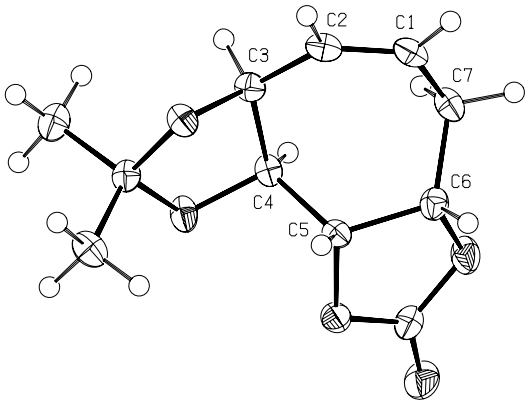
Supporting Information:

X-Ray data for 25a, 28b and 29b

1)- 25a



ORTEP drawing

Molecular formula $C_{11}H_{14}O_5$
Molecular weight 226.22
Crystal habit colorless plate
Crystal dimensions(mm) 0.20x0.20x0.12
Crystal system Orthorhombic
Space group $P2_12_12_1$
a(Å) 5.748(5)
b(Å) 13.271(5)
c(Å) 13.964(5)
V(Å3) 1065.2(11)
Z 4
d(g/cm3) 1.411
F000 480
$\mu(cm^{-1})$ 0.112
Difractometer KappaCCD
X-ray source MoKa
λ(Å) 0.71069
Monochromator graphite
T (K) 150.0(1)
Scan mode phi and omega scans
Maximum θ 27.46
HKL ranges -4 7 ; -17 13 ; -18 13
Reflections measured 4435
Independant reflections 2368
Rint 0.0384
Reflections used 2212
Criterion >2sigma(I)
Refinement type Fsqd
Hydrogen atoms mixed
Parameters refined 147

Reflections / parameter 15
wR2 0.0811
R1 0.0334
Flack's parameter 0.3(8)
Weighs a, b1 0.0356 ; 0.1062
GoF 1.036
difference peak / hole (e Å-3) .230(.039) / -.199(.039)

TABLE 1. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 25a

atom	x	y	z	U(eq)
O(1)	5490(2)	9919(1)	9140(1)	21(1)
O(3)	10320(2)	10017(1)	6909(1)	24(1)
O(5)	13812(2)	9951(1)	6195(1)	33(1)
O(2)	8491(2)	10853(1)	8550(1)	23(1)
C(7)	10610(3)	7741(1)	8338(1)	26(1)
C(10)	4542(2)	11437(1)	8331(1)	27(1)
C(11)	12312(3)	9563(1)	6660(1)	23(1)
C(1)	8307(3)	7535(1)	8813(1)	24(1)
C(2)	6984(2)	8245(1)	9206(1)	22(1)
C(4)	9238(2)	9827(1)	8573(1)	18(1)
O(4)	12422(2)	8621(1)	7001(1)	28(1)
C(8)	6228(2)	10929(1)	8999(1)	20(1)
C(9)	6503(3)	11483(1)	9940(1)	31(1)
C(5)	9030(2)	9379(1)	7569(1)	19(1)
C(3)	7580(2)	9341(1)	9299(1)	20(1)
C(6)	10208(2)	8350(1)	7434(1)	22(1)

U(eq) is defined as 1/3 the trace of the Uij tensor.

TABLE 2. Bond lengths (A) and angles (deg) for 25a

O(1)-C(8)	1.420(2)	O(1)-C(3)	1.442(2)
O(3)-C(11)	1.340(2)	O(3)-C(5)	1.455(2)
O(5)-C(11)	1.196(2)	O(2)-C(4)	1.428(2)
O(2)-C(8)	1.448(2)	C(7)-C(1)	1.506(2)
C(7)-C(6)	1.516(2)	C(10)-C(8)	1.505(2)
C(11)-O(4)	1.340(2)	C(1)-C(2)	1.329(2)
C(2)-C(3)	1.501(2)	C(4)-C(5)	1.527(2)
C(4)-C(3)	1.534(2)	O(4)-C(6)	1.455(2)
C(8)-C(9)	1.514(2)	C(5)-C(6)	1.536(2)

C(8)-O(1)-C(3)	105.9(1)	C(11)-O(3)-C(5)	109.8(1)
C(4)-O(2)-C(8)	109.1(1)	C(1)-C(7)-C(6)	109.2(1)

