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The nature of the light absorption and emission transitions of 4-hydroxybenzophenone in different solvents. A combined computational and experimental study.

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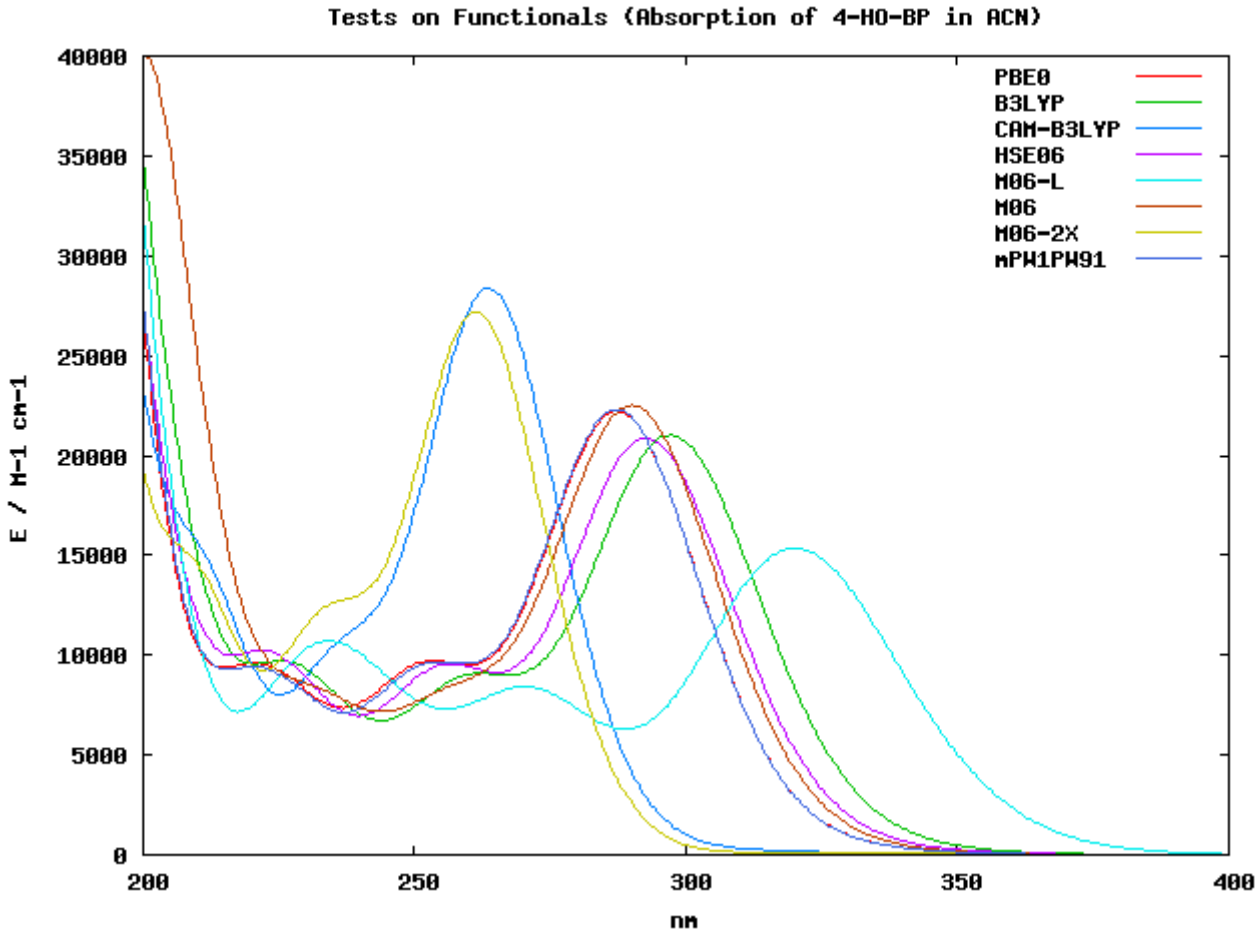
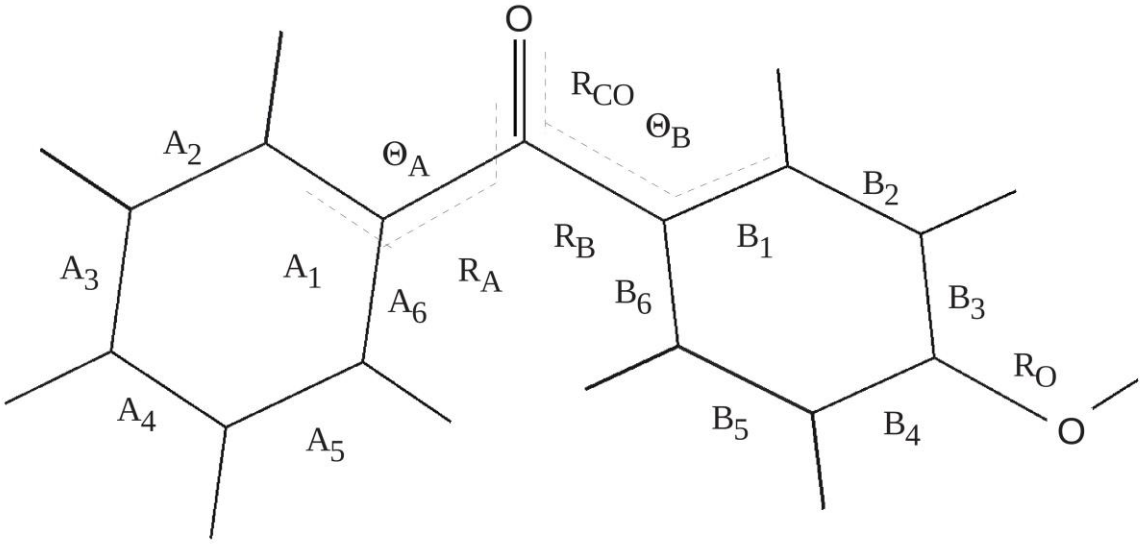
Figure 1: Tests on functionals.



