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Change in energy of hydrogen bonds upon excitation of 6-aminocoumarin: TDDFT/EFP1 study

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Optimized coordinates of 6AC at S_0 state

C	6.0	-3.0967340188	0.4493620886	3.0259300744
H	1.0	-3.8305374705	0.5280128013	3.8326380429
C	6.0	-1.7700505857	0.7817581524	3.2754845027
H	1.0	-1.4488172138	1.1257124150	4.2598693812
C	6.0	-0.8233655575	0.6774514019	2.2522262858
O	8.0	0.4708558614	1.0177139150	2.5423794608
C	6.0	1.4902191871	0.9607664051	1.5925969888
O	8.0	2.6009180745	1.2894666054	1.9334913486
C	6.0	1.0998814187	0.5010861266	0.2593322615
H	1.0	1.9053861492	0.4549605853	-0.4742026310
C	6.0	-0.1776499661	0.1611109048	-0.0352715319
H	1.0	-0.4451786911	-0.1774851131	-1.0405693823
C	6.0	-1.2105647485	0.2393526768	0.9716341122
C	6.0	-2.5588001484	-0.0909931445	0.7345181090
H	1.0	-2.8505369802	-0.4309447416	-0.2633414423
C	6.0	-3.5169583882	0.0053626187	1.7496083251
N	7.0	-4.8428657439	-0.3903666312	1.5416079973
H	1.0	-5.1433368800	-0.3601914842	0.5713180880
H	1.0	-5.5187242984	0.0774944177	2.1392800092

Optimized coordinates of 6AC(H2O)5 complex at S_0 state

C	6.0	-3.6239911317	-0.1741059790	1.5978777327
H	1.0	-4.2936061470	-0.1914748090	2.4602924504
C	6.0	-2.2656111392	-0.4190995859	1.7708684832
H	1.0	-1.8512157091	-0.6290902821	2.7584769267
C	6.0	-1.4137290364	-0.4037121191	0.6643192253
O	8.0	-0.0774771067	-0.6565810533	0.8755101711
C	6.0	0.8476883256	-0.6549109172	-0.1513777574
O	8.0	2.0061158715	-0.8783129109	0.1458101497
C	6.0	0.3428922180	-0.3870306151	-1.4900431601
H	1.0	1.0859517932	-0.3955772535	-2.2876323887
C	6.0	-0.9731518492	-0.1426767851	-1.7120694818
H	1.0	-1.3351916642	0.0574734782	-2.7247004015
C	6.0	-1.9187983345	-0.1398374320	-0.6229269905
C	6.0	-3.2964693597	0.1069088468	-0.7844161934
H	1.0	-3.6874597128	0.3119181892	-1.7841966326
C	6.0	-4.1652956248	0.0952964723	0.3144771561
N	7.0	-5.5229066852	0.4016232939	0.1697135790
H	1.0	-5.8893759019	0.1743090039	-0.7498345476
H	1.0	-6.0998703491	0.0217737410	0.9164541641

FRAGNAME=H2ODFT

O1	2.4729885697	-1.9132038845	2.6574706423
H2	1.7349328677	-2.4629602485	2.8670420503
H3	2.1815778615	-1.3095317132	1.9929872618

FRAGNAME=H2ODFT

O1	4.0998416455	-2.6928287728	0.4265517706
H2	3.7546341278	-2.6163564959	1.3016873113
H3	3.6444613154	-2.0565009315	-0.1012683572

FRAGNAME=H2ODFT

O1	-6.7637250457	0.4199933538	2.8204174312
H2	-6.6411437044	1.3439283977	2.6714331926
H3	-7.6076073986	0.3211034464	3.2314670811

FRAGNAME=H2ODFT

O1	-6.3160401739	-0.5165198904	-2.5572976128
H2	-7.0381691255	-0.1907669702	-3.0704187156
H3	-6.2843693723	-1.4497047087	-2.6952885887

FRAGNAME=H2ODFT

O1	-6.0510996795	2.7273989599	1.6637803509
H2	-5.3254050810	3.2859536139	1.8923902858
H3	-5.7776328968	2.2194368868	0.9167402548