O(5)-C(11)-O(3)	124.4(1)	O(5)-C(11)-O(4)	124.1(1)
O(3)-C(11)-O(4)	111.6(1)	C(2)-C(1)-C(7)	123.8(1)
C(1)-C(2)-C(3)	126.3(1)	O(2)-C(4)-C(5)	109.1(1)
O(2)-C(4)-C(3)	103.2(1)	C(5)-C(4)-C(3)	113.2(1)
C(11)-O(4)-C(6)	109.7(1)	O(1)-C(8)-O(2)	105.2(1)
O(1)-C(8)-C(10)	108.5(1)	O(2)-C(8)-C(10)	109.9(1)
O(1)-C(8)-C(9)	111.7(1)	O(2)-C(8)-C(9)	108.4(1)
C(10)-C(8)-C(9)	112.8(1)	O(3)-C(5)-C(4)	108.3(1)
O(3)-C(5)-C(6)	102.4(1)	C(4)-C(5)-C(6)	115.1(1)
O(1)-C(3)-C(2)	108.2(1)	O(1)-C(3)-C(4)	101.1(1)
C(2)-C(3)-C(4)	119.5(1)	O(4)-C(6)-C(7)	110.2(1)
O(4)-C(6)-C(5)	102.5(1)	C(7)-C(6)-C(5)	116.1(1)

TABLE 3. Anisotropic displacement parameters (A^2 x 10^3) for 25a

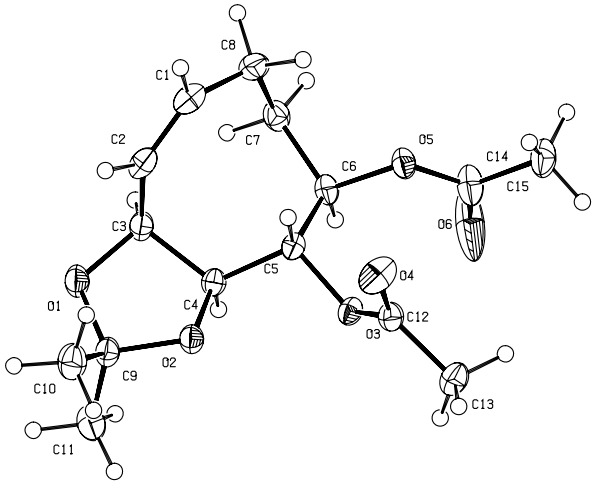
atom	U11	U22	U33	U23	U13	U12
O(1)	14(1)	21(1)	30(1)	3(1)	2(1)	-1(1)
O(3)	24(1)	22(1)	26(1)	4(1)	8(1)	2(1)
O(5)	30(1)	32(1)	37(1)	0(1)	14(1)	-3(1)
O(2)	18(1)	17(1)	35(1)	-1(1)	9(1)	-2(1)
C(7)	27(1)	19(1)	32(1)	2(1)	-1(1)	4(1)
C(10)	21(1)	22(1)	37(1)	4(1)	-2(1)	-4(1)
C(11)	23(1)	24(1)	23(1)	-5(1)	4(1)	-1(1)
C(1)	27(1)	19(1)	25(1)	6(1)	-7(1)	-2(1)
C(2)	19(1)	25(1)	23(1)	5(1)	-3(1)	-5(1)
C(4)	14(1)	17(1)	25(1)	-1(1)	-1(1)	-1(1)
O(4)	24(1)	24(1)	38(1)	0(1)	11(1)	4(1)
C(8)	15(1)	20(1)	24(1)	-2(1)	4(1)	-3(1)
C(9)	33(1)	30(1)	28(1)	-6(1)	3(1)	1(1)
C(5)	15(1)	18(1)	22(1)	3(1)	1(1)	-1(1)
C(3)	15(1)	23(1)	22(1)	3(1)	-1(1)	1(1)
C(6)	20(1)	21(1)	25(1)	-2(1)	4(1)	-1(1)

The anisotropic displacement factor exponent takes the form
  2 pi^2 [h^2a*^2U(11) +...+ 2hka*b*U(12)]

TABLE 4. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 25a

atom	x	y	z	U(eq)
H(7A)	11385	7097	8176	31
H(7B)	11634	8120	8780	31
H(10A)	2974	11410	8605	40
H(10B)	4552	11090	7711	40
H(10C)	5001	12142	8241	40
H(1)	7768	6858	8833	29
H(2)	5518	8038	9451	27
H(4)	10881	9782	8805	22
H(9A)	7607	11120	10348	46
H(9B)	4992	11524	10263	46
H(9C)	7088	12165	9817	46
H(5)	7359	9341	7374	22
H(3)	8165	9474	9962	24
H(6)	9283	7939	6970	26