The choice of the functional is limited on the availability of the gradient for the excited states and its implementation in the program Gaussian 09A. Among the 8 functional tested (PBE0, B3LYP, CAM-B3LYP, HSE06, M06-L, M06, M06-2X, mPW91PW91) PBE0 and mPW91PW91 are the ones that better fit the experimental curve. We chose the former.

Figure 2: Structures of the S_0, S_1, S_2, and T_1 states of 4HOBP in ACN.



Coord	Values ----------				Deviations ----------		
	S_0	T_1	S_1	S_2	T_1	S_1	S_2
R_{CO}	1.230	1.294	1.293	1.275	**0.01**	**0.01**	**0.01**
R_A	1.494	1.467	1.408	1.448	0.00	**0.03**	**0.01**
R_B	1.483	1.431	1.480	1.495	**0.01**	0.00	0.00
R_O	1.352	1.347	1.332	1.329	0.00	0.00	0.00
A_1	1.402	1.410	1.427	1.430	0.00	0.00	0.00
A_2	1.391	1.391	1.386	1.383	0.00	0.00	0.00
A_3	1.397	1.397	1.403	1.405	0.00	0.00	0.00
A_4	1.395	1.398	1.404	1.403	0.00	0.00	0.00
A_5	1.394	1.391	1.385	1.386	0.00	0.00	0.00
A_6	1.401	1.409	1.426	1.429	0.00	0.00	0.00
B_1	1.403	1.454	1.418	1.425	**0.01**	0.00	0.00
B_2	1.386	1.372	1.376	1.375	0.00	0.00	0.00
B_3	1.401	1.414	1.411	1.417	0.00	0.00	0.00
B_4	1.398	1.428	1.411	1.417	0.00	0.00	0.00
B_5	1.388	1.367	1.375	1.375	0.00	0.00	0.00
B_6	1.404	1.444	1.418	1.422	**0.01**	0.00	0.00
Θ_A	-33.06	-22.71	0.02	-15.50	**0.03**	**0.33**	**0.09**
Θ_B	-23.90	-21.70	-86.87	-25.13	0.00	**1.21**	0.00
	Standard deviations from S_0 =				**0.068**	**0.297**	**0.083**

Generation of Figure 2 in manuscript.

