Table 1: Hydrogen bond energies along with various properties calculated at MP2(full)/6-311++G(2d,2p) level of theory. The energies in a.u. of the original molecule (E_M) and that calculated by fragmentation (E_e) are also shown in the first column. See text for details.

Molecules	**O-H…O Distances in Å**	**E (HB) (kcal mol^{-1})**	**ρ at (3, -1) BCP (a.u.)**	**Frequency (cm^{-1})**	**$\Delta E^{**} = \|E_M - E_e\|$ (kcal mol^{-1})**
1,2,3-propanetriol	2.16(HB1)	1.90 (2.00)#		3784	
E_M : –344.21170	2.08(HB2)	2.47 (2.56)#	0.02178	3765	0.50
E_e : –344.21091	2.58(HB3)	1.63 (1.66)#		3845	
1,2,3-butanetriol	2.13(HB1)	2.13		3768	
E_M : –383.44517	2.05(HB2)	2.72	0.02287	3745	0.50
E_e : –383.44437	2.58(HB3)	1.60		3844	
1,2,4-butanetriol	1.98(HB1)	2.90	0.02339	3789	
E_M : –383.43912	2.22(HB2)	1.75		3828	0.40
E_e : –383.43849				3875	
1,2,3-pentanetriol	2.13(HB1)	2.11		3769	
E_M : –422.67178	2.05(HB2)	2.77	0.02298	3743	0.51
E_e : –422.67097	2.57(HB3)	1.61		3844	
1,2,4-pentanetriol	1.97(HB1)	3.04	0.02421	3785	
E_M : –422.67251	2.22(HB2)	1.77		3827	0.42
E_e : –422.67184				3858	
1,2,5-pentanetriol	1.80(HB1)	4.97	0.03581	3669	
E_M : –422.66590	2.25(HB2)	1.78		3825	0.55
E_e : –422.66502				3865	
1,3,5-pentanetriol	1.94(HB1)	2.91	0.02558	3763	
E_M : –422.66727	1.96(HB2)	2.90	0.02404	3792	0.58
E_e : –422.66635				3875	
2,3,4-pentanetriol	2.12(HB1)	2.18		3759	
E_M : –422.67861	2.02(HB2)	2.94	0.02418	3731	0.52
E_e : –422.67778	2.56(HB3)	1.50		3820	
2,3,5-pentanetriol	1.91(HB1)	2.86	0.02704	3756	
E_M : –422.67242	2.23(HB2)	2.58		3805	0.50
E_e : –422.67163				3874	
2,4,6-heptanetriol	1.92(HB1)	3.02	0.02665	3753	
E_M : –501.13408	1.93(HB2)	2.94	0.02585	3773	0.65
E_e : –501.13304				3857	
α-D-fructose	2.08(HB1)	3.08	0.02001	3755	
E_M : –686.05951	2.44(HB2)	2.85	0.01004	3816	0.14
E_e : –686.05929	2.48(HB3)	2.83		3839	
β-D-xylose	2.41(HB1)	1.81		3834	
E_M ; –571.71462	2.45(HB2)	1.75	–	3837	0.01
E_e : –571.71463	2.48(HB3)	2.12		3842	
α-cyclodextrin*	1.94(HB1)	4.58	0.02426	3605	0.28
E_M: –3665.68068	2.38(HB2)	2.40		3780	
E_e: –3665.68024					

* Optimized geometry at B3LYP/6-311++G(d,p) level is used.

** The average error $|E_M – Ee|$ of all the 12 cases (excluding Cyclodextrin) turns out to be 0.44 kcal mol $^{-1}$.

The respective hydrogen bond energy calculated at MP2(full)/ AUG-cc-pVTZ level