Compound 28b



ORTEP drawing

Molecular formula	$C_{15}H_{22}O_6$
Molecular weight	298.33
Crystal habit	colorless cube
Crystal dimensions(mm)	0.20x0.20x0.20
Crystal system	orthorhombic
Space group ?	$P2_12_12_1$
a(Å)	7.516(5)
b(Å)	10.884(5)
c(Å)	19.063(5)
V(Å^3)	1559.4(13)
Z	4
d(g-cm^{-3})	1.271
F000	640
μ(cm^{-1})	0.098
Difractometer	KappaCCD
X-ray source	MoKα
λ(Å)	0.71069
Monochromator	graphite
T (K)	150.0(1)
Scan mode	? phi and omega scans
Maximum θ	27.48
HKL ranges	-7 9 ; -14 11 ; -19 24
Reflections measured	6844
Independant reflections	3529
Rint	0.0381
Reflections used	3100
Criterion	>2sigma(I)
Refinement type	Fsqd
Hydrogen atoms	mixed
Parameters refined	194
Reflections / parameter	15
wR2	0.1151
R1	0.0455

Flack's parameter 0.1(10)
Weighs a, b1 0.0498 ; 0.4693
GoF 1.033
difference peak / hole (e Å^{-3}).614(.042) / -.486(.042)

TABLE 1. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 28b

atom	x	y	z	U(eq)
O(1)	823(2)	2186(1)	759(1)	36(1)
O(2)	2456(2)	1720(1)	1731(1)	27(1)
O(3)	1722(2)	1756(1)	3138(1)	25(1)
O(4)	2057(2)	-286(1)	3275(1)	44(1)
O(5)	-1622(2)	1394(1)	3621(1)	29(1)
O(6)	-1159(5)	3050(2)	4282(1)	100(1)
C(1)	-2392(3)	166(2)	1679(1)	36(1)
C(2)	-1146(3)	694(2)	1284(1)	33(1)
C(3)	-392(2)	1979(2)	1326(1)	28(1)
C(4)	797(2)	2215(2)	1965(1)	24(1)
C(5)	295(2)	1565(2)	2639(1)	24(1)
C(6)	-1383(3)	2096(2)	2974(1)	27(1)
C(7)	-3063(3)	1965(2)	2541(1)	32(1)
C(8)	-3468(3)	661(2)	2282(1)	36(1)
C(9)	2616(2)	2015(2)	1002(1)	28(1)
C(10)	3479(3)	950(2)	632(1)	39(1)
C(11)	3625(3)	3204(2)	907(1)	39(1)
C(12)	2436(3)	745(2)	3439(1)	27(1)
C(13)	3712(3)	1089(2)	4002(1)	36(1)
C(14)	-1454(3)	1975(2)	4233(1)	40(1)
C(15)	-1622(4)	1117(2)	4837(1)	42(1)

U(eq) is defined as 1/3 the trace of the Uij tensor.

TABLE 2. Bond lengths (A) and angles (deg) for 28b

O(1)-C(3)	1.434(2)	O(1)-C(9)	1.438(2)
O(2)-C(4)	1.429(2)	O(2)-C(9)	1.431(2)
O(3)-C(12)	1.352(2)	O(3)-C(5)	1.449(2)
O(4)-C(12)	1.199(2)	O(5)-C(14)	1.333(2)
O(5)-C(6)	1.461(2)	O(6)-C(14)	1.194(3)
C(1)-C(2)	1.333(3)	C(1)-C(8)	1.505(3)
C(1)-H(1)	0.9500	C(2)-C(3)	1.511(3)
C(2)-H(2)	0.9500	C(3)-C(4)	1.532(3)
C(3)-H(3)	1.0000	C(4)-C(5)	1.515(2)
C(4)-H(4)	1.0000	C(5)-C(6)	1.528(3)
C(5)-H(5)	1.0000	C(6)-C(7)	1.515(3)
C(6)-H(6)	1.0000	C(7)-C(8)	1.533(3)
C(7)-H(7A)	0.9900	C(7)-H(7B)	0.9900
C(8)-H(8A)	0.9900	C(8)-H(8B)	0.9900