Figure 2 is intended to be purely illustrative. **R**, although related to the deformation of the structures with respect to the optimized geometries, is the same for all states and , indeed, dimensionless. All curves are parabolas whore parameters are defined as follows:

a. the parabola for the ground state is: $\mathbf{S_0(R) = k_0\ (R-R_0)^2}$ where $\mathbf{R_0} = 0$ and $\mathbf{k_0}$ set arbitrarily to 0.82 in order to get a reasonable agreement between the value of $\mathbf{S_0(R_1)}$ and the energies of the ground state at the excited states $\mathbf{S_1}$ (see below)

b. the parabola for the excited state $\mathbf{S_1}$ is: $\mathbf{S_1(R) = k_1\ (R-R_1)^2 + c_1}$ where the $\mathbf{R_1}$ is set arbitrarily to 1. $\mathbf{c_1}$ is set to the value of the energy of state $\mathbf{S_1}$ at its optimized energy; $\mathbf{k_1}$ and $\mathbf{R_1}$ are found solving system of the equations defining the following conditions:

$\mathbf{S_1(R_1)}$ is the energies of the $\mathbf{S_1}$ states at its optimized geometry;
$\mathbf{S_1(R=0)}$ corresponds to the vertical excitation energy fro $\mathbf{S_0}$ to $\mathbf{S_1}$.

c. the parabolas for the excited states $\mathbf{S_2}$ and $\mathbf{T_1}$ are: $\mathbf{S_2/T_1(R) = k_i\ (R-R_i)^2 + c_i}$ where the $\mathbf{R_i}$ are chosen so that the $\mathbf{S_0(R_i)}$ correspond to the energies of the ground state at the optimized geometries of the excited states **i**-esim. $\mathbf{k_i}$ and $\mathbf{c_i}$ are found solving system of the equations defining the following conditions:

$\mathbf{S_2/T_1(R_i)}$ are the energies of the excited states at their corresponding optimized geometries.
$\mathbf{S_2/T_1(R=0)}$ corresponds to the vertical excitation energies from $\mathbf{S_0}$ to $\mathbf{S_i}$.

Despite of being far to be rigorous, this approach allowed us to get a semi-quantitative picture that quite well describe the electronic states of 4HOBP in ACN

Tables 2.1-2.4: Energies, Cartesian coordinates and vertical transitions of the S_0, S_1, S_2 and T_1 states of 4HOBP in 2-Propanol.

Table 1.1a

****

4HOBP in ACN - S_0:

SCF Done: E(RPBE1PBE) = -651.149221428

Sum of electronic and thermal Free Energies= -650.991786

1	6	0	-0.013953	-0.011151	-0.005343
2	6	0	-0.027235	-0.026449	1.395623
3	6	0	1.170919	-0.024324	2.108091
4	6	0	2.389133	-0.029206	1.429013
5	6	0	2.409349	-0.017071	0.032363
6	6	0	1.214689	0.006065	-0.680046
7	1	0	-0.971871	-0.012529	1.932811
8	1	0	1.151818	-0.019363	3.195144
9	1	0	3.322697	-0.038873	1.986577
10	1	0	3.357671	-0.021459	-0.499590
11	1	0	1.221950	0.027608	-1.766739
12	6	0	-1.268680	0.067781	-0.812779
13	8	0	-1.275479	0.721269	-1.854903
14	6	0	-2.493011	-0.634030	-0.357411
15	6	0	-2.456027	-1.786033	0.444446
16	6	0	-3.623780	-2.448800	0.795405
17	6	0	-4.858015	-1.954327	0.362292
18	6	0	-4.915244	-0.805590	-0.437710
19	6	0	-3.739975	-0.165397	-0.799175
20	1	0	-1.504444	-2.190900	0.777158
21	1	0	-3.592674	-3.350188	1.401664
22	8	0	-5.967339	-2.626414	0.742513
23	1	0	-5.878164	-0.422665	-0.770990
24	1	0	-3.780009	0.721373	-1.426074
25	1	0	-6.757766	-2.195369	0.373488

