A Precision Structural Model for Fullerenols

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Supporting Information

Table S1. Relative Gibbs Free-energies (G_{rel}, in kcal/mol) Calculated in Gas Phase and Water (in Parentheses) for Different Groups of C_{60} Diols and Related Structures[a]

species	G_{rel}	species	G_{rel}	species	G_{rel}	Species	G_{rel}
1a	0.0 (0.0)	**2h**$^{\cdot}$	13.3 (12.1)	**2a**$^{-}$	9.7 (9.6)	**3d**$^{2-}$	13.9 (16.7)
1b	16.5 (15.6)	**2i**$^{\cdot}$	24.6 (24.1)	**2b**$^{-}$	0.0 (0.1)	**3e**$^{2-}$	0.0 (0.0)
1c	35.2 (31.1)	**3a**	35.8 (33.5)	**2c**$^{-}$	25.1 (24.4)	**3g**$^{2-}$	44.7 (32.5)
1d	32.6 (29.7)	**3b**	0.0 (0.0)	**2d**$^{-}$	39.1 (36.7)	**3f**$^{2-}$	47.2 (32.9)
2a$^{\cdot}$	5.7 (5.6)	**3c**	20.9 (19.0)	**2e**$^{-}$	45.7 (42.8)	**3a**$^{\cdot-}$	31.7 (36.4)
2b$^{\cdot}$	0.0 (0.0)	**3d**	10.1 (3.4)	**2f**$^{-}$	10.3 (0.0)	**3b**$^{\cdot-}$	–2.3 (4.7)
2c$^{\cdot}$	25.7 (23.6)	**3e**	16.8 (9.3)	**2g**$^{-}$	28.9 (17.4)	**3c**$^{\cdot-}$	18.2 (24.2)
2d$^{\cdot}$	39.5 (37.7)	**4a**	0.0 (0.0)	**2h**$^{-}$	7.5 (17.4)	**3d**$^{\cdot-}$	4.5 (6.0)
2e$^{\cdot}$	49.3 (47.2)	**4b**	2.4 (1.6)	**3a**$^{2-}$	43.2 (47.3)	**3e**$^{\cdot-}$	0.0 (0.0)
2f$^{\cdot}$	23.4 (21.2)	**4c**	93.1 (90.6)	**3b**$^{2-}$	11.1 (17.4)	**3f**$^{\cdot-}$	31.7 (36.4)
2g$^{\cdot}$	36.7 (30.8)	**4d**	69.2 (66.1)	**3c**$^{2-}$	31.3 (37.6)		

[a]**1a-1d**, **2a**$^{\cdot}$**-2j**$^{\cdot}$, **3a-3e**, **4a-4d**, **2a**$^{-}$**-2h**$^{-}$, **3a**$^{2-}$**-3f**$^{2-}$ and **3a**$^{\cdot-}$**-3f**$^{\cdot-}$ are in different groups, respectively.

Table S2. Relative Gibbs Free-energies of 23 symmetrically unique C_{60} diol (G_{rel}, in kcal/mol) Calculated in Gas Phase.

Num	Spin states	G_{rel}	Num	Spin states	G_{rel}	Num	Spin states	G_{rel}
1	CS	0.0	**13**	OS	32.8		CS	44.4
2	CS	9.5		triplet	33.5	**19**	OS	33.0
3	CS	20.4		CS	40.1		triplet	32.6
4	CS	16.5	**14**	OS	40.1		CS	45.3
5	CS	25.8		triplet	34.2	**20**	OS	35.1
6	CS	28.6		CS	37.9		triplet	32.7
7	CS	31.2	**15**	OS	33.8		CS	46.0
	CS	31.0		triplet	32.1	**21**	OS	34.6

8	OS	30.3		CS	38.0		triplet	32.9
	triplet	37.2	**16**	OS	33.1		CS	42.1
	CS	31.5		triplet	32.7	**22**	OS	35.9
9	OS	30.6		CS	42.1		triplet	35.2
	triplet	37.4	**17**	OS	34.3		CS	35.7
10	CS	31.0		triplet	33.0	**23**	OS	33.3
11	CS	34.1		CS	43.8		triplet	35.1
12	CS	34.8	**18**	OS	34.8			
	CS	35.0		triplet	33.2			

Presents in red shown in the lowest energy for every unique C_{60} diols.

Table S3.the calculated NMR of fullerenols.