C(9)-C(10)	1.504(3)	C(9)-C(11)	1.510(3)
C(10)-H(10A)	0.9800	C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800	C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800	C(11)-H(11C)	0.9800
C(12)-C(13)	1.487(3)	C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800	C(13)-H(13C)	0.9800
C(14)-C(15)	1.488(3)	C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800	C(15)-H(15C)	0.9800

C(3)-O(1)-C(9)	109.4(1)	C(4)-O(2)-C(9)	106.9(1)
C(12)-O(3)-C(5)	117.1(1)	C(14)-O(5)-C(6)	118.6(2)
C(2)-C(1)-C(8)	130.9(2)	C(2)-C(1)-H(1)	114.5
C(8)-C(1)-H(1)	114.5	C(1)-C(2)-C(3)	129.2(2)
C(1)-C(2)-H(2)	115.4	C(3)-C(2)-H(2)	115.4
O(1)-C(3)-C(2)	110.1(2)	O(1)-C(3)-C(4)	101.7(1)
C(2)-C(3)-C(4)	114.7(2)	O(1)-C(3)-H(3)	110.0
C(2)-C(3)-H(3)	110.0	C(4)-C(3)-H(3)	110.0
O(2)-C(4)-C(5)	107.8(1)	O(2)-C(4)-C(3)	101.4(1)
C(5)-C(4)-C(3)	116.8(2)	O(2)-C(4)-H(4)	110.1
C(5)-C(4)-H(4)	110.1	C(3)-C(4)-H(4)	110.1
O(3)-C(5)-C(4)	107.8(1)	O(3)-C(5)-C(6)	106.4(1)
C(4)-C(5)-C(6)	112.6(2)	O(3)-C(5)-H(5)	110.0
C(4)-C(5)-H(5)	110.0	C(6)-C(5)-H(5)	110.0
O(5)-C(6)-C(7)	107.9(2)	O(5)-C(6)-C(5)	104.8(1)
C(7)-C(6)-C(5)	115.1(2)	O(5)-C(6)-H(6)	109.6
C(7)-C(6)-H(6)	109.6	C(5)-C(6)-H(6)	109.6
C(6)-C(7)-C(8)	115.4(2)	C(6)-C(7)-H(7A)	108.4
C(8)-C(7)-H(7A)	108.4	C(6)-C(7)-H(7B)	108.4
C(8)-C(7)-H(7B)	108.4	H(7A)-C(7)-H(7B)	107.5
C(1)-C(8)-C(7)	118.1(2)	C(1)-C(8)-H(8A)	107.8
C(7)-C(8)-H(8A)	107.8	C(1)-C(8)-H(8B)	107.8
C(7)-C(8)-H(8B)	107.8	H(8A)-C(8)-H(8B)	107.1
O(2)-C(9)-O(1)	105.3(1)	O(2)-C(9)-C(10)	108.6(2)
O(1)-C(9)-C(10)	110.7(2)	O(2)-C(9)-C(11)	110.5(2)
O(1)-C(9)-C(11)	108.7(2)	C(10)-C(9)-C(11)	112.8(2)
C(9)-C(10)-H(10A)	109.5	C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5	C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5	H(10B)-C(10)-H(10C)	109.5
C(9)-C(11)-H(11A)	109.5	C(9)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5	C(9)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5	H(11B)-C(11)-H(11C)	109.5
O(4)-C(12)-O(3)	123.8(2)	O(4)-C(12)-C(13)	125.3(2)

O(3)-C(12)-C(13)	110.9(2)	C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5	H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5	H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5	O(6)-C(14)-O(5)	123.4(2)
O(6)-C(14)-C(15)	124.7(2)	O(5)-C(14)-C(15)	111.8(2)
C(14)-C(15)-H(15A)	109.5	C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5	C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5	H(15B)-C(15)-H(15C)	109.5

