A New Chiral Pool Approach to Anthracyclinones.

The Stereoselective Synthesis of Idarubicinone

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Supporting Information

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Fig. S1. An ORTEP drawing of pyranose **12**.

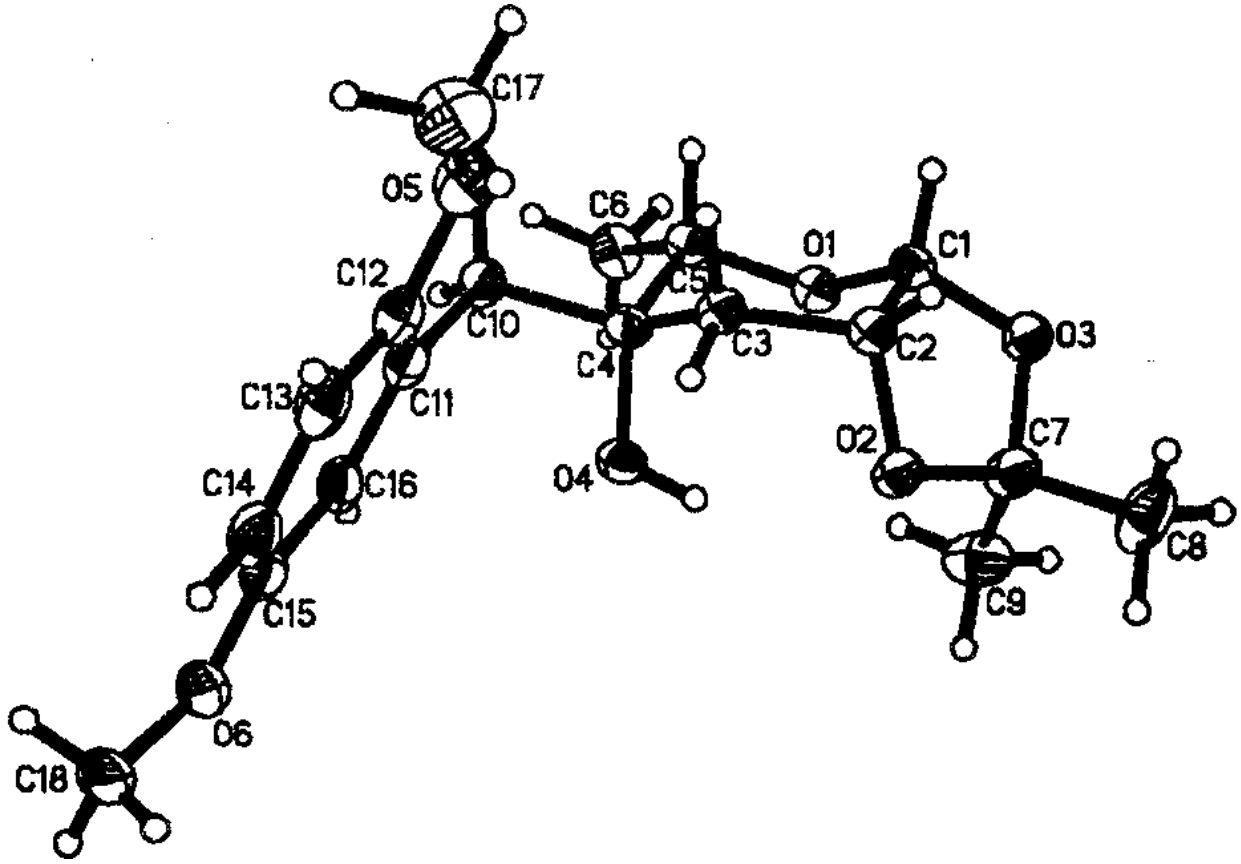

Table S1. Crystal data and structure refinement for **12**.