Num of carbon (style)	shifts	Num of carbon (style)	shifts	Num of carbon (style)	shifts
15(sp2)	148.749	16(sp2)	134.7453	21(sp2)	120.4138
2(hemiacetal-sp2)	148.6674	5(sp2)	134.3496	52(sp2)	119.8437
42(ether-sp2)	148.306	22(sp2)	134.2365	43(sp2)	118.1794
56(sp2)	147.929	55(sp2)	134.0968	36(sp2)	117.9926
41(carboxyl)	147.7964	25(sp2)	133.9438	54(sp3)	117.7887
38(sp2)	146.4774	47(sp2)	132.9691	31(sp2)	117.021
24(sp2)	143.583	45(sp2)	132.5956	1(hemiacetal-sp3)	94.1192
51(sp2)	142.879	48(sp2)	132.3729	84(sp3)	83.7303
10(sp2)	142.5825	3(sp2)	132.0865	50(epoxy-sp3)	83.5734
34(sp2)	141.9954	33(sp2)	131.9419	49(epoxy-sp3)	78.8649
19(sp2)	140.3255	85(ether-sp2)	130.0681	17(sp3)	75.5008
27(sp2)	140.2837	12(sp2)	129.6251	18(sp3)	73.4978
46 (sp2)	140.1541	6(sp2)	129.0487	78(sp3)	72.4526
13(ether-sp2)	140.0786	11(sp2)	127.9299	4(sp3)	70.5097
37(hemiacetal-sp2)	139.969	28(sp2)	126.5777	29(sp3)	70.3644
40(ether-sp2)	138.7931	9(sp2)	125.4781	53(sp3)	69.03
35(sp2)	137.6909	32(sp2)	123.6216	26(sp3)	66.5438
44(sp2)	137.0218	39(sp2)	123.5947	30(sp3)	66.2728
20(sp2)	136.6618	7(sp2)	123.3549	79(sp3)	62.1558
23(sp2)	135.9361	8(sp2)	122.4596	14(sp3)	61.1841

The calculated at the level of DFT B3LYP/6-31G(d,p)

Sp^2 C: 148.7-117, sp^3 C: 83.7-61.2,

hemiacetal sp^2 C: 148.6674, 139.969, hemiacetal sp^3 C: 94.1192

ether sp^2 C: 148.306, 140.0786, 138.7931, 130.0681,

Epoxy sp^3 C: 83.5734, 78.8649.

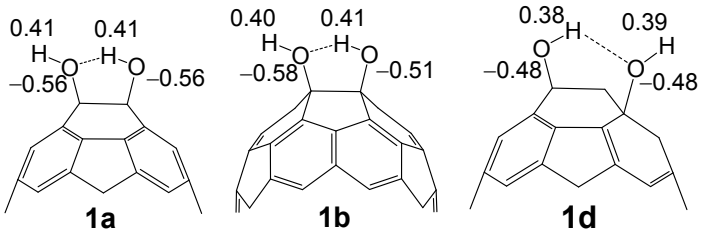

Figure S1. Mulliken charges for the atoms in **1a**, **1b** and **1d**.

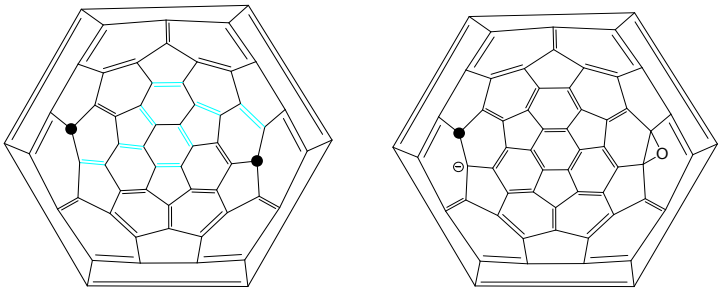

Figure S2. Skeletal structures and π-electron configurations for **1c** and **2h**$^-$. **1c** has 8 double bonds at pentagonal edges but the corresponding conjugate base **2h**$^-$ has no such double bonds.

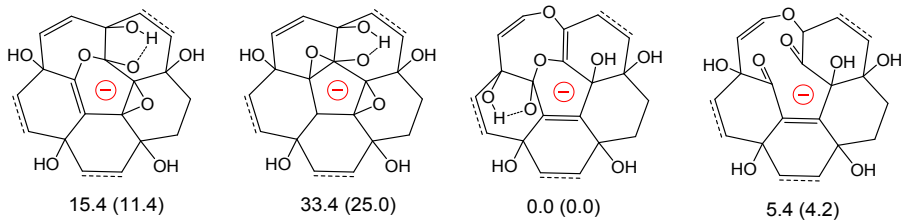

Figure S3. Relative Gibbs free energies (kcal/mol) for four isomers of the deprotonated structure of Figure 3b. The energies were calculated in gas phase; the energies calculated in water are in the parentheses.