4)	0.0442(2)	4.0(1)	1.0000
C(17)	0.0017(4)	0.3096(4)	0.0416(2)	4.1(1)	1.0000
C(18)	-0.0332(4)	0.2188(5)	0.0403(2)	4.4(1)	1.0000
C(19)	0.0274(4)	0.1398(4)	0.0427(2)	4.7(1)	1.0000
C(20)	0.1251(4)	0.1533(4)	0.0461(2)	4.8(1)	1.0000
C(21)	0.1634(4)	0.2445(4)	0.0452(2)	4.4(1)	1.0000
C(22)	0.7201(6)	0.417(1)	0.1257(3)	10.9(4)	1.0000
C(23)	0.729(2)	0.348(2)	0.1592(8)	26(1)	1.0000
C(24)	0.8090(7)	0.412(1)	0.1033(5)	14.8(5)	1.0000

C(25)	0.7080(8)	0.515(1)	0.1422(4)	13.6(5)	1.0000
C(26)	0.4071(5)	0.7887(5)	0.0688(2)	5.1(1)	1.0000
C(27)	0.477(1)	0.7852(9)	0.1015(5)	15.9(6)	1.0000
C(28)	0.451(1)	0.8364(7)	0.0362(2)	10.0(3)	1.0000
C(29)	0.327(1)	0.8482(8)	0.0824(6)	17.5(6)	1.0000
C(30)	0.6195(7)	0.6195	0.0000	7.5(2)	0.5000
C(31)	0.607(3)	0.558(1)	0.0246(9)	43(2)	1.0000
C(32)	-0.2573(8)	0.0081(8)	-0.0148(3)	8.8(3)	1.0000
C(33)	-0.335(1)	-0.057(1)	-0.0169(5)	13.6(5)	1.0000
C(34)	-0.209(3)	0.043(2)	-0.0455(9)	32(1)	1.0000
C(35)	0.3990(6)	0.1106(5)	0.0927(3)	6.6(2)	1.0000
C(36)	0.5006(6)	0.0897(6)	0.1055(3)	7.4(2)	1.0000
C(37)	0.3396(7)	0.1596(8)	0.1217(3)	8.7(3)	1.0000
H(1)	0.7026	0.2912	0.0689	6.2602	1.0000
H(O1)	0.4043	0.2583	0.0188	5.3064	1.0000
H(2)	0.5321	0.4613	0.1318	6.3185	1.0000
H(3)	0.4234	0.6154	0.1025	5.0402	1.0000
H(04)	-0.1385	0.1360	0.0354	7.2252	1.0000
H(4)	0.3043	0.7307	0.0094	5.0690	1.0000
H(5)	-0.0403	0.3629	0.0407	5.0110	1.0000
H(05)	0.0450	0.0120	0.0310	7.7592	1.0000
H(6)	0.2312	0.2533	0.0454	5.2990	1.0000
H(06)	0.2449	0.0748	0.0548	7.3920	1.0000
H(7)	0.3156	0.3865	0.0944	4.8563	1.0000
H(8)	0.3606	0.4545	0.1243	4.8563	1.0000
H(9)	0.1806	0.6346	-0.0257	5.0915	1.0000
H(10)	0.1766	0.5245	-0.0194	5.0915	1.0000
H(23a)	0.6710	0.3476	0.1739	30.2987	1.0000
H(23b)	0.7382	0.2829	0.1499	30.2987	1.0000
H(23c)	0.7811	0.3638	0.1749	30.2987	1.0000
H(24a)	0.8186	0.3462	0.0962	18.5152	1.0000
H(24b)	0.8046	0.4513	0.0828	18.5152	1.0000
H(24c)	0.8611	0.4301	0.1197	18.5152	1.0000
H(25a)	0.7635	0.5305	0.1569	16.1467	1.0000
H(25b)	0.6988	0.5597	0.1231	16.1467	1.0000