TABLE 3. Anisotropic displacement parameters (A^2 x 10^3) for 28b

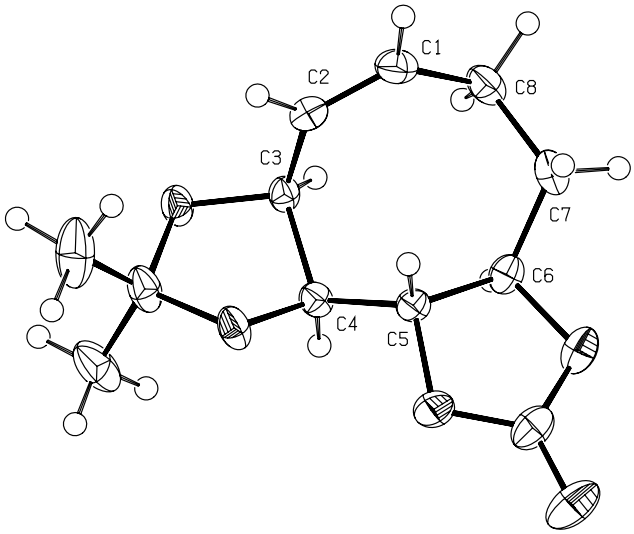
atom	U11	U22	U33	U23	U13	U12
O(1)	29(1)	56(1)	22(1)	5(1)	0(1)	8(1)
O(2)	27(1)	34(1)	22(1)	2(1)	0(1)	5(1)
O(3)	31(1)	21(1)	23(1)	1(1)	-5(1)	-1(1)
O(4)	54(1)	23(1)	54(1)	1(1)	-19(1)	3(1)
O(5)	39(1)	27(1)	21(1)	2(1)	2(1)	-2(1)
O(6)	243(3)	28(1)	31(1)	-3(1)	18(2)	-10(2)
C(1)	35(1)	34(1)	38(1)	-3(1)	-12(1)	0(1)
C(2)	32(1)	38(1)	29(1)	-7(1)	-9(1)	5(1)
C(3)	27(1)	36(1)	21(1)	0(1)	-1(1)	5(1)
C(4)	27(1)	23(1)	23(1)	0(1)	-1(1)	2(1)
C(5)	28(1)	23(1)	21(1)	-1(1)	-4(1)	0(1)
C(6)	34(1)	25(1)	22(1)	3(1)	2(1)	1(1)
C(7)	30(1)	37(1)	28(1)	7(1)	2(1)	7(1)
C(8)	28(1)	44(1)	36(1)	7(1)	-7(1)	-5(1)
C(9)	29(1)	34(1)	21(1)	1(1)	-1(1)	5(1)
C(10)	44(1)	41(1)	30(1)	-5(1)	2(1)	8(1)
C(11)	49(1)	36(1)	31(1)	2(1)	5(1)	-2(1)
C(12)	29(1)	27(1)	24(1)	2(1)	-1(1)	2(1)
C(13)	36(1)	41(1)	31(1)	0(1)	-8(1)	4(1)
C(14)	65(1)	29(1)	25(1)	2(1)	3(1)	3(1)
C(15)	63(1)	40(1)	25(1)	7(1)	-6(1)	-5(1)

The anisotropic displacement factor exponent takes the form
2 pi^2 [h^2a*^2U(11) +...+ 2hka*b*U(12)]

TABLE 4. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 28b

atom	x	y	z	U(eq)
H(1)	-2643	-664	1561	43
H(2)	-663	190	923	39
H(3)	-1376	2596	1311	33
H(4)	914	3118	2049	29
H(5)	134	666	2549	29
H(6)	-1186	2982	3091	32
H(7A)	-2967.9998	2513	2128	38
H(7B)	-4082	2253	2825	38
H(8A)	-3317	94	2684	43
H(8B)	-4738	633	2145	43
H(10A)	4699	849	804	58
H(10B)	3501	1109	126	58
H(10C)	2800	199	725	58
H(11A)	3005	3865	1156	58
H(11B)	3694	3404	407	58
H(11C)	4829	3113	1097	58
H(13A)	3107	1065	4457	54
H(13B)	4160	1921	3916	54
H(13C)	4709	509	4004	54
H(15A)	-687	1295	5181	64
H(15B)	-1497	269	4671	64
H(15C)	-2791	1222	5056	64