Optimized coordinates of 6AC(H2O)5 complex at S_1 state

C	6.0	-3.6368802969	-0.2109226615	1.6668033147
H	1.0	-4.3007716582	-0.2535583123	2.5297219444
C	6.0	-2.2689341684	-0.4159559575	1.7790459119
H	1.0	-1.8090314294	-0.6168824102	2.7488762441
C	6.0	-1.4168294912	-0.3946291584	0.6523367165
O	8.0	-0.0976206606	-0.6345461057	0.8854857289
C	6.0	0.8590153148	-0.6477281205	-0.2202100020

O	8.0	1.9977132293	-0.8979139956	0.1457010292
C	6.0	0.3552296172	-0.3765129525	-1.5135296405
H	1.0	1.0963846527	-0.3898703768	-2.3124572388
C	6.0	-1.0004769272	-0.1142328439	-1.7626930418
H	1.0	-1.3674922557	0.0918298137	-2.7672422829
C	6.0	-1.9116714331	-0.1387736137	-0.6500259178
C	6.0	-3.2989077591	0.0586693196	-0.7627024476
H	1.0	-3.7357541037	0.2534751753	-1.7458178472
C	6.0	-4.1616800369	0.0056291969	0.3675376385
N	7.0	-5.5061622361	0.1624530066	0.1692750889
H	1.0	-5.8766640167	0.1518430662	-0.7757556186
H	1.0	-6.1374034801	0.0780871127	0.9628298346

FRAGNAME=H2ODFT

O1	2.3929797132	-1.8563580961	2.6774909959
H2	1.6543961585	-2.4260861467	2.8216531797
H3	2.1529772689	-1.2735789814	1.9748916903

FRAGNAME=H2ODFT

O1	4.1021513862	-2.6521156262	0.4746018438
H2	3.7512172980	-2.5735917501	1.3472745893
H3	3.6065718432	-2.0626700255	-0.0711391703

FRAGNAME=H2ODFT

O1	-6.8234498644	0.5040945020	2.5881480381
H2	-6.6545648357	1.4321361928	2.5550584442
H3	-7.7159213416	0.4009178753	2.8775054298

FRAGNAME=H2ODFT

O1 -6.3017812329 -0.4244723132 -2.5190111229

H2 -6.9841291712 -0.0863497791 -3.0766426294

H3 -6.2078693054 -1.3397128277 -2.7297094965

FRAGNAME=H2ODFT

O1 -5.8484313558 2.8204235951 1.7523427326

H2 -5.4894829153 3.5602536829 2.2156848440

H3 -5.1890251551 2.5388152268 1.1385360502

Mulliken's population analyses of 6AC(H2O)5 complex

	S_1		S_0	
	MULL.POP.	**CHARGE**	**MULL.POP.**	**CHARGE**
1 C	5.989404	0.010596	5.978162	0.021838
2 H	0.983072	0.016928	0.955201	0.044799
3 C	5.93792	0.06208	5.941786	0.058214
4 H	1.014658	-0.014658	1.018002	-0.018002
5 C	5.891867	0.108133	5.906172	0.093828
6 O	8.286016	-0.286016	8.231067	-0.231067
7 C	5.819065	0.180935	5.797106	0.202894
8 O	8.323168	-0.323168	8.29348	-0.29348
9 C	6.07075	-0.07075	6.055767	-0.055767
10 H	1.023955	-0.023955	0.998068	0.001932
11 C	5.978102	0.021898	5.868367	0.131633
12 H	1.05981	-0.05981	1.019255	-0.019255
13 C	5.968101	0.031899	5.990726	0.009274
14 C	5.965096	0.034904	5.987956	0.012044
15 H	1.001105	-0.001105	1.020021	-0.020021
16 C	6.088202	-0.088202	6.05975	-0.05975
17 N	7.147209	-0.147209	7.309385	-0.309385
18 H	0.740387	0.259613	0.779585	0.220415
19 H	0.712114	0.287886	0.790143	0.209857