Supplementary Material (ESI) for Organic and Biomolecular Chemistry

Experimental and computational evidence for α-lactone intermediates in the addition of aqueous bromine to disodium dimethyl-maleate and -fumarate

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Electronic Supplementary Information

Cartesian coordinates (Ångström) for optimised structures in PCM water

Label in Table below	Label in main paper
M1	**13**
M2	**15**
M3	**17**
M4	**19**
M5	**21**
M6	**23**
M7	**29**
M8	neutral bromo-β-lactone (Fig. 3a)
M10	constrained Cs symmetry version of 27
F1	**14**
F2	**16**
F3	**18**
F4	**20**
F5	**22**
F6	**24**
F7	failed attempt to find a frontside TS for 16 -> 23
F8	neutral bromo-β-lactone (Fig. 3b)
F10	**28**

M1				M2				M3			
Br	0.00000	0.45969	1.51762	Br	0.00000	0.00000	1.52818	C	0.38877	-1.18401	0.40332
C	0.73855	0.45969	-0.51937	C	0.73501	0.00000	-0.52510	C	0.05572	-0.00602	-0.52614
C	1.53125	1.71405	-0.76408	C	1.47472	1.30806	-0.84335	C	0.71680	-0.13456	-1.88949
C	1.48595	-0.85117	-0.84334	C	1.50157	-1.26415	-0.77809	C	-0.47028	-2.35821	0.39726
C	-0.73855	0.45969	-0.51937	C	-0.73501	0.00000	-0.52510	C	1.43844	-1.09941	1.47539
C	-1.48595	-0.85117	-0.84334	C	-1.47472	-1.30806	-0.84335	C	-1.49174	0.27030	-0.56641
C	-1.53125	1.71405	-0.76408	C	-1.50157	1.26415	-0.77809	H	0.50339	0.75760	-2.48136
O	1.67314	-0.87514	-2.08375	O	2.02107	1.97880	0.04751	H	1.80036	-0.26043	-1.79482
O	-1.67314	-0.87514	-2.08375	O	-2.02107	-1.97880	0.04751	H	0.30530	-0.99954	-2.41946
O	-1.81468	-1.64694	0.05144	O	1.41669	1.47099	-2.08809	O	0.53886	-2.53337	-0.44618
O	1.81468	-1.64694	0.05144	O	-1.41669	-1.47099	-2.08809	O	-1.39919	-3.01614	0.78169
H	1.05264	2.61448	-0.37424	H	1.64576	-1.33916	-1.86415	H	1.62583	-2.09113	1.89848
H	2.53016	1.61786	-0.32642	H	-1.64576	1.33916	-1.86415	H	2.37282	-0.68689	1.08027
H	1.64630	1.82073	-1.85078	H	0.96700	-2.15528	-0.43765	H	1.08148	-0.44399	2.27728
H	-1.05264	2.61448	-0.37424	H	-0.96700	2.15528	-0.43765	O	-2.08616	0.12060	0.52847
H	-2.53016	1.61786	-0.32642	H	2.48586	-1.21370	-0.30158	O	-1.96223	0.61502	-1.67535
H	-1.64630	1.82073	-1.85078	H	-2.48586	1.21370	-0.30158	Br	0.79004	1.68910	0.28676