Compound 29b



ORTEP drawing

Molecular formula	$C_{12}H_{16}O_5$
Molecular weight	240.25
Crystal habit	colorless plate
Crystal dimensions(mm)	0.24x0.24x0.16
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a(Å)	6.810(5)
b(Å)	11.333(5)
c(Å)	15.396(5)
V(Å3)	1188.2(11)
Z	4
d(g-cm^{-3})	1.343
F000	512
μ(cm^{-1})	0.105
Difractometer	KappaCCD
X-ray source	MoKα
λ(Å)	0.71069
Monochromator	graphite
T (K)	150.0(1)
Scan mode	phi and omega scans
Maximum θ	27.46
HKL ranges	-6 8 ; -14 11 ; -19 17
Reflections measured	5917
Independant reflections	2672
Rint	0.0545
Reflections used	2488
Criterion	>2sigma(I)
Refinement type	Fsqd
Hydrogen atoms	mixed
Parameters refined	156
Reflections / parameter	15

wR2 0.1027
R1 0.0418
Flack's parameter -0.6(10)
Weighs a, b1 0.0466 ; 0.1132
GoF 1.045
difference peak / hole (e Å^{-3}).170(.042) / -.236(.042)
TABLE 1. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 29b

atom	x	y	z	U(eq)
O(1)	3952(2)	166(1)	8458(1)	27(1)
O(2)	5167(2)	1991(1)	8808(1)	28(1)
O(3)	8192(2)	3329(1)	7957(1)	32(1)
O(4)	9503(2)	3092(1)	6650(1)	32(1)
O(5)	10854(2)	4381(1)	7583(1)	48(1)
C(1)	3554(2)	1427(2)	6277(1)	30(1)
C(2)	3310(2)	1201(1)	7115(1)	26(1)
C(3)	4839(2)	656(1)	7695(1)	21(1)
C(4)	6266(2)	1557(1)	8089(1)	22(1)
C(5)	6822(2)	2570(1)	7503(1)	21(1)
C(6)	7981(2)	2192(1)	6695(1)	24(1)
C(7)	6909(3)	2175(1)	5835(1)	28(1)
C(8)	5392(3)	1182(1)	5766(1)	30(1)
C(9)	4129(3)	1005(1)	9162(1)	31(1)
C(10)	2127(3)	1418(2)	9447(1)	54(1)
C(11)	5297(4)	431(2)	9881(1)	46(1)
C(12)	9615(2)	3668(1)	7409(1)	32(1)

U(eq) is defined as 1/3 the trace of the Uij tensor.

TABLE 2. Bond lengths (A) and angles (deg) for 29b

O(1)-C(3)	1.433(2)	O(1)-C(9)	1.447(2)
O(2)-C(4)	1.425(2)	O(2)-C(9)	1.430(2)
O(3)-C(12)	1.341(2)	O(3)-C(5)	1.449(2)
O(4)-C(12)	1.341(2)	O(4)-C(6)	1.456(2)
O(5)-C(12)	1.199(2)	C(1)-C(2)	1.327(2)
C(1)-C(8)	1.503(2)	C(1)-H(1)	0.9500
C(2)-C(3)	1.505(2)	C(2)-H(2)	0.9500
C(3)-C(4)	1.534(2)	C(3)-H(3)	1.0000
C(4)-C(5)	1.508(2)	C(4)-H(4)	1.0000
C(5)-C(6)	1.534(2)	C(5)-H(5)	1.0000
C(6)-C(7)	1.512(2)	C(6)-H(6)	1.0000
C(7)-C(8)	1.532(2)	C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900	C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900	C(9)-C(10)	1.507(3)
C(9)-C(11)	1.510(2)	C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800	C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800	C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800		