H(25c)	0.6534	0.5146	0.1590	16.1467	1.0000
H(27a)	0.4481	0.7544	0.1222	19.1278	1.0000
H(27b)	0.5323	0.7497	0.0936	19.1278	1.0000
H(27c)	0.4955	0.8483	0.1079	19.1278	1.0000
H(28a)	0.5033	0.7980	0.0274	12.2623	1.0000
H(28b)	0.4053	0.8436	0.0168	12.2623	1.0000
H(28c)	0.4747	0.8973	0.0438	12.2623	1.0000
H(29a)	0.3505	0.9092	0.0897	21.0262	1.0000
H(29b)	0.2815	0.8558	0.0624	21.0262	1.0000
H(29c)	0.2972	0.8177	0.1032	21.0262	1.0000
H(30a)	0.6695	0.5240	0.0283	49.4777	1.0000
H(30b)	0.5979	0.5911	0.0491	49.4777	1.0000
H(30c)	0.5604	0.5165	0.0200	49.4777	1.0000
H(33a)	-0.3922	-0.0230	-0.0099	16.3374	1.0000
H(33b)	-0.3394	-0.0797	-0.0415	16.3374	1.0000
H(33c)	-0.3237	-0.1066	0.0007	16.3374	1.0000
H(34a)	-0.2335	0.0131	-0.0668	36.8684	1.0000
H(34b)	-0.1442	0.0313	-0.0415	36.8684	1.0000
H(34c)	-0.2213	0.1107	-0.0462	36.8684	1.0000
H(36a)	0.5127	0.0231	0.1033	8.8546	1.0000
H(36b)	0.5444	0.1240	0.0896	8.8546	1.0000
H(36c)	0.5092	0.1097	0.1309	8 .8546	1.0000
H(37a)	0.3751	0.1670	0.1444	10.4327	1.0000
H(37b)	0.3209	0.2210	0.1125	10.4327	1.0000
H(37c)	0.2838	0.1222	0.1265	10.4327	1.0000

$$B_{eq} = \frac{8}{3}\pi^2\left(U_{11}\left(aa^*\right)^2 + U_{22}\left(bb^*\right)^2 + U_{33}\left(cc^*\right)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha\right)$$

Table 2. Anisotropic Displacement Parameters

atom	U11	U22	U33	U12	U13	U23
O(1)	0.036(2)	0.054(2)	0.078(3)	0.003(2)	-0.001(2)	-0.010(2)
O(2)	0.040(2)	0.041(2)	0.075(2)	-0.002(1)	0.003(2)	-0.002(2)
O(3)	0.048(2)	0.056(2)	0.096(3)	0.000(2)	0.013(2)	-0.014(2)
O(4)	0.039(2)	0.071(3)	0.118(4)	-0.009(2)	-0.008(2)	-0.009(3)
O(5)	0.072(3)	0.051(2)	0.124(4)	-0.012(2)	0.016(3)	-0.002(3)
O(6)	0.061(3)	0.050(2)	0.123(4)	0.007(2)	0.003(3)	0.019(3)
O(7)	0.142(7)	0.1416	0.41(3)	-0.047(10)	0.0483	-0.05(1)
O(8)	0.071(3)	0.068(3)	0.152(6)	0.011(2)	0.004(4)	0.018(4)
O(9)	0.146(7)	0.123(6)	0.159(7)	-0.011(5)	-0.038(6)	-0.011(6)
C(1)	0.045(3)	0.050(3)	0.053(3)	0.004(2)	0.004(2)	0.006(2)
C(2)	0.039(3)	0.089(5)	0.070(4)	0.017(3)	-0.001(3)	-0.007(3)
C(3)	0.052(3)	0.104(6)	0.071(4)	0.014(3)	-0.009(3)	-0.025(4)
C(4)	0.048(3)	0.081(4)	0.071(4)	0.010(3)	-0.005(3)	-0.016(3)
C(5)	0.048(3)	0.055(3)	0.055(3)	0.002(2)	0.004(2)	0.008(2)
C(6)	0.043(3)	0.045(3)	0.062(3)	0.004(2)	0.001(2)	0.007(2)
C(7)	0.044(3)	0.057(3)	0.052(3)	0.003(2)	0.008(2)	0.003(2)
C(8)	0.041(3)	0.045(3)	0.054(3)	-0.002(2)	0.006(2)	0.001(2)
C(9)	0.048(3)	0.054(3)	0.058(3)	-0.002(2)	0.006(2)	-0.006(2)
C(10)	0.049(3)	0.050(3)	0.057(3)	-0.002(2)	0.008(2)	-0.005(2)
C(11)	0.057(3)	0.044(3)	0.058(3)	0.003(2)	0.006(2)	0.001(2)
C(12)	0.043(3)	0.040(3)	0.061(3)	0.004(2)	0.002(2)	-0.002(2)
C(13)	0.042(3)	0.040(3)	0.062(3)	-0.002(2)	0.007(2)	-0.004(2)
C(14)	0.049(3)	0.044(3)	0.069(3)	0.010(2)	-0.006(3)	-0.004(3)
C(15)	0.037(3)	0.052(3)	0.064(3)	0.000(2)	0.003(2)	-0.001(3)
C(16)	0.039(3)	0.052(3)	0.062(3)	-0.002(2)	-0.001(2)	0.001(3)
C(17)	0.039(3)	0.053(3)	0.064(3)	-0.001(2)	0.000(2)	0.003(3)
C(18)	0.045(3)	0.062(3)	0.060(3)	-0.001(2)	0.003(3)	0.001(3)
C(19)	0.056(3)	0.051(3)	0.071(4)	-0.009(2)	0.009(3)	0.008(3)
C(20)	0.051(3)	0.051(3)	0.079(4)	-0.002(2)	0.007(3)	0.007(3)
C(21)	0.048(3)	0.048(3)	0.070(3)	-0.001(2)	0.006(3)	0.005(3)
C(22)	0.063(5)	0.21(1)	0.142(9)	0.027(6)	-0.029(5)	-0.104(9)
C(23)	0.33(3)	0.34(3)	0.35(3)	0.01(3)	-0.30(3)	0.03(3)
C(24)	0.056(5)	0.25(2)	0.25(2)	-0.007(8)	-0.031(8)	-0.15(2)