Empirical formula	$C_{18}\ H_{26}\ O_6$
Formula weight	338.39
Temperature	293(2) K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	P2(1)2(1)2(1)
Unit cell dimensions	a = 9.8252(5) Å, α= 90°. b = 11.7622(9) Å, β= 90°. c = 14.2416(9) Å, γ = 90°.
Volume	1645.84(18) $Å^3$
Z	4
Density (calculated)	1.366 Mg/m^3
Absorption coefficient	0.841 mm^{-1}
F(000)	728
Crystal size	0.77 x 0.35 x 0.14 mm^3
Theta range for data collection	4.88 to 88.59°.
Index ranges	$0\leq h\leq 12$, $-14\leq k\leq 0$, $-17\leq l\leq 0$
Reflections collected	1749
Independent reflections	1749 [R(int) = 0.0000]
Absorption correction	Not applied
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1749 / 0 / 224
Goodness-of-fit on F^2	0.999
Final R indices [I>2sigma(I)]	R1 = 0.0490, wR2 = 0.1418
R indices (all data)	R1 = 0.0498, wR2 = 0.1432
Absolute structure parameter	0.0(4)
Extinction coefficient	0.0108(14)
Largest diff. peak and hole	0.222 and -0.250 $e.Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **12**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	1572(2)	323(2)	3857(2)	51(1)
O(2)	471(2)	-1827(2)	4227(2)	57(1)
O(3)	1626(2)	-705(2)	5210(2)	59(1)
O(4)	585(2)	-929(2)	2339(2)	55(1)
O(5)	-3319(3)	430(3)	2526(2)	81(1)
O(6)	-1774(3)	-2357(2)	-360(2)	77(1)
C(5)	836(3)	869(3)	3148(2)	49(1)
C(4)	-86(3)	-1(3)	2743(2)	47(1)
C(3)	-901(3)	-422(3)	3539(2)	48(1)
C(2)	-180(3)	-778(2)	4398(2)	49(1)
C(1)	885(3)	-6(3)	4656(2)	51(1)
C(7)	1498(4)	-1850(3)	4863(3)	69(1)
C(6)	1742(4)	1361(4)	2451(2)	68(1)
C(8)	1203(6)	-2622(4)	5681(4)	100(2)
C(9)	2644(4)	-2182(5)	4337(4)	93(2)
C(10)	-847(3)	533(3)	1949(2)	55(1)
C(11)	-1774(4)	-267(3)	1512(2)	55(1)
C(12)	-3019(4)	-316(3)	1828(3)	63(1)
C(13)	-3819(4)	-1088(4)	1418(3)	73(1)
C(14)	-3442(4)	-1786(4)	697(3)	72(1)
C(15)	-2247(4)	-1723(3)	361(3)	60(1)
C(16)	-1430(4)	-966(3)	783(2)	59(1)
C(17)	-4578(5)	468(6)	2833(4)	108(2)
C(18)	-2607(6)	-3035(4)	-878(4)	97(2)

Table S3. Bond lengths [Å] and angles [°] for **12**.

O(1)-C(1)	1.379(4)
O(1)-C(5)	1.398(4)
O(2)-C(7)	1.357(4)
O(2)-C(2)	1.411(4)
O(3)-C(1)	1.353(4)
O(3)-C(7)	1.439(4)
O(4)-C(4)	1.398(4)
O(5)-C(17)	1.312(5)
O(5)-C(12)	1.358(5)
O(6)-C(15)	1.351(5)
O(6)-C(18)	1.360(5)
C(5)-C(6)	1.453(4)
C(5)-C(4)	1.484(4)
C(4)-C(3)	1.474(4)
C(4)-C(10)	1.494(4)
C(3)-C(2)	1.474(4)
C(2)-C(1)	1.434(4)
C(7)-C(9)	1.408(7)
C(7)-C(8)	1.505(6)
C(10)-C(11)	1.451(5)
C(11)-C(12)	1.305(5)
C(11)-C(16)	1.367(5)
C(12)-C(13)	1.336(6)
C(13)-C(14)	1.366(6)
C(14)-C(15)	1.269(6)
C(15)-C(16)	1.341(5)

C(1)-O(1)-C(5)	118.2(2)
C(7)-O(2)-C(2)	103.8(2)
C(1)-O(3)-C(7)	108.7(2)
C(17)-O(5)-C(12)	118.0(4)
C(15)-O(6)-C(18)	121.9(4)
O(1)-C(5)-C(6)	111.1(3)
O(1)-C(5)-C(4)	106.2(2)
C(6)-C(5)-C(4)	112.5(3)
O(4)-C(4)-C(3)	108.1(2)
O(4)-C(4)-C(5)	114.2(3)
C(3)-C(4)-C(5)	105.3(2)
O(4)-C(4)-C(10)	104.7(2)
C(3)-C(4)-C(10)	116.8(3)
C(5)-C(4)-C(10)	108.0(3)

C(4)-C(3)-C(2)	118.2(2)
O(2)-C(2)-C(1)	105.5(2)
O(2)-C(2)-C(3)	108.9(3)
C(1)-C(2)-C(3)	112.5(3)
O(3)-C(1)-O(1)	112.9(3)
O(3)-C(1)-C(2)	99.1(3)
O(1)-C(1)-C(2)	108.9(3)
O(2)-C(7)-C(9)	104.2(3)
O(2)-C(7)-O(3)	106.0(3)
C(9)-C(7)-O(3)	111.9(4)
O(2)-C(7)-C(8)	112.6(3)
C(9)-C(7)-C(8)	113.5(4)
O(3)-C(7)-C(8)	108.4(4)
C(11)-C(10)-C(4)	111.5(3)
C(12)-C(11)-C(16)	117.9(4)
C(12)-C(11)-C(10)	118.0(4)
C(16)-C(11)-C(10)	124.1(3)
C(11)-C(12)-C(13)	115.5(4)
C(11)-C(12)-O(5)	115.3(4)
C(13)-C(12)-O(5)	129.2(4)
C(12)-C(13)-C(14)	125.3(4)
C(15)-C(14)-C(13)	120.0(4)
C(14)-C(15)-C(16)	115.0(4)
C(14)-C(15)-O(6)	124.9(4)
C(16)-C(15)-O(6)	120.1(4)
C(15)-C(16)-C(11)	126.3(4)