M4				M5				M6			
C	1.61316	0.79880	-1.31569	O	-1.34463	0.14409	2.02923	C	-1.03977	-0.13570	-1.66733
C	0.78981	0.15864	-0.20719	C	-0.86386	-0.05942	0.19350	C	-0.40411	0.12335	-0.31902
C	1.55520	-1.07906	0.38282	O	-0.05123	-1.25423	-1.58728	C	1.14627	0.16374	-0.15866
O	2.59984	-0.85040	1.02599	C	0.92188	-0.48888	-1.29154	C	1.84163	-0.62831	0.92594
Br	0.59830	1.56776	1.22359	C	0.60668	0.22893	0.05031	C	-0.34145	1.56554	0.16833
C	-0.61443	-0.24661	-0.58932	O	-1.61572	-2.08477	1.48303	O	-1.13566	2.44707	0.38981
C	-1.57993	-0.72781	0.46523	C	-1.32671	-0.91507	1.30107	O	0.99624	1.59803	0.29955
O	-1.31770	0.80401	-1.58045	Br	0.88369	2.20064	-0.15265	Br	-1.34395	-0.94617	1.06454
C	-0.96267	-0.40266	-1.99356	C	-1.90223	0.64357	-0.62623	C	1.91171	0.06536	-1.50450
O	-1.04386	-1.03109	-3.01543	H	-1.48097	0.98345	-1.57444	O	2.39259	1.11571	-1.98434
O	1.04126	-2.18157	0.06629	H	-2.75043	-0.02054	-0.82016	O	1.96372	-1.10935	-1.94893
H	1.13248	1.69609	-1.71471	H	-2.26329	1.52189	-0.07902	H	-2.10063	0.13194	-1.63568
H	2.59674	1.06406	-0.92045	O	1.99410	-0.31333	-1.88317	H	-0.54771	0.47518	-2.43426
H	1.75845	0.07660	-2.13146	C	1.51367	-0.23867	1.17619	H	-0.93692	-1.18757	-1.94672
H	-1.03552	-1.27386	1.23869	H	2.55331	-0.04337	0.89941	H	2.89741	-0.33437	0.96302
H	-2.33892	-1.38959	0.03703	H	1.39057	-1.31993	1.32681	H	1.39221	-0.44358	1.90609
H	-2.07832	0.13205	0.92576	H	1.28475	0.27628	2.11266	H	1.78952	-1.69632	0.69789

M7				M8				M10			
O	0.56739	-2.19850	0.12070	Br	0.34286	-0.68575	-1.80886	C	0.80134	-2.49601	0.12705
C	-0.81334	-0.28015	-0.47993	O	0.34286	-0.68575	1.75059	C	-0.46682	-2.18729	-0.19988
C	0.66024	-0.09178	-0.65279	O	2.49464	-0.68575	0.93164	C	1.92593	-2.11443	-0.82336
C	1.30864	-1.16649	0.22706	O	-2.21416	1.74609	0.90864	O	3.10995	-2.39066	-0.47656
O	2.37844	-1.02162	0.82589	H	-2.59640	2.52030	1.41421	O	1.58411	-1.53437	-1.89735
H	1.01740	-1.14573	-2.50046	O	-0.97166	1.46733	2.77784	C	-0.87398	-1.67431	-1.55418
C	1.21077	-0.15448	-2.07324	C	1.33099	-0.40454	0.85885	O	-1.14840	-0.38852	-1.71991
H	2.29268	0.00492	-2.03960	C	0.41711	0.32384	-0.12328	O	-1.19450	-2.46476	-2.44832
H	0.77104	0.60829	-2.72120	C	-0.70483	-0.06235	0.90867	C	-1.65808	-2.53333	0.66285
Br	0.92689	1.78337	-0.01158	C	0.73154	1.77732	-0.41266	C	1.15365	-3.17374	1.42841
C	-1.41466	-0.58672	0.89986	H	0.80370	2.35293	0.51887	Br	-0.60159	0.95098	-0.25762
O	-2.38653	-1.37294	0.83198	H	-0.04431	2.22035	-1.04405	Br	0.02568	2.76397	1.52121
O	-0.88920	-0.02629	1.88342	H	1.69404	1.84499	-0.92959	H	-1.40689	-2.49829	1.72812
H	-1.59976	-1.05678	-2.24626	C	-1.77147	-1.07682	0.54728	H	-2.01871	-3.54784	0.43569
C	-1.72375	-0.15035	-1.62328	H	-1.31218	-1.99320	0.16808	H	-2.49516	-1.84670	0.48499
H	-1.44238	0.68949	-2.27221	H	-2.44222	-0.66979	-0.21459	H	0.89041	-2.55473	2.29859
H	-2.76829	-0.09784	-1.31265	H	-2.35952	-1.32294	1.43864	H	2.22824	-3.36603	1.46415
				C	-1.29522	1.13540	1.65777	H	0.62554	-4.13023	1.54360