C(25)	0.074(6)	0.23(2)	0.21(1)	-0.004(8)	-0.023(7)	-0.15(1)
C(26)	0.073(4)	0.057(3)	0.063(3)	-0.013(3)	0.011(3)	-0.010(3)
C(27)	0.26(2)	0.080(7)	0.27(2)	-0.068(9)	-0.16(2)	0.009(9)
C(28)	0.21(1)	0.090(6)	0.077(5)	-0.080(7)	0.038(7)	-0.019(5)
C(29)	0.20(1)	0.075(6)	0.39(2)	-0.060(8)	0.18(2)	-0.13(1)
C(30)	0.084(5)	0.0841	0.117(9)	-0.003(6)	0.0238	-0.024(5)
C(31)	0.87(9)	0.14(2)	0.64(7)	0.17(3)	0.67(7)	0.15(3)
C(32)	0.115(8)	0.108(7)	0.110(7)	-0.007(6)	-0.033(6)	-0.008(6)
C(33)	0.13(1)	0.15(1)	0.24(2)	-0.004(9)	-0.06(1)	-0.04(1)
C(34)	0.61(7)	0.23(3)	0.38(4)	-0.10(3)	0.34(5)	0.00(3)
C(35)	0.064(4)	0.057(4)	0.129(7)	0.011(3)	0.022(5)	0.039(5)
C(36)	0.070(5)	0.077(5)	0.134(7)	0.010(4)	0.012(5)	0.029(5)
C(37)	0.095(6)	0.108(7)	0.128(7)	0.031(5)	0.042(6)	0.060(6)

The general temperature factor expression

$$\exp\left(-2\pi^2\left(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl\right)\right)$$

Table 3. Bond Lengths (Å)

atom	atom	distance	atom	atom	distance
O(1)	C(6)	1.373(6)	O(2)	C(13)	1.416(6)
O(2)	C(15)	1.385(6)	O(3)	C(15)	1.219(7)
O(4)	C(18)	1.384(7)	O(5)	C(19)	1.364(7)
O(6)	C(20)	1.370(7)	O(7)	C(32)	1.23(1)
O(8)	C(35)	1.20(1)	O(10)	C(30)	1.11(2)
C(1)	C(2)	1.373(8)	C(1)	C(6)	1.401(7)
C(1)	C(14)	1.515(8)	C(2)	C(3)	1.404(10)
C(3)	C(4)	1.398(9)	C(3)	C(22)	1.51(1)
C(4)	C(5)	1.380(8)	C(5)	C(6)	1.390(8)
C(5)	C(7)	1.516(7)	C(7)	C(8)	1.516(8)
C(8)	C(9)	1.401(8)	C(8)	C(13)	1.378(8)
C(9)	C(10)	1.383(8)	C(10)	C(11)	1.396(8)
C(10)	C(26)	1.528(8)	C(11)	C(12)	1.392(8)
C(12)	C(13)	1.394(8)	C(12)	C(14)	1.516(8)
C(15)	C(16)	1.457(8)	C(16)	C(17)	1.411(8)
C(16)	C(21)	1.393(8)	C(17)	C(18)	1.358(9)
C(18)	C(19)	1.390(9)	C(19)	C(20)	1.380(9)
C(20)	C(21)	1.379(8)	C(22)	C(23)	1.53(3)
C(22)	C(24)	1.47(2)	C(22)	C(25)	1.49(2)
C(26)	C(27)	1.51(2)	C(26)	C(28)	1.46(1)
C(26)	C(29)	1.47(1)	C(30)	C(31)	1.24(2)
C(30)	C(31)	1.24(2)	C(32)	C(33)	1.41(2)
C(32)	C(34)	1.37(2)	C(35)	C(36)	1.51(1)
C(35)	C(37)	1.48(1)			