Table 1.1b

4HOBP in ACN - S_0 - Vertical transitions:

Excited State 1:	Singlet-A	3.7971 eV	326.52 nm	f=0.0047
Excited State 2:	Singlet-A	4.3082 eV	287.79 nm	f=0.4050
Excited State 3:	Singlet-A	4.6950 eV	264.08 nm	f=0.0191
Excited State 4:	Singlet-A	4.7923 eV	258.71 nm	f=0.0050
Excited State 5:	Singlet-A	4.9281 eV	251.59 nm	f=0.1505
Excited State 6:	Singlet-A	5.3913 eV	229.97 nm	f=0.0891
Excited State 7:	Singlet-A	5.6475 eV	219.54 nm	f=0.0684
Excited State 8:	Singlet-A	5.7063 eV	217.28 nm	f=0.0387
Excited State 9:	Singlet-A	5.7548 eV	215.44 nm	f=0.0134
Excited State 10:	Singlet-A	5.8921 eV	210.42 nm	f=0.0040
Excited State 11:	Singlet-A	5.9339 eV	208.94 nm	f=0.0127
Excited State 12:	Singlet-A	6.1057 eV	203.06 nm	f=0.0035
Excited State 13:	Singlet-A	6.1158 eV	202.73 nm	f=0.0476
Excited State 14:	Singlet-A	6.1740 eV	200.82 nm	f=0.0899

Excited State	15:	Singlet-A	6.3600 eV	194.94 nm	f=0.0587
Excited State	16:	Singlet-A	6.3802 eV	194.33 nm	f=0.2212
Excited State	17:	Singlet-A	6.4278 eV	192.89 nm	f=0.1384
Excited State	18:	Singlet-A	6.4819 eV	191.28 nm	f=0.0118
Excited State	19:	Singlet-A	6.5508 eV	189.27 nm	f=0.1360
Excited State	20:	Singlet-A	6.6536 eV	186.34 nm	f=0.0103
Excited State	21:	Singlet-A	6.6705 eV	185.87 nm	f=0.0182
Excited State	22:	Singlet-A	6.7138 eV	184.67 nm	f=0.4215
Excited State	23:	Singlet-A	6.7201 eV	184.50 nm	f=0.0178
Excited State	24:	Singlet-A	6.8002 eV	182.32 nm	f=0.2365
Excited State	25:	Singlet-A	6.8175 eV	181.86 nm	f=0.3821
Excited State	26:	Singlet-A	6.8718 eV	180.42 nm	f=0.0654
Excited State	27:	Singlet-A	6.9124 eV	179.37 nm	f=0.0685
Excited State	28:	Singlet-A	6.9622 eV	178.08 nm	f=0.0368
Excited State	29:	Singlet-A	7.0066 eV	176.95 nm	f=0.0299
Excited State	30:	Singlet-A	7.0493 eV	175.88 nm	f=0.0445
Excited State	31:	Singlet-A	7.0685 eV	175.40 nm	f=0.0032
Excited State	32:	Singlet-A	7.1050 eV	174.50 nm	f=0.0171
Excited State	33:	Singlet-A	7.1480 eV	173.45 nm	f=0.0083
Excited State	34:	Singlet-A	7.1869 eV	172.51 nm	f=0.0043
Excited State	35:	Singlet-A	7.2472 eV	171.08 nm	f=0.0111
Excited State	36:	Singlet-A	7.2976 eV	169.90 nm	f=0.0157

Table 1.1c

4HOBP in ACN - S_0 - Triplet Vertical transitions:

