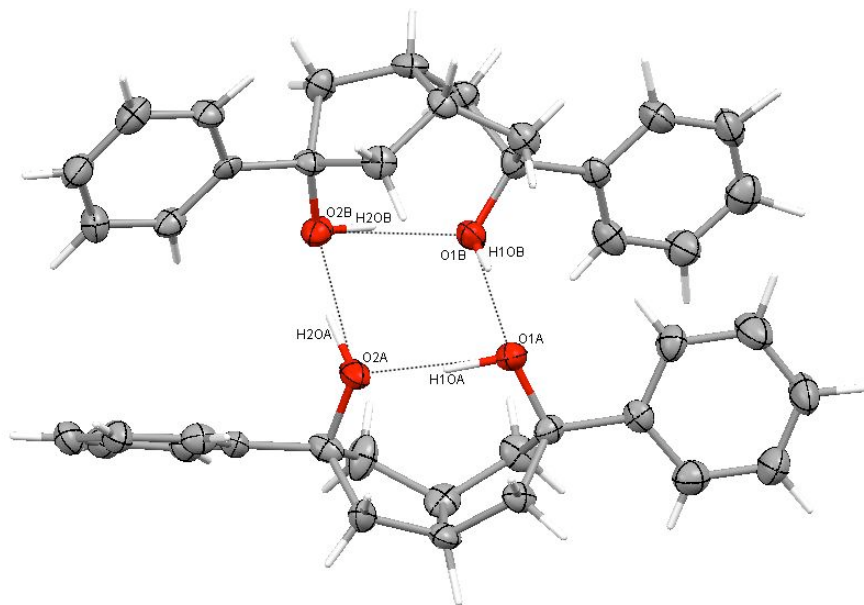
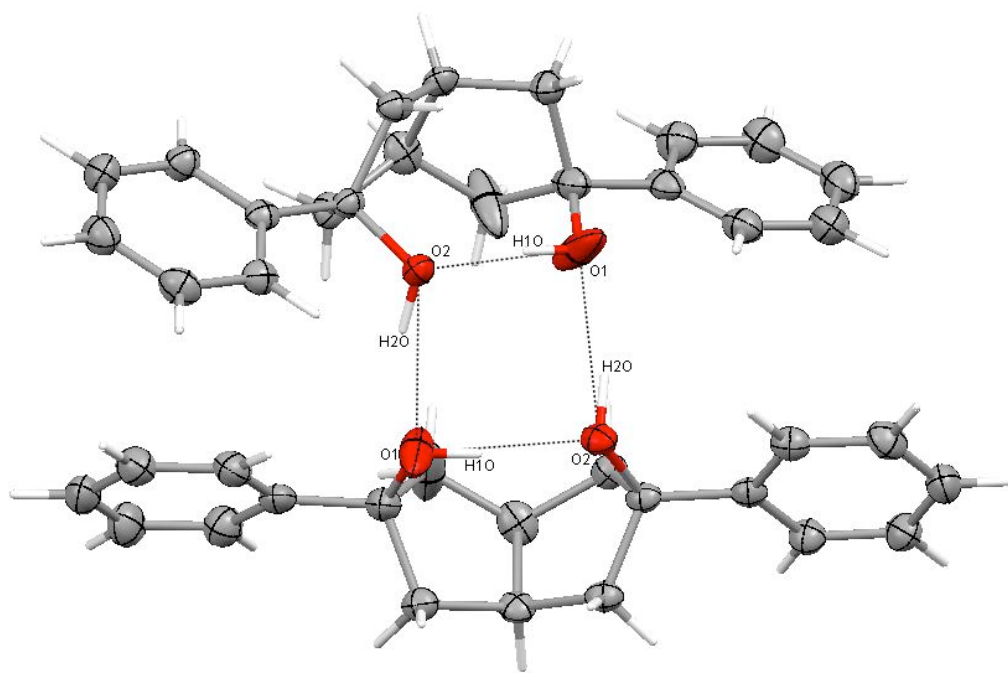


Details of the hydrogen bonding present in the four crystal structures



Diol 2 (apohost): CCDC 784997

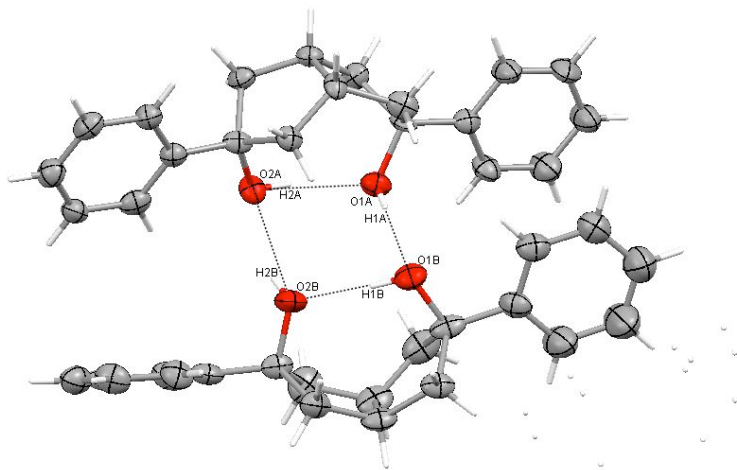
Nr	Typ	Res	Donor --- H....	Acceptor [ARU]	D - H	H...A	D...A	D - H...A
1	Intra 1	O1A	--H1OA ..O2A	[]	1.13(10)	1.53(10)	2.640(6)	164(7)
2	1	O2A	--H2OA ..O2B	[]	1.18(14)	1.64(14)	2.798(7)	167(10)
3	2	O1B	--H1OB ..O1A	[]	0.77(10)	1.96(10)	2.723(7)	170(9)
4	Intra 2	O2B	--H2OB ..O1B	[]	1.13(12)	1.66(12)	2.650(6)	143(11)
5	Intra 1	C14A	--H14A ..O1A	[]	0.94(6)	2.32(6)	2.685(7)	103(4)
6	Intra 2	C14B	--H14B ..O1B	[]	0.91(6)	2.34(6)	2.716(9)	105(5)