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 12. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	41(1)	57(1)	57(1)	-5(1)	-1(1)	-5(1)
O(2)	53(1)	45(1)	72(1)	-2(1)	-24(1)	-1(1)
O(3)	57(1)	56(1)	66(1)	-4(1)	-23(1)	-3(1)
O(4)	51(1)	55(1)	59(1)	-14(1)	-1(1)	6(1)
O(5)	53(1)	103(2)	87(2)	-9(2)	-9(1)	15(2)
O(6)	77(2)	72(2)	82(2)	-13(2)	-30(2)	1(1)
C(5)	45(1)	48(2)	53(2)	-3(1)	1(1)	-6(1)
C(4)	46(1)	44(1)	51(2)	-5(1)	1(1)	-2(1)

C(3)	41(1)	47(1)	57(2)	2(1)	-2(1)	-1(1)
C(2)	44(1)	48(2)	53(2)	1(1)	-4(1)	-3(1)
C(1)	53(2)	50(2)	49(2)	-5(1)	-4(1)	-2(1)
C(7)	62(2)	55(2)	90(2)	-5(2)	-38(2)	4(2)
C(6)	62(2)	76(2)	65(2)	4(2)	5(2)	-20(2)
C(8)	106(3)	79(3)	117(4)	33(3)	-64(3)	-23(3)
C(9)	58(2)	83(3)	138(4)	-28(3)	-30(3)	15(2)
C(10)	57(2)	50(2)	59(2)	3(2)	-10(2)	-4(1)
C(11)	55(2)	53(2)	58(2)	13(1)	-14(2)	0(1)
C(12)	53(2)	69(2)	68(2)	13(2)	-11(2)	7(2)
C(13)	49(2)	84(2)	86(2)	16(2)	-20(2)	-3(2)
C(14)	64(2)	66(2)	85(2)	10(2)	-29(2)	-8(2)
C(15)	63(2)	54(2)	62(2)	5(2)	-18(2)	2(2)
C(16)	60(2)	59(2)	57(2)	8(2)	-16(2)	-3(2)
C(17)	57(2)	144(5)	123(4)	-11(4)	7(3)	21(3)
C(18)	97(3)	77(3)	116(4)	-32(3)	-60(3)	15(2)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **12**.

	x	y	z	U(eq)
H(4)	794	-1384	2750	82
H(5)	287	1476	3428	59
H(3A)	-1431	-1065	3318	58
H(3B)	-1540	171	3711	58
H(2)	-828	-858	4917	58
H(1)	534	649	5005	61
H(6A)	1216	1769	1993	101
H(6B)	2244	766	2146	101

H(6C)	2363	1874	2753	101
H(8A)	1953	-2603	6113	151
H(8B)	1077	-3385	5457	151
H(8C)	391	-2371	5993	151
H(9A)	3433	-2187	4735	139
H(9B)	2782	-1656	3831	139
H(9C)	2499	-2930	4087	139
H(10A)	-1357	1181	2182	66
H(10B)	-204	807	1484	66
H(13)	-4705	-1155	1640	88
H(14)	-4059	-2308	453	86
H(16)	-544	-912	559	70
H(17A)	-4646	1019	3328	162
H(17B)	-4834	-267	3068	162
H(17C)	-5173	679	2328	162
H(18A)	-2108	-3345	-1398	145
H(18B)	-3360	-2597	-1108	145
H(18C)	-2941	-3644	-492	145

Table S6. Torsion angles [°] for **12**.

C(1)-O(1)-C(5)-C(6)	168.4(3)
C(1)-O(1)-C(5)-C(4)	-69.0(3)
O(1)-C(5)-C(4)-O(4)	-61.3(3)
C(6)-C(5)-C(4)-O(4)	60.4(4)
O(1)-C(5)-C(4)-C(3)	57.1(3)
C(6)-C(5)-C(4)-C(3)	178.8(3)
O(1)-C(5)-C(4)-C(10)	-177.3(2)
C(6)-C(5)-C(4)-C(10)	-55.6(4)
O(4)-C(4)-C(3)-C(2)	72.4(3)
C(5)-C(4)-C(3)-C(2)	-50.1(4)

C(10)-C(4)-C(3)-C(2)	-170.0(3)
C(7)-O(2)-C(2)-C(1)	35.0(3)
C(7)-O(2)-C(2)-C(3)	156.0(3)
C(4)-C(3)-C(2)-O(2)	-73.4(3)
C(4)-C(3)-C(2)-C(1)	43.2(4)
C(7)-O(3)-C(1)-O(1)	-83.2(3)
C(7)-O(3)-C(1)-C(2)	31.8(3)
C(5)-O(1)-C(1)-O(3)	168.4(2)
C(5)-O(1)-C(1)-C(2)	59.4(3)
O(2)-C(2)-C(1)-O(3)	-41.1(3)
C(3)-C(2)-C(1)-O(3)	-159.7(3)
O(2)-C(2)-C(1)-O(1)	77.0(3)
C(3)-C(2)-C(1)-O(1)	-41.6(4)
C(2)-O(2)-C(7)-C(9)	-132.7(3)
C(2)-O(2)-C(7)-O(3)	-14.5(4)
C(2)-O(2)-C(7)-C(8)	103.9(4)
C(1)-O(3)-C(7)-O(2)	-11.9(4)
C(1)-O(3)-C(7)-C(9)	101.1(4)
C(1)-O(3)-C(7)-C(8)	-133.1(3)
O(4)-C(4)-C(10)-C(11)	57.8(4)
C(3)-C(4)-C(10)-C(11)	-61.6(4)
C(5)-C(4)-C(10)-C(11)	179.9(3)
C(4)-C(10)-C(11)-C(12)	91.2(4)
C(4)-C(10)-C(11)-C(16)	-89.4(4)
C(16)-C(11)-C(12)-C(13)	2.3(5)
C(10)-C(11)-C(12)-C(13)	-178.3(3)
C(16)-C(11)-C(12)-O(5)	-177.4(3)
C(10)-C(11)-C(12)-O(5)	2.0(5)
C(17)-O(5)-C(12)-C(11)	175.9(5)
C(17)-O(5)-C(12)-C(13)	-3.7(7)
C(11)-C(12)-C(13)-C(14)	-1.6(6)