Excited State	1:	Triplet-A	3.0062 eV	412.43 nm	f=0.0000
Excited State	2:	Triplet-A	3.2868 eV	377.21 nm	f=0.0000
Excited State	3:	Triplet-A	3.4855 eV	355.71 nm	f=0.0000
Excited State	4:	Triplet-A	4.1007 eV	302.35 nm	f=0.0000
Excited State	5:	Triplet-A	4.1984 eV	295.32 nm	f=0.0000
Excited State	6:	Triplet-A	4.2965 eV	288.57 nm	f=0.0000
Excited State	7:	Triplet-A	4.4053 eV	281.44 nm	f=0.0000
Excited State	8:	Triplet-A	4.4133 eV	280.93 nm	f=0.0000
Excited State	9:	Triplet-A	4.8870 eV	253.70 nm	f=0.0000
Excited State	10:	Triplet-A	5.0392 eV	246.04 nm	f=0.0000
Excited State	11:	Triplet-A	5.2519 eV	236.07 nm	f=0.0000
Excited State	12:	Triplet-A	5.6520 eV	219.36 nm	f=0.0000
Excited State	13:	Triplet-A	5.6986 eV	217.57 nm	f=0.0000
Excited State	14:	Triplet-A	5.7870 eV	214.25 nm	f=0.0000
Excited State	15:	Triplet-A	5.8131 eV	213.29 nm	f=0.0000
Excited State	16:	Triplet-A	5.8692 eV	211.25 nm	f=0.0000
Excited State	17:	Triplet-A	5.9684 eV	207.74 nm	f=0.0000
Excited State	18:	Triplet-A	6.0289 eV	205.65 nm	f=0.0000
Excited State	19:	Triplet-A	6.0939 eV	203.46 nm	f=0.0000
Excited State	20:	Triplet-A	6.3076 eV	196.56 nm	f=0.0000
Excited State	21:	Triplet-A	6.3880 eV	194.09 nm	f=0.0000
Excited State	22:	Triplet-A	6.4157 eV	193.25 nm	f=0.0000
Excited State	23:	Triplet-A	6.4585 eV	191.97 nm	f=0.0000
Excited State	24:	Triplet-A	6.5077 eV	190.52 nm	f=0.0000
Excited State	25:	Triplet-A	6.5490 eV	189.32 nm	f=0.0000
Excited State	26:	Triplet-A	6.6453 eV	186.58 nm	f=0.0000
Excited State	27:	Triplet-A	6.6707 eV	185.86 nm	f=0.0000
Excited State	28:	Triplet-A	6.7792 eV	182.89 nm	f=0.0000

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Excited State  29:      Triplet-A      6.8051 eV  182.19 nm  f=0.0000
Excited State  30:      Triplet-A      6.8217 eV  181.75 nm  f=0.0000
Excited State  31:      Triplet-A      6.8519 eV  180.95 nm  f=0.0000
Excited State  32:      Triplet-A      6.9139 eV  179.33 nm  f=0.0000
Excited State  33:      Triplet-A      6.9781 eV  177.68 nm  f=0.0000
Excited State  34:      Triplet-A      6.9821 eV  177.58 nm  f=0.0000
Excited State  35:      Triplet-A      7.0410 eV  176.09 nm  f=0.0000
Excited State  36:      Triplet-A      7.0529 eV  175.79 nm  f=0.0000
-----------------------------------------------------------------------