F1				F2				F3			
Br	0.00000	0.00000	1.52818	C	-0.93777	0.39516	-2.09687	C	-0.30482	0.48727	-1.93508
C	0.73501	0.00000	-0.5251	C	-0.99936	0.46395	-0.59615	C	-0.22963	0.49144	-0.41084
C	1.47472	1.30806	-0.84335	Br	1.56961	0.39156	0.42239	C	1.19591	0.55862	0.14043
C	1.50157	-1.26415	-0.77809	C	-0.21667	-0.54217	0.23487	C	1.60942	1.66419	1.07280
C	-0.73501	0.00000	-0.5251	O	-1.18630	-2.41877	-0.74498	H	0.96579	1.6395	1.96138
C	-1.47472	-1.30806	-0.84335	C	-0.06111	-1.91034	-0.50838	H	1.48227	2.63948	0.59428
C	-1.50157	1.26415	-0.77809	O	1.07673	-2.35653	-0.76137	H	2.64734	1.53283	1.39265
O	2.02107	1.97880	0.04751	C	-1.57102	1.62667	0.05753	O	2.32382	0.31066	-1.00258
O	-2.02107	-1.97880	0.04751	O	-2.50736	0.70895	-0.07266	O	2.57364	-1.61503	0.31095
O	1.41669	1.47099	-2.08809	O	-1.48331	2.74193	0.50645	C	2.10760	-0.56071	-0.04117
O	-1.41669	-1.47099	-2.08809	C	-0.74462	-0.75833	1.64767	Br	-0.96383	-1.30345	0.17601
H	1.64576	-1.33916	-1.86415	H	-1.46168	-0.50164	-2.44388	O	-1.95588	1.38106	1.07251
H	-1.64576	1.33916	-1.86415	H	-1.73151	-1.22813	1.59296	C	-1.11727	1.64649	0.18728
H	0.96700	-2.15528	-0.43765	H	0.10806	0.31949	-2.41681	O	-0.83438	2.7543	-0.33162
H	-0.96700	2.15528	-0.43765	H	-0.82222	0.17929	2.20799	H	-1.35429	0.43584	-2.24089
H	2.48586	-1.21370	-0.30158	H	-1.38261	1.28252	-2.55599	H	0.12438	1.41711	-2.31898
H	-2.48586	1.21370	-0.30158	H	-0.06806	-1.42895	2.18686	H	0.23185	-0.36069	-2.36705

F4				F5				F6			
C	-0.01791	-0.02951	-0.02345	C	0.00000	0.00000	0.00000	C	0.02930	-0.05625	-0.02811
C	-0.02810	0.12414	1.47665	C	0.00000	0.00000	1.50069	C	0.07914	-0.10477	1.47961
C	1.29989	-0.02166	2.18932	C	1.32319	0.00000	2.21665	C	1.42373	0.09618	2.21171
C	2.31237	1.03729	1.79507	C	2.34819	1.00670	1.73403	C	2.47969	1.07527	1.75317
O	-0.87744	1.41953	1.91768	C	-1.27750	0.21758	2.19466	C	-1.25087	0.12968	2.19101
C	-1.29327	0.18637	2.17858	O	-2.16847	-0.46070	2.67590	O	-1.87486	-0.80676	2.71191
O	-2.26068	-0.31665	2.68696	O	-1.09266	1.48045	2.03791	O	-1.50589	1.38214	2.25176
C	1.78790	-1.51021	2.02313	C	1.71824	-1.50542	2.08850	C	1.59227	-1.38710	2.07540
O	3.02350	-1.67964	1.94809	O	2.88395	-1.86474	2.30081	O	2.48848	-2.16561	2.32896
Br	1.01648	0.15027	4.17548	Br	1.07043	0.26271	4.18232	Br	1.14040	0.39900	4.16216
O	0.86464	-2.36060	1.99386	O	0.70524	-2.19540	1.75422	O	0.35910	-1.60813	1.66694
H	0.57565	0.76752	-0.48536	H	0.13644	1.02684	-0.36160	H	0.02383	0.99025	-0.36315
H	-1.03524	0.00931	-0.42348	H	-0.94722	-0.38486	-0.38885	H	-0.88937	-0.53383	-0.38322
H	0.42235	-0.99513	-0.29114	H	0.82136	-0.60662	-0.38987	H	0.89413	-0.55409	-0.47470
H	2.54654	0.94877	0.72735	H	2.53780	0.86696	0.66203	H	2.70058	0.93007	0.68753
H	3.23999	0.88433	2.35002	H	3.28835	0.84728	2.26917	H	3.40453	0.91173	2.31635
H	1.92953	2.04353	1.99438	H	2.00076	2.03111	1.90220	H	2.13820	2.10205	1.90846