O(5)-C(12)-C(13)-C(14)	178.0(4)
C(12)-C(13)-C(14)-C(15)	-0.6(6)
C(13)-C(14)-C(15)-C(16)	1.9(5)
C(13)-C(14)-C(15)-O(6)	-178.8(3)
C(18)-O(6)-C(15)-C(14)	8.5(5)
C(18)-O(6)-C(15)-C(16)	-172.2(4)
C(14)-C(15)-C(16)-C(11)	-1.2(5)
O(6)-C(15)-C(16)-C(11)	179.5(3)
C(12)-C(11)-C(16)-C(15)	-1.1(5)
C(10)-C(11)-C(16)-C(15)	179.5(3)

Fig. S2. ORTEP drawing of **22**.

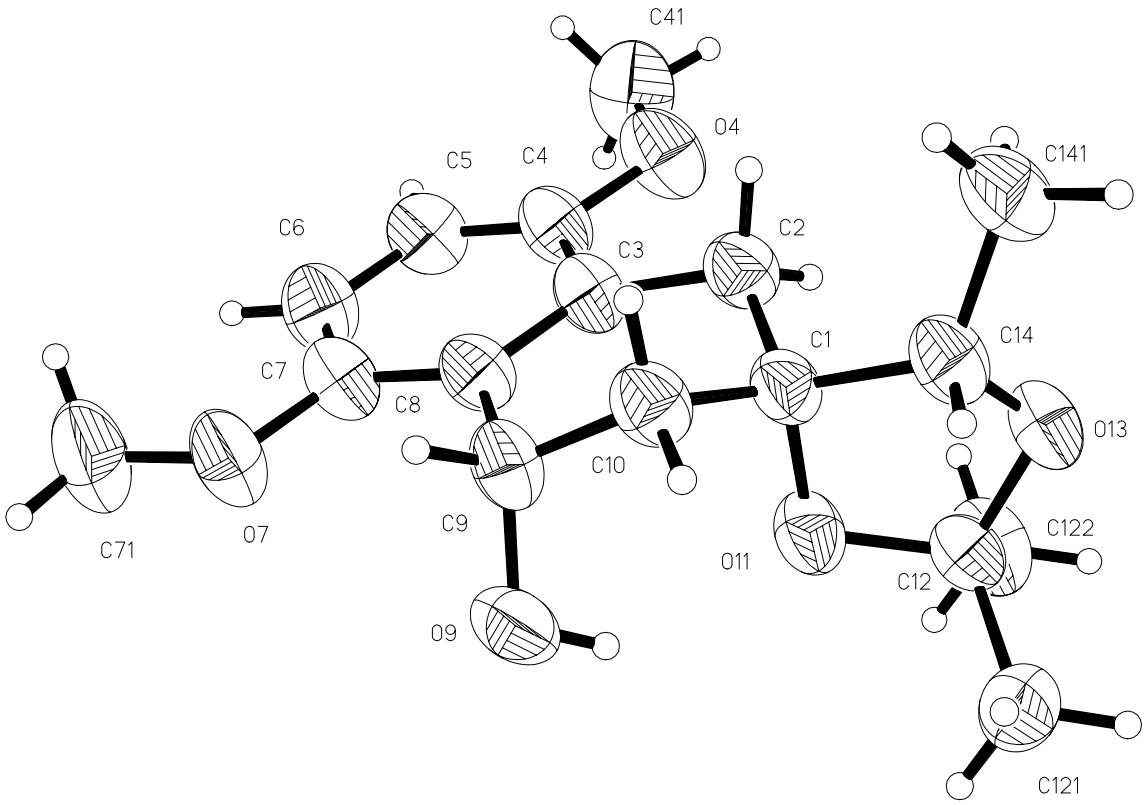

Table S7. Crystal Data and Details of the Structure Determination for **22**.