(Diol 2)₂.(benzene): CCDC 78500

Nr	Typ	Res	Donor --- H...Acceptor	[ARU]	D - H	H...A	D...A	D - H...A
1	1	O(2) --H(2O) ..O(1)	[2555.01]		0.94(3)	1.86(3)	2.755(2)	159(3)
2	Intra 1	O(1) --H(1O) ..O(2)	[]		0.89(4)	1.74(4)	2.625(2)	172(3)
3	Intra 1	C(5) --H(1) ..O(1)	[]		0.99(2)	2.38(2)	2.756(2)	101.7(13)
4	Intra 1	C(18) --H(20) ..O(2)	[]		0.93(2)	2.28(3)	2.654(3)	103.6(18)

[2555.] = -x,y,1/2-z



(Diol 2).(o-xylene): CCDC 784999

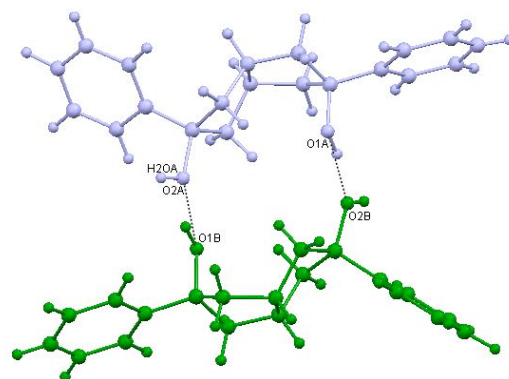
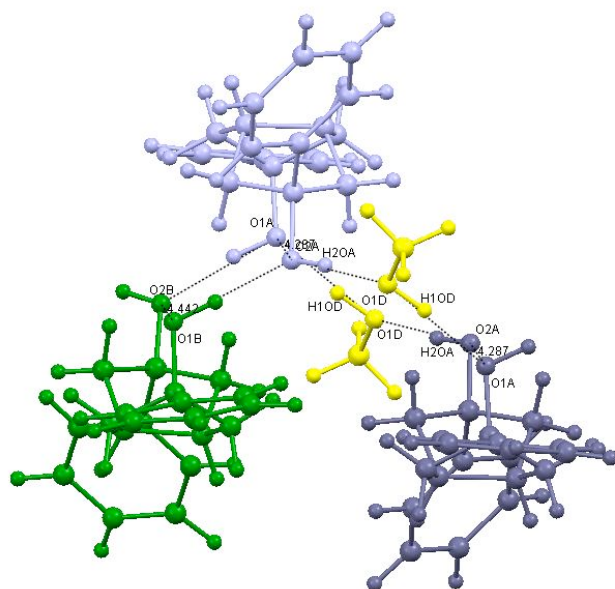
Nr	Typ	Res	Donor --- H....Acceptor	[ARU]	D - H	H...A	D...A	D - H...A
1		1	O1A --H1A ..O1B	[1565.02]	0.84	1.92	2.735(10)	163
2	Intra	2	O1B --H1B ..O2B	[]	0.84	1.80	2.636(10)	177
3	Intra	1	O2A --H2A ..O1A	[]	0.84	1.87	2.674(10)	161
4		2	O2B --H2B ..O2A	[1545.01]	0.84	2.02	2.747(10)	144
5	Intra	1	C14A --H14A ..O1A	[]	0.95	2.36	2.733(11)	102
6	Intra	2	C14B --H14B ..O1B	[]	0.95	2.33	2.706(11)	103
7	Intra	1	C16A --H16A ..O2A	[]	0.95	2.37	2.731(11)	102

Translation of ARU-code to Equivalent Position Code

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[1565.] = x,1+y,z

[1545.] = x,-1+y,z



(Diol 2).(Methanol): CCDC 784998

Nr	Typ	Res	Donor --- H....Acceptor	[ARU]	D - H	H...A	D...A	D - H...A
1		2	O2B --H2OB ..O1C	[1455.03]	0.89(4)	1.75(4)	2.627(4)	170(4)
2		2	O1B --H1OB ..O2A	[1456.01]	0.93(5)	1.77(5)	2.663(3)	162(5)
3		1	O2A --H2OA ..O1D	[1655.04]	0.88(4)	1.78(4)	2.651(4)	172(3)
4		1	O1A --H1OA ..O2B	[1654.02]	0.93(4)	1.73(4)	2.650(4)	169(4)
5		3	O1C --H1OC ..O1B	[2657.02]	0.82(4)	1.83(4)	2.643(4)	174(5)
6		4	O1D --H1OD ..O1A	[2665.01]	0.93(5)	1.74(5)	2.663(4)	171(5)
7	Intra	2	C6B --H2B6 ..O1B	[]	1.02(4)	2.50(3)	3.162(5)	122(2)

Translation of ARU-code to Equivalent Position Code

[1654.] = 1+x,y,-1+z

[1655.] = 1+x,y,z

[2665.] = 1-x,1-y,-z

[1456.] = -1+x,y,1+z

[1455.] = -1+x,y,z

[2657.] = 1-x,-y,2-z