F7				F8				F10			
C	0.00000	0.00000	0.00000	C	0.00000	0.00000	0.00000	C	1.91223	-1.90346	0.54122
C	0.00000	0.00000	1.52059	C	0.00000	0.00000	1.51070	C	0.58960	-1.85859	0.29283
Br	1.90826	0.00000	2.11940	Br	1.85838	0.00000	2.18333	C	0.03102	-1.82719	-1.09407
C	-0.73909	1.12069	2.20307	C	-0.74475	1.10253	2.25851	O	-0.52863	-0.77149	-1.67578
C	-1.51151	2.07238	1.38268	O	-0.75269	2.30163	2.27525	O	-0.01010	-2.78565	-1.86244
O	-0.42230	2.73089	1.21187	O	-1.51228	0.24783	2.98913	C	-0.44044	-1.93009	1.35932
C	-0.74298	-1.23633	2.09297	C	-0.94831	-0.94900	2.32455	C	2.91095	-1.74631	-0.54951
O	-1.84183	-0.84986	2.60463	C	-0.30005	-1.84799	3.37831	H	0.07648	-2.08789	2.33906
C	-0.56475	1.42889	3.65817	O	0.18838	-2.95137	2.80859	H	-1.01236	-0.99353	1.39797
O	-0.28721	-2.38066	1.97891	C	-2.02184	-1.68693	1.54294	H	-1.14252	-2.75414	1.18556
O	-2.66859	2.22411	1.02965	O	-0.27287	-1.59610	4.56337	H	3.45044	-0.79799	-0.41797
H	-1.03470	0.00948	-0.36933	H	0.47498	-0.90977	-0.38121	H	3.65537	-2.5531	-0.51456
H	0.52894	0.86821	-0.40135	H	0.55472	0.86862	-0.36863	H	2.47069	-1.74221	-1.55577
H	0.48288	-0.91393	-0.35721	H	-1.02300	0.05868	-0.38794	Br	-0.81910	0.77747	-0.71983
H	-1.51482	1.75880	4.09144	H	-2.72486	-2.15959	2.23860	C	2.51762	-2.13565	1.93968
H	-0.19753	0.55547	4.20163	H	-1.56982	-2.46658	0.92207	O	3.76616	-2.19836	2.06109
H	0.16762	2.23675	3.77336	H	-2.58175	-0.99497	0.90660	O	1.77649	-2.29313	2.94652
				H	0.57652	-3.55531	3.49946	Br	-1.40797	2.68580	0.02069

Crystallographic data for bromohydrins

erythro-2-bromo-3-hydroxy-2,3-dimethylsuccinic acid

Table 1. Crystal data and structure refinement for compound **7**.