Crystal Data	
Empirical Formula	$C_{17}H_{24}O5$
Formula Weight	308.36
Crystal System	Monoclinic
Space group	P21 (No. 4)
a, b, c [Å]	9.119(2) 8.115(2) 11.043(2)
alpha, beta, gamma [deg]	90 91.48(3) 90
V [$Å^3$]	816.9(3)
Z	2
D(obs), D(calc) [g/cm^3]	0.000, 1.254
F(000)	332
Mu(CuKa) [/mm]	0.8
Crystal Size [mm]	0.00 x 0.00 x 0.00
Data Collection	
Temperature (K)	293
Radiation [Å]	CuKa 1.54178
Theta Min-Max [Deg]	4.0, 74.9
Scan,(Type & Range) [Deg]	0.00 + 0.14 Tan(Theta)
Dataset	-11: 11 ; -9: 10 ; 0: 13
Tot., Uniq. Data, R(int)	6656, 3328, 0.173
Observed data [I > 2.0 sigma(I)]	3128
Refinement	
Nref, Npar	3328, 199
R, wR, S	0.0667, 0.0618, 1.02
w = 1/[^2^(FO^2^)+(0.0140P)^2^+0.0024P] WHERE P=(FO^2^+2FC^2^)/3'	
Max. and Av. Shift/Error	4.50, 0.02
Min. and Max. resd. dens. [$e/Å^3$]	-0.18, 0.34

Table S8. Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for **22**.

Atom	x	y	z	U(eq) [Ang^2]
O4	0.72085(7)	0.29624(19)	0.50688(6)	0.0685(3)
O7	1.22825(7)	0.2508(2)	0.78530(7)	0.0746(3)
O9	1.09781(7)	0.5815(2)	0.86290(7)	0.0690(3)
O11	0.83171(6)	0.71274(18)	0.78452(5)	0.0550(2)
O13	0.59071(6)	0.77628(18)	0.80461(5)	0.0577(2)
C1	0.75887(9)	0.56680	0.83077(7)	0.0499(3)
C2	0.72527(9)	0.44762(19)	0.72647(8)	0.0513(3)
C3	0.86046(9)	0.36422(19)	0.68064(7)	0.0489(3)
C4	0.85242(9)	0.2830(2)	0.56881(8)	0.0561(3)
C5	0.96938(11)	0.1928(2)	0.52712(8)	0.0628(4)
C6	1.09721(11)	0.1806(2)	0.59801(9)	0.0644(4)
C7	1.10749(9)	0.2592(2)	0.70756(8)	0.0571(3)
C8	0.98959(9)	0.3525(2)	0.75002(7)	0.0522(3)
C9	1.00635(9)	0.4397(2)	0.87165(8)	0.0562(3)
C10	0.85944(9)	0.4826(2)	0.92331(7)	0.0530(3)
C12	0.72613(8)	0.8430(2)	0.76590(8)	0.0527(3)
C14	0.62299(9)	0.6459(2)	0.88556(7)	0.0555(3)
C41	0.70721(15)	0.2144(3)	0.39305(9)	0.0858(6)
C71	1.34428(13)	0.1462(3)	0.75147(14)	0.0894(5)
C121	0.77605(12)	0.9883(2)	0.84233(10)	0.0653(4)
C122	0.70816(12)	0.8857(3)	0.63413(9)	0.0738(4)
C141	0.48826(12)	0.5459(3)	0.89980(11)	0.0746(4)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S9. Hydrogen Atom Positions and Isotropic Displacement Parameters for **22**

Atom	x	y	z	U(iso) [Ang^2]
H2A	0.67850	0.50700	0.66090	0.0770
H2B	0.65760	0.36550	0.75330	0.0770
H5A	0.96270	0.13830	0.45000	0.0940
H6A	1.17890	0.11780	0.57010	0.0970
H9	1.04650	0.66240	0.83730	0.1040
H9A	1.05400	0.36480	0.92730	0.0840
H10A	0.81340	0.38360	0.95090	0.0800
H10B	0.87390	0.55410	0.99180	0.0800
H12A	0.78420	0.95650	0.92600	0.0980
H12B	0.87010	1.02390	0.81520	0.0980
H12C	0.70690	1.07700	0.83350	0.0980
H12D	0.67500	0.79000	0.59020	0.1110

H12E	0.63820	0.97310	0.62290	0.1110
H12F	0.80140	0.92000	0.60460	0.1110
H14A	0.65020	0.69100	0.96330	0.0830
H14B	0.41420	0.61230	0.93610	0.1120
H14C	0.45410	0.50960	0.82130	0.1120
H14D	0.50880	0.45180	0.95020	0.1120
H41A	0.61110	0.23290	0.35810	0.1290
H41B	0.77980	0.25520	0.33920	0.1290
H41C	0.72170	0.09840	0.40570	0.1290
H71A	1.42090	0.14990	0.81270	0.1340
H71B	1.31070	0.03480	0.74160	0.1340
H71C	1.38140	0.18550	0.67620	0.1340

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S10. (An)isotropic Displacement Parameters for **22**.