C(3)-O(1)-C(9)	108.9(1)	C(4)-O(2)-C(9)	106.6(1)
C(12)-O(3)-C(5)	109.4(1)	C(12)-O(4)-C(6)	109.8(1)
C(2)-C(1)-C(8)	125.2(2)	C(2)-C(1)-H(1)	117.4
C(8)-C(1)-H(1)	117.4	C(1)-C(2)-C(3)	124.8(2)
C(1)-C(2)-H(2)	117.6	C(3)-C(2)-H(2)	117.6
O(1)-C(3)-C(2)	110.7(1)	O(1)-C(3)-C(4)	101.7(1)
C(2)-C(3)-C(4)	113.6(1)	O(1)-C(3)-H(3)	110.2
C(2)-C(3)-H(3)	110.2	C(4)-C(3)-H(3)	110.2
O(2)-C(4)-C(5)	109.5(1)	O(2)-C(4)-C(3)	101.8(1)
C(5)-C(4)-C(3)	115.4(1)	O(2)-C(4)-H(4)	109.9
C(5)-C(4)-H(4)	109.9	C(3)-C(4)-H(4)	109.9
O(3)-C(5)-C(4)	109.0(1)	O(3)-C(5)-C(6)	103.0(1)
C(4)-C(5)-C(6)	113.7(1)	O(3)-C(5)-H(5)	110.3
C(4)-C(5)-H(5)	110.3	C(6)-C(5)-H(5)	110.3
O(4)-C(6)-C(7)	108.1(1)	O(4)-C(6)-C(5)	102.1(1)
C(7)-C(6)-C(5)	117.7(1)	O(4)-C(6)-H(6)	109.5
C(7)-C(6)-H(6)	109.5	C(5)-C(6)-H(6)	109.5
C(6)-C(7)-C(8)	113.3(1)	C(6)-C(7)-H(7A)	108.9
C(8)-C(7)-H(7A)	108.9	C(6)-C(7)-H(7B)	108.9
C(8)-C(7)-H(7B)	108.9	H(7A)-C(7)-H(7B)	107.7
C(1)-C(8)-C(7)	112.9(1)	C(1)-C(8)-H(8A)	109.0
C(7)-C(8)-H(8A)	109.0	C(1)-C(8)-H(8B)	109.0
C(7)-C(8)-H(8B)	109.0	H(8A)-C(8)-H(8B)	107.8
O(2)-C(9)-O(1)	105.7(1)	O(2)-C(9)-C(10)	108.4(1)
O(1)-C(9)-C(10)	110.3(2)	O(2)-C(9)-C(11)	110.8(2)
O(1)-C(9)-C(11)	108.0(1)	C(10)-C(9)-C(11)	113.4(2)
C(9)-C(10)-H(10A)	109.5	C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5	C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5	H(10B)-C(10)-H(10C)	109.5
C(9)-C(11)-H(11A)	109.5	C(9)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5	C(9)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5	H(11B)-C(11)-H(11C)	109.5
O(5)-C(12)-O(4)	124.2(2)	O(5)-C(12)-O(3)	124.1(2)
O(4)-C(12)-O(3)	111.6(1)		

TABLE 3. Anisotropic displacement parameters (A^2 x 10^3) for 29b

atom	U11	U22	U33	U23	U13	U12

O(1)	37(1)	21(1)	22(1)	2(1)	5(1)	-6(1)
O(2)	48(1)	18(1)	19(1)	-1(1)	7(1)	-4(1)
O(3)	38(1)	25(1)	32(1)	-2(1)	-3(1)	-12(1)
O(4)	28(1)	24(1)	42(1)	3(1)	9(1)	-3(1)
O(5)	40(1)	32(1)	73(1)	-4(1)	1(1)	-15(1)
C(1)	29(1)	32(1)	28(1)	0(1)	-7(1)	-1(1)
C(2)	23(1)	26(1)	29(1)	-1(1)	-1(1)	-4(1)
C(3)	26(1)	16(1)	20(1)	0(1)	3(1)	-3(1)
C(4)	27(1)	17(1)	20(1)	1(1)	-1(1)	0(1)
C(5)	26(1)	16(1)	22(1)	0(1)	-1(1)	-3(1)
C(6)	25(1)	17(1)	30(1)	2(1)	3(1)	-1(1)
C(7)	38(1)	24(1)	22(1)	2(1)	6(1)	3(1)
C(8)	42(1)	30(1)	20(1)	-2(1)	0(1)	0(1)
C(9)	50(1)	19(1)	22(1)	1(1)	7(1)	-2(1)
C(10)	67(1)	39(1)	55(1)	2(1)	36(1)	6(1)
C(11)	85(2)	31(1)	24(1)	7(1)	-5(1)	-5(1)
C(12)	30(1)	22(1)	46(1)	3(1)	1(1)	-4(1)

The anisotropic displacement factor exponent takes the form
2 pi^2 [h^2a*^2U(11) +...+ 2hka*b*U(12)]

TABLE 4. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 29b

atom	x	y	z	U(eq)
H(1)	2482	1772	5974	36
H(2)	2080	1397	7368	31
H(3)	5582	33	7373	25
H(4)	7476	1147	8300	26
H(5)	5626	3025	7330	25
H(6)	8598	1404	6801	29
H(7A)	7880	2085	5360	33
H(7B)	6236	2940	5753	33
H(8A)	5041	1067	5148	36
H(8B)	5987	439	5978	36
H(10A)	2266	1966	9936	80
H(10B)	1338	738	9627	80
H(10C)	1474	1821	8963	80
H(11A)	6593	204	9660	70
H(11B)	4602	-273	10086	70
H(11C)	5453	989	10362	70