Identification code	CCDC 652216
Empirical formula	C6 H9 Br O5
Formula weight	241.04
Temperature	30(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 11.4120(5)Å $\alpha = 90^o$
	b = 5.8870(3)Å $\beta = 93.337(2)^o$
	c = 12.3790(7)Å $\gamma = 90^o$
Volume	830.24(7) $Å^3$
Z	4
Density (calculated)	1.928 Mg/m^3
Absorption coefficient	4.932 mm^{-1}
F(000)	480
Crystal size	0.20 x 0.20 x 0.10 mm
Theta range for data collection	3.30 to 27.46^o
Index ranges	-14<=h<=12; -6<=k<=7; -16<=l<=14
Reflections collected	5751
Independent reflections	1883 [R(int) = 0.0707]
Reflections observed (>2σ)	1420
Data Completeness	0.988
Max. and min. transmission	0.6383 and 0.4387
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1883 / 0 / 115
Goodness-of-fit on F^2	1.021
Final R indices [I>2σ(I)]	$R_1 = 0.0381$ $wR_2 = 0.0761$
R indices (all data)	$R_1 = 0.0626$ $wR_2 = 0.0832$
Largest diff. peak and hole	0.793 and -0.722 $eÅ^{-3}$

Hydrogen bonds with H..A < r(A) + 2.000 Angstroms and <DHA > 110 deg.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
O2-**H2**	0.840	1.91	162	2.716(3)	**O3** [-x+1, -y, -z+1]
O4-**H4**	0.840	1.79	170	2.618(3)	**O5** [x, -y+1/2, z+1/2]
O5-**H5**	0.840	2.15	117	2.629(3)	**O1**
O5-**H5**	0.840	2.15	140	2.841(3)	**O1** [-x+1, y+1/2, -z+1/2]

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **7**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Br(1)	752(1)	1932(1)	3276(1)	12(1)
O(1)	5081(2)	0(4)	3056(2)	12(1)
O(2)	4235(2)	-2377(4)	4189(2)	13(1)
O(3)	3597(2)	2429(4)	4781(2)	11(1)
O(4)	1978(2)	1601(4)	5651(2)	13(1)
O(5)	3087(2)	1968(4)	2433(2)	12(1)
C(1)	4221(3)	-800(6)	3421(3)	11(1)
C(2)	2975(3)	-162(6)	2974(3)	11(1)
C(3)	2095(3)	110(6)	3876(3)	12(1)
C(4)	2632(3)	1546(6)	4821(3)	10(1)
C(5)	2561(3)	-1893(6)	2091(3)	8(1)
C(6)	1580(3)	-2121(6)	4279(3)	12(1)

Table 3. Bond lengths [Å] and angles [^{o}] for **7**

Br(1)-C(3)	1.979(3)	O(1)-C(1)	1.200(4)
O(2)-C(1)	1.328(4)	O(3)-C(4)	1.221(4)
O(4)-C(4)	1.305(4)	O(5)-C(2)	1.430(4)
C(1)-C(2)	1.542(4)	C(2)-C(5)	1.548(5)
C(2)-C(3)	1.553(5)	C(3)-C(6)	1.534(5)
C(3)-C(4)	1.541(5)		
O(1)-C(1)-O(2)	124.6(3)	O(1)-C(1)-C(2)	121.8(3)
O(2)-C(1)-C(2)	113.5(3)	O(5)-C(2)-C(1)	106.0(3)
O(5)-C(2)-C(5)	106.2(3)	C(1)-C(2)-C(5)	109.3(3)
O(5)-C(2)-C(3)	109.0(3)	C(1)-C(2)-C(3)	112.9(3)
C(5)-C(2)-C(3)	113.1(3)	C(6)-C(3)-C(4)	111.5(3)
C(6)-C(3)-C(2)	114.9(3)	C(4)-C(3)-C(2)	110.9(3)
C(6)-C(3)-Br(1)	106.5(2)	C(4)-C(3)-Br(1)	104.7(2)
C(2)-C(3)-Br(1)	107.7(2)	O(3)-C(4)-O(4)	125.4(3)
O(3)-C(4)-C(3)	121.5(3)	O(4)-C(4)-C(3)	113.0(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for **7** The anisotropic displacement factor exponent takes the form: -2 gpi^2 [h^2 a^{*2} U11 + ... + 2 h k a* b* U