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
O4	0.0603(4)	0.0919(8)	0.0525(3)	-0.0115(4)	-0.0141(3)	0.0033(4)
O7	0.0495(3)	0.0988(8)	0.0751(4)	-0.0140(5)	-0.0074(3)	0.0171(4)
O9	0.0504(3)	0.0812(7)	0.0751(4)	-0.0124(4)	-0.0065(3)	-0.0072(3)
O11	0.0477(3)	0.0588(5)	0.0590(3)	0.0054(3)	0.0095(2)	0.0053(3)
O13	0.0407(3)	0.0735(6)	0.0592(3)	0.0056(3)	0.0069(2)	0.0020(3)
C1	0.0454(4)	0.0562(7)	0.0482(4)	-0.0017(4)	0.0050(3)	-0.0017(4)
C2	0.0483(4)	0.0526(6)	0.0530(4)	-0.0049(4)	-0.0015(3)	0.0014(4)
C3	0.0440(4)	0.0563(6)	0.0463(4)	0.0014(4)	0.0019(3)	-0.0012(3)
C4	0.0535(4)	0.0677(8)	0.0470(4)	0.0023(4)	-0.0031(3)	-0.0009(4)
C5	0.0627(5)	0.0751(9)	0.0509(4)	-0.0041(5)	0.0062(3)	-0.0011(5)
C6	0.0567(5)	0.0792(10)	0.0578(4)	-0.0045(5)	0.0111(3)	0.0075(5)
C7	0.0441(4)	0.0670(7)	0.0603(4)	-0.0028(5)	0.0049(3)	0.0010(4)
C8	0.0500(4)	0.0615(8)	0.0449(4)	0.0013(4)	-0.0011(3)	0.0023(4)
C9	0.0487(4)	0.0697(8)	0.0498(4)	0.0034(4)	-0.0064(3)	0.0041(4)
C10	0.0523(4)	0.0607(7)	0.0461(4)	-0.0022(4)	0.0007(3)	0.0019(4)
C12	0.0431(4)	0.0617(7)	0.0537(4)	0.0047(4)	0.0076(3)	0.0009(4)
C14	0.0436(4)	0.0739(8)	0.0494(4)	-0.0041(4)	0.0104(3)	0.0023(4)
C41	0.1035(8)	0.1016(14)	0.0512(4)	-0.0155(7)	-0.0193(5)	0.0218(8)
C71	0.0596(6)	0.1044(13)	0.1039(8)	-0.0147(9)	-0.0011(5)	0.0278(7)
C121	0.0655(5)	0.0584(8)	0.0719(5)	-0.0064(5)	0.0013(4)	0.0094(5)
C122	0.0746(6)	0.0930(11)	0.0540(5)	0.0113(6)	0.0068(4)	0.0065(6)
C141	0.0565(5)	0.0863(11)	0.0818(6)	0.0064(7)	0.0197(4)	-0.0083(5)

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S11. Bond Distances (Å) for **22**.

O4	-C4	1.3698(11)	C14	-C141	1.484(2)
O4	-C41	1.4243(17)	C2	-H2A	0.9604
O7	-C7	1.3804(12)	C2	-H2B	0.9603
O7	-C71	1.414(2)	C5	-H5A	0.9602
O9	-C9	1.426(2)	C6	-H6A	0.9599
O11	-C1	1.4568(14)	C9	-H9A	0.9603
O11	-C12	1.4410(18)	C10	-H10A	0.9598
O13	-C12	1.4241(12)	C10	-H10B	0.9597
O13	-C14	1.4112(18)	C14	-H14A	0.9600
O9	-H9	0.8503	C41	-H41A	0.9603
C1	-C10	1.5178(13)	C41	-H41B	0.9601
C1	-C14	1.5337(13)	C41	-H41C	0.9603
C1	-C2	1.5289(14)	C71	-H71A	0.9601
C2	-C3	1.5054(15)	C71	-H71B	0.9598
C3	-C4	1.4001(15)	C71	-H71C	0.9601
C3	-C8	1.3914(12)	C121	-H12A	0.9604
C4	-C5	1.3823(17)	C121	-H12B	0.9602
C5	-C6	1.3908(14)	C121	-H12C	0.9602
C6	-C7	1.3687(16)	C122	-H12D	0.9604
C7	-C8	1.4054(16)	C122	-H12E	0.9599
C8	-C9	1.5224(15)	C122	-H12F	0.9597
C9	-C10	1.5102(13)	C141	-H14B	0.9598
C12	-C122	1.5007(15)	C141	-H14C	0.9599
C12	-C121	1.513(2)	C141	-H14D	0.9605

Table S12. Bond Angles (Degrees) for **22**.

C4 -O4 -C41	117.35(11)	O9 -C9 -C8	111.16(9)
C7 -O7 -C71	117.11(11)	C1 -C10 -C9	112.08(8)
C1 -O11 -C12	109.72(7)	O11 -C12 -O13	105.05(12)
C12 -O13 -C14	107.87(8)	O11 -C12 -C121	107.56(8)