Table 3. Bond Angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
C(13)	O(2)	C(15)	117.1(4)	C(2)	C(1)	C(6)	118.3(5)
C(2)	C(1)	C(14)	119.8(5)	C(6)	C(1)	C(14)	121.9(5)
C(1)	C(2)	C(3)	122.7(5)	C(2)	C(3)	C(4)	116.1(6)
C(2)	C(3)	C(22)	121.1(6)	C(4)	C(3)	C(22)	122.8(6)
C(3)	C(4)	C(5)	123.4(6)	C(4)	C(5)	C(6)	117.7(5)
C(4)	C(5)	C(7)	121.6(5)	C(6)	C(5)	C(7)	120.6(5)
O(1)	C(6)	C(1)	122.0(5)	O(1)	C(6)	C(5)	116.5(5)
C(1)	C(6)	C(5)	121.5(5)	C(5)	C(7)	C(8)	112.4(4)
C(7)	C(8)	C(9)	120.1(5)	C(7)	C(8)	C(13)	123.0(5)
C(9)	C(8)	C(13)	116.8(5)	C(8)	C(9)	C(10)	123.0(5)
C(9)	C(10)	C(11)	117.2(5)	C(9)	C(10)	C(26)	122.8(5)
C(11)	C(10)	C(26)	119.9(5)	C(10)	C(11)	C(12)	122.2(5)
C(11)	C(12)	C(13)	117.5(5)	C(11)	C(12)	C(14)	119.8(5)
C(13)	C(12)	C(14)	122.6(5)	O(2)	C(13)	C(8)	118.1(5)
O(2)	C(13)	C(12)	118.9(5)	C(8)	C(13)	C(12)	122.9(5)
C(1)	C(14)	C(12)	110.9(4)	O(2)	C(15)	O(3)	121.5(5)
O(2)	C(15)	C(16)	111.8(4)	O(3)	C(15)	C(16)	126.7(5)
C(15)	C(16)	C(17)	117.9(5)	C(15)	C(16)	C(21)	121.8(5)
C(17)	C(16)	C(21)	120.3(5)	C(16)	C(17)	C(18)	118.8(5)
O(4)	C(18)	C(17)	118.9(5)	O(4)	C(18)	C(19)	119.9(6)
C(17)	C(18)	C(19)	121.2(5)	O(5)	C(19)	C(18)	119.0(5)
O(5)	C(19)	C(20)	121.2(6)	C(18)	C(19)	C(20)	119.9(6)
O(6)	C(20)	C(19)	115.4(6)	O(6)	C(20)	C(21)	124.1(5)
C(19)	C(20)	C(21)	120.4(6)	C(16)	C(21)	C(20)	119.2(5)
C(3)	C(22)	C(23)	106(1)	C(3)	C(22)	C(24)	112.4(8)
C(3)	C(22)	C(25)	112.2(9)	C(23)	C(22)	C(24)	108(1)
C(23)	C(22)	C(25)	106(1)	C(24)	C(22)	C(25)	110(1)
C(10)	C(26)	C(27)	112.4(7)	C(10)	C(26)	C(28)	112.0(5)
C(10)	C(26)	C(29)	108.5(6)	C(27)	C(26)	C(28)	109.9(10)
C(27)	C(26)	C(29)	105(1)	C(28)	C(26)	C(29)	108(1)
O(10)	C(30)	C(31)	126(2)	O(10)	C(30)	C(31)	126(2)
C(31)	C(30)	C(31)	107(4)	O(7)	C(32)	C(33)	121(1)
O(7)	C(32)	C(34)	114(1)	C(33)	C(32)	C(34)	123(2)

O(8)	C(35)	C(36)	120.8(8)	O(8)	C(35)	C(37)	125.2(8)
C(36)	C(35)	C(37)	113.9(10)				