Atom	U11	U22	U33	U23	U13	U12
Br(1)	10(1)	16(1)	9(1)	0(1)	-3(1)	1(1)
O(1)	12(1)	16(1)	9(1)	1(1)	-1(1)	1(1)
O(2)	10(1)	17(1)	11(1)	2(1)	-4(1)	1(1)
O(3)	13(1)	14(1)	7(1)	0(1)	-1(1)	0(1)
O(4)	12(1)	21(2)	7(1)	-5(1)	-2(1)	-2(1)
O(5)	10(1)	16(1)	9(1)	5(1)	-3(1)	-3(1)
C(1)	16(2)	11(2)	6(2)	-7(2)	-3(2)	2(2)
C(2)	12(2)	10(2)	9(2)	0(2)	-4(1)	-4(2)
C(3)	9(2)	20(2)	6(2)	-2(2)	-5(1)	4(2)
C(4)	13(2)	10(2)	8(2)	1(2)	-3(1)	5(2)
C(5)	9(2)	6(2)	10(2)	-5(2)	7(1)	-4(2)
C(6)	12(2)	13(2)	9(2)	1(2)	-2(2)	-3(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **7**.

Atom	x	y	z	U(eq)
H(2)	4932	-2631	4414	15
H(4)	2358	2189	6182	16
H(5)	3777	2452	2539	15
H(5A)	1777	-1471	1793	12
H(5B)	2534	-3415	2409	12
H(5C)	3111	-1889	1511	12
H(6A)	2213	-3068	4603	17
H(6B)	1186	-2930	3668	17
H(6C)	1012	-1790	4821	17

threo-2-bromo-3-hydroxy-2,3-dimethylsuccinic acid

Table 6. Crystal data and structure refinement for compound **8**.

Identification code	CCDC 652217
Empirical formula	C6 H11 Br O6
Formula weight	259.06
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 6.2390(3)Å α = 85.342(2)^o
	b = 7.2280(4)Å β = 82.801(2)^o
	c = 11.1710(8)Å γ = 69.105(3)^o
Volume	466.56(5) Å^3
Z	2
Density (calculated)	1.844 Mg/m^3
Absorption coefficient	4.403 mm^{-1}
F(000)	260
Crystal size	0.20 x 0.20 x 0.10 mm
Theta range for data collection	3.51 to 27.34^o
Index ranges	-8<=h<=8; -9<=k<=9; -14<=l<=14
Reflections collected	8440
Independent reflections	2075 [R(int) = 0.0683]
Reflections observed (>2σ)	1623
Data Completeness	0.982
Max. and min. transmission	0.652 and 0.502
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2075 / 2 / 134
Goodness-of-fit on F^2	1.000
Final R indices [I>2σ(I)]	R1 = 0.0378 wR2 = 0.0757
R indices (all data)	R1 = 0.0614 wR2 = 0.0839
Largest diff. peak and hole	0.677 and -0.759 eÅ^{-3}

Notes: Lattice dominated by hydrogen bonding. Included water acts as a 'cement'. Wayer hydrogens located and refined at 0.89 Å from O6.

Hydrogen bonds with H..A < r(A) + 2.000 Angstroms and <DHA > 110 deg.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
O2-**H2**	0.840	1.78	167	2.608(4)	O6 [x, y+1, z]
O4-**H4**	0.840	1.82	171	2.654(4)	O3 [-x, -y, -z+1]
O5-**H5**	0.840	2.08	147	2.819(4)	O6
O5-**H5**	0.840	2.75	114	3.178(3)	Br1
O6-**H6A**	0.884	1.93	178	2.816(4)	O1 [-x+1, -y, -z+2]
O6-**H6B**	0.890	1.86	173	2.749(4)	O5 [-x, -y, -z+2]

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **8**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Br(1)	5535(1)	289(1)	7242(1)	29(1)
O(1)	2540(4)	3213(4)	9630(2)	34(1)
O(2)	2197(4)	5624(3)	8197(2)	35(1)
O(3)	191(4)	2071(3)	5242(2)	31(1)
O(4)	2057(4)	-789(3)	6173(2)	33(1)
O(5)	362(4)	1435(3)	8446(2)	25(1)
O(6)	3000(4)	-2083(3)	9634(2)	28(1)
C(1)	2007(5)	3939(5)	8654(3)	27(1)
C(2)	921(5)	3019(5)	7808(3)	25(1)
C(3)	2637(5)	2192(5)	6673(3)	25(1)
C(4)	1523(6)	1113(5)	5958(3)	26(1)
C(5)	-1363(5)	4555(5)	7496(3)	28(1)
C(6)	3302(6)	3717(5)	5836(3)	27(1)

Table 8. Bond lengths [Å] and angles [º] for **8**.