C9 -O9 -H9	109.14	O13 -C12 -C121	112.30(9)
O11 -C1 -C10	109.21(8)	O13 -C12 -C122	107.76(8)
O11 -C1 -C14	100.28(8)	C121-C12 -C122	112.62(14)
O11 -C1 -C2	109.54(8)	O11 -C12 -C122	111.32(10)
C2 -C1 -C14	114.44(8)	O13 -C14 -C141	108.50(10)
C10 -C1 -C14	113.77(7)	C1 -C14 -C141	119.50(13)
C2 -C1 -C10	109.16(8)	O13 -C14 -C1	102.79(7)
C1 -C2 -C3	112.81(8)	C1 -C2 -H2A	109.09
C2 -C3 -C4	118.91(8)	C1 -C2 -H2B	108.93
C2 -C3 -C8	122.30(9)	C3 -C2 -H2A	108.88
C4 -C3 -C8	118.54(10)	C3 -C2 -H2B	109.27
O4 -C4 -C3	115.38(10)	H2A -C2 -H2B	107.72
O4 -C4 -C5	123.28(10)	C4 -C5 -H5A	120.50
C3 -C4 -C5	121.32(9)	C6 -C5 -H5A	119.97
C4 -C5 -C6	119.53(10)	C5 -C6 -H6A	120.21
C5 -C6 -C7	120.11(11)	C7 -C6 -H6A	119.68
O7 -C7 -C6	124.20(11)	O9 -C9 -H9A	107.36
C6 -C7 -C8	120.69(9)	C8 -C9 -H9A	107.69
O7 -C7 -C8	115.09(10)	C10 -C9 -H9A	107.18
C3 -C8 -C7	119.80(10)	C1 -C10 -H10A	109.20
C7 -C8 -C9	118.98(8)	C1 -C10 -H10B	109.07
C3 -C8 -C9	121.22(10)	C9 -C10 -H10A	109.06
O9 -C9 -C10	111.45(13)	C9 -C10 -H10B	109.38
C8 -C9 -C10	111.75(8)	H10A -C10 -H10B	107.95
O13 -C14 -H14A	109.00	C12 -C121-H12C	109.89
C1 -C14 -H14A	108.64	H12A-C121-H12B	109.48
C141-C14 -H14A	108.02	H12A-C121-H12C	109.48
O4 -C41 -H41A	109.87	H12B-C121-H12C	109.41
O4 -C41 -H41B	109.87	C12 -C122 -H12D	109.16
O4 -C41 H41C	108.67	C12 -C122-H12E	110.58
H41A-C41 -H41B	109.50	C12 -C122-H12F	108.72
H41A-C41 -H41C	109.42	H12D-C122-H12E	109.43
H41B-C41 -H41C	109.49	H12D-C122-H12F	109.45
O7 -C71 -H71A	109.33	H12E-C122-H12F	109.48
O7 -C71 -H71B	110.89	C14 -C141-H14B	109.31
O7 -C71 -H71C	108.19	C14 -C141-H14C	108.80
H71A-C71 -H71B	109.49	C14 -C141-H14D	110.27
H71A -C71 -H71C	109.44	H14B-C141-H14C	109.52
H71B-C71 -H71C	109.46	H14B-C141-H14D	109.46
C12 -C121-H12A	109.99	H14C-C141-H14D	109.46
C12 -C121-H12B	108.58		

Table S13. Torsion Angles (Degrees) for **22**

.

C41	-O4	-C4	-C3	-179.49(15)
C41	-O4	-C4	-C5	-1.1(2)
C71	-O7	-C7	-C8	174.40(15)
C71	-O7	-C7	-C6	-3.8(2)
C12	-O11	-C1	-C2	98.00(9)
C1	-O11	-C12	-C122	-114.64(11)
C1	-O11	-C12	-O13	1.72(10)
C1	-O11	-C12	-C121	121.54(9)
C12	-O11	-C1	-C10	-142.49(8)
C12	-O11	-C1	-C14	-22.69(9)
C14	-O13	-C12	-O11	22.73(11)
C12	-O13	-C14	-C141	-164.31(11)
C14	-O13	-C12	-C122	141.51(13)
C14	-O13	-C12	-C121	-93.88(13)
C12	-O13	-C14	-C1	-36.83(12)
C14	-C1	-C10	-C9	-167.38(11)
C10	-C1	-C14	-C141	-87.95(11)
C2	-C1	-C10	-C9	63.45(13)
C14	-C1	-C2	-C3	-176.22(10)
O11	-C1	-C14	-C141	155.62(9)
O11	-C1	-C10	-C9	-56.29(13)
O11	-C1	-C14	-O13	35.47(9)
C2	-C1	-C14	-C141	38.50(12)
C10	-C1	-C14	-O13	151.90(9)
C10	-C1	-C2	-C3	-47.42(12)
C2	-C1	-C14	-O13	-81.65(11)
O11	-C1	-C2	-C3	72.11(11)
C1	-C2	-C3	-C8	20.66(18)
C1	-C2	-C3	-C4	-165.09(12)
C2	-C3	-C8	-C9	-6.6(2)
C8	-C3	-C4	-C5	0.0(2)
C8	-C3	-C4	-O4	178.35(13)
C2	-C3	-C8	-C7	173.66(13)
C4	-C3	-C8	-C7	-0.6(2)
C4	-C3	-C8	-C9	179.16(13)
C2	-C3	-C4	-C5	-174.50(13)
C2	-C3	-C4	-O4	3.9(2)
C3	-C4	-C5	-C6	0.7(2)
O4	-C4	-C5	-C6	-177.50(14)
C4	-C5	-C6	-C7	-0.8(2)
C5	-C6	-C7	-O7	178.30(14)
C5	-C6	-C7	-C8	0.2(2)
O7	-C7	-C8	-C3	-177.75(13)
C6	-C7	-C8	-C3	0.5(2)