Br(1)-C(3)	1.984(3)
O(1)-C(1)	1.204(4)
O(2)-C(1)	1.321(4)
O(3)-C(4)	1.215(4)
O(4)-C(4)	1.303(4)
O(5)-C(2)	1.425(4)
C(1)-C(2)	1.543(5)
C(2)-C(5)	1.522(4)
C(2)-C(3)	1.561(4)
C(3)-C(6)	1.524(4)
C(3)-C(4)	1.535(5)
O(1)-C(1)-O(2)	124.9(3)
O(1)-C(1)-C(2)	123.0(3)
O(2)-C(1)-C(2)	112.1(3)
O(5)-C(2)-C(5)	105.9(2)
O(5)-C(2)-C(1)	108.9(3)
C(5)-C(2)-C(1)	108.9(3)
O(5)-C(2)-C(3)	108.9(2)
C(5)-C(2)-C(3)	113.2(3)
C(1)-C(2)-C(3)	110.8(2)
C(6)-C(3)-C(4)	109.0(3)
C(6)-C(3)-C(2)	116.0(3)
C(4)-C(3)-C(2)	107.2(2)
C(6)-C(3)-Br(1)	106.7(2)
C(4)-C(3)-Br(1)	110.0(2)
C(2)-C(3)-Br(1)	107.9(2)
O(3)-C(4)-O(4)	124.0(3)
O(3)-C(4)-C(3)	118.6(3)
O(4)-C(4)-C(3)	117.3(3)

Symmetry transformations used to generate equivalent atoms:

Table 9. Anisotropic displacement parameters ($Å^2$ x 10^3) for **8**. The anisotropic displacement factor exponent takes the form: -2 gpi^2 [h^2 a^{*2} U11 + ... + 2 h k a* b* U

Atom	U11	U22	U33	U23	U13	U12
Br(1)	18(1)	29(1)	38(1)	1(1)	-2(1)	-4(1)
O(1)	30(1)	35(1)	34(2)	-2(1)	-10(1)	-7(1)
O(2)	45(2)	31(1)	34(2)	-4(1)	-7(1)	-19(1)
O(3)	34(1)	23(1)	37(1)	0(1)	-14(1)	-8(1)
O(4)	41(1)	21(1)	42(2)	0(1)	-17(1)	-11(1)
O(5)	19(1)	27(1)	29(1)	3(1)	-1(1)	-10(1)
O(6)	23(1)	31(1)	32(1)	-3(1)	-2(1)	-13(1)
C(1)	22(2)	24(2)	32(2)	-3(2)	-2(2)	-6(1)
C(2)	19(2)	27(2)	28(2)	1(1)	-1(1)	-8(1)
C(3)	20(2)	23(2)	30(2)	3(1)	-2(1)	-6(1)
C(4)	26(2)	23(2)	28(2)	0(2)	0(2)	-8(1)
C(5)	20(2)	28(2)	33(2)	-2(2)	-5(1)	-4(1)
C(6)	25(2)	26(2)	31(2)	1(2)	0(1)	-13(1)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **8**.

Atom	x	y	z	U(eq)
H(2)	2494	6213	8737	46(12)
H(4)	1252	-1206	5793	40
H(5)	1553	604	8707	43(12)
H(4A)	-2304	5111	8240	41
H(4B)	-2186	3924	7070	41
H(4C)	-1071	5617	6977	41
H(5A)	1912	4699	5539	40
H(5B)	4360	3050	5150	40
H(5C)	4061	4381	6279	40
H(6A)	4420(40)	-2460(60)	9850(40)	61(14)
H(6B)	1990(60)	-1960(70)	10290(30)	64(15)