C6	-C7	-C8	-C9	-179.24(13)
O7	-C7	-C8	-C9	2.5(2)
C3	-C8	-C9	-O9	-105.16(13)
C3	-C8	-C9	-C10	20.05(19)
C7	-C8	-C9	-C10	-160.18(13)
C7	-C8	-C9	-O9	74.61(16)
O9	-C9	-C10	-C1	76.45(11)
C8	-C9	-C10	-C1	-48.60(16)

Table S14. Contact Distances(Å) for **22**.

O7	.O9	3.067(2)	C12	.H2A	2.9903
O9	.O7	3.067(2)	C14	.H12A	2.9461
O9	.O11	2.7682(13)	C122	.C6_a	3.567(2)
O11	.C8	3.285(2)	C122	.C4_f	3.563(3)
O11	.O9	2.7682(13)	C41	.H71B_a	2.9976
O4	.H2B	2.8521	C41	.H5A	2.4757
O4	.H2A	2.4497	C71	.H6A	2.4866
O4	.H6A_a	2.8996	C121	.H14A	3.0002
O7	.H9A	2.4430	C122	.H2A	3.0998
O9	.H41B_a	2.8883	C122	.H41C_f	3.0617
O9	.H12A_b	2.7371	C141	.H2B	2.6970
O11	.H9	2.0698	H2A	.O4	2.4497
O13	.H2A	2.8285	H2A	.O13	2.8285
O13	.H41A_c	2.5629	H2A	.C12	2.9903
C4	.C122_d	3.563(3)	H2A	.C122	3.0998
C6	.C122_e	3.567(2)	H2A	.H12D	2.4256
C8	.O11	3.285(2)	H2B	.O4	2.8521
C1	.H9	2.7344	H2B	.C141	2.6970
C2	.H14C	2.7565	H2B	.H10A	2.5771
C3	.H10A	3.0302	H2B	.H12C_d	2.5391
C4	.H12F_d	3.0099	H2B	.H14C	2.3339
C5	.H41B	2.7141	H5A	.C41	2.4757
C5	.H12F_d	2.8367	H5A	.H41B	2.2524
C5	.H41C	2.7073	H5A	.H41C	2.2624
C6	.H71C	2.7106	H6A	.C71	2.4866
C6	.H71B	2.7468	H6A	.H71B	2.3168
C8	.H12B_d	2.9760	H6A	.H71C	2.2300
C9	.H12A_b	2.9051	H6A	.O4_e	2.8996
H9	.O11	2.0698	H12F	.H12B	2.5371
H9	.C1	2.7344	H14A	.C121	3.0002
H9	.H10B	2.5098	H14A	.H10B	2.3370
H9A	.O7	2.4430	H14A	.H12A	2.5161
H9A	.H12A_b	2.2873	H14A	.H71A_g	2.5949

H10A	.C3	3.0302	H14C	.C2	2.7565
H10A	.H2B	2.5771	H14C	.H2B	2.3339
H10B	.H9	2.5098	H41A	.O13_h	2.5629
H10B	.H14A	2.3370	H41B	.C5	2.7141
H12A	.C14	2.9461	H41B	.H5A	2.2524
H12A	.H14A	2.5161	H41B	.O9_e	2.8883
H12A	.O9_g	2.7371	H41B	.H71B_a	2.5666
H12A	.C9_g	2.9051	H41C	.C5	2.7073
H12A	.H9A_g	2.2873	H41C	.C122_d	3.0617
H12B	.C8_f	2.9760	H41C	.H5A	2.2624
H12B	.H12F	2.5371	H71A	.H14A_b	2.5949
H12C	.H2B_f	2.5391	H71B	.C6	2.7468
H12C	.H12E	2.5371	H71B	.H6A	2.3168
H12D	.H2A	2.4256	H71B	.C41_e	2.9976
H12E	.H12C	2.5371	H71B	.H41B_e	2.5666
H12F	.C4_f	3.0099	H71C	.C6	2.7106
H12F	.C5_f	2.8367	H71C	.H6A	2.2300

Table S15. Hydrogen Bonds (Å, Deg) for **22**.

O9 -- H9 .. O11	0.8503	2.0698	2.7682(13)	138.99	.	yes
C41 -- H41A .. O13	0.9603	2.5629	3.4772(16)	159.17	2_646	yes

Translation of Symmetry Code to Equiv.Pos

a =[2756.00] = 2-x,1/2+y,1-z

b =[2747.00] = 2-x,-1/2+y,2-z

c =[2656.00] = 1-x,1/2+y,1-z

d =[1545.00] = x,-1+y,z

e =[2746.00] = 2-x,-1/2+y,1-z

f =[1565.00] = x,1+y,z

g =[2757.00] = 2-x,1/2+y,2-z

h =[2646.00] = 1-x,-1/2+y,1-z