Table 1.2
***********************************************************************
4HOBP in ACN - S_1:
Total Energy, E(TD-HF/TD-KS) =  -651.028704626
Energy, force constant and most relevant orbital transitions:
Excited State   1:      Singlet-A      2.4600 eV  503.99 nm  f=0.0003
MO: Occ  Virt         Coeff.
     50 -> 53         0.18957
     52 -> 53         0.67219
-----------------------------------------------------------------------
     1          6           0        0.011600   -0.167843   -0.061943
     2          6           0       -0.106048    0.234081    1.301099
     3          6           0        1.017057    0.573248    2.036815
     4          6           0        2.298109    0.530604    1.462876
     5          6           0        2.428468    0.136881    0.122881
     6          6           0        1.319027   -0.206966   -0.632843
     7          1           0       -1.089996    0.273369    1.764345
     8          1           0        0.900444    0.876805    3.075532
     9          1           0        3.173982    0.798403    2.047724
    10          1           0        3.415642    0.099467   -0.334437
    11          1           0        1.434811   -0.510359   -1.670563
    12          6           0       -1.119687   -0.515543   -0.825558
    13          8           0       -1.164743   -0.895318   -2.061140
    14          6           0       -2.538273   -0.536339   -0.403394
    15          6           0       -3.117414   -1.727141    0.104335
    16          6           0       -4.430833   -1.745148    0.510758
    17          6           0       -5.216737   -0.582866    0.357425
    18          6           0       -4.677667    0.590694   -0.211151
    19          6           0       -3.361808    0.597883   -0.614668
    20          1           0       -2.500296   -2.615092    0.208032
    21          1           0       -4.880246   -2.633310    0.945229
    22          8           0       -6.484281   -0.656137    0.761120
    23          1           0       -5.303425    1.472702   -0.327182
    24          1           0       -2.932932    1.489919   -1.062326
    25          1           0       -6.945904    0.188658    0.600725
-----------------------------------------------------------------------

Table 1.3
***********************************************************************
4HOBP in ACN - S_2:
Total Energy, E(TD-HF/TD-KS) =  -651.004593591
Energy, force constant and most relevant orbital transitions:
Excited State   2:      Singlet-A      3.6801 eV  336.90 nm  f=0.4715
MO: Occ  Virt         Coeff.
     49 -> 53         0.14972
```

51 -> 53	0.35767				
52 -> 53	0.58022				
1	6	0	0.014534	-0.135868	-0.040932
2	6	0	0.066878	-0.300509	1.377212
3	6	0	1.263743	-0.186355	2.067246
4	6	0	2.461881	0.104948	1.398881
5	6	0	2.427284	0.306101	0.009048
6	6	0	1.239348	0.210691	-0.692827
7	1	0	-0.839811	-0.483712	1.944673
8	1	0	1.264746	-0.316030	3.147795
9	1	0	3.397273	0.181945	1.947188
10	1	0	3.345839	0.539967	-0.526296
11	1	0	1.220340	0.369809	-1.766947
12	6	0	-1.181268	-0.199228	-0.855590
13	8	0	-1.191644	0.324146	-2.018498
14	6	0	-2.462023	-0.740197	-0.306836
15	6	0	-2.535151	-1.805577	0.631556
16	6	0	-3.745442	-2.341444	1.003479
17	6	0	-4.943037	-1.793567	0.480904
18	6	0	-4.900178	-0.715832	-0.437741
19	6	0	-3.681566	-0.194407	-0.803550
20	1	0	-1.625520	-2.254615	1.015264
21	1	0	-3.805717	-3.186442	1.683186
22	8	0	-6.083065	-2.347340	0.879155
23	1	0	-5.826410	-0.328290	-0.857102
24	1	0	-3.628226	0.615494	-1.524227
25	1	0	-6.850512	-1.895599	0.475080

Table 1.4a

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4HOBP in ACN - T_1:

Total Energy, E(TD-HF/TD-KS) = -651.049249622

Energy, force constant and most relevant orbital transitions:

Excited State 1: Triplet-?Sym 2.3820 eV 520.51 nm f=0.000

MO: Occ Virt	Coeff.				
51 -> 53	0.18005				
52 -> 53	-0.64038				
52 -> 54	-0.14465				
52 -> 55	-0.10040				
1	6	0	-0.018678	0.106712	0.038206
2	6	0	0.008482	0.097238	1.446630
3	6	0	1.208883	-0.057200	2.132650
4	6	0	2.412046	-0.193441	1.433934
5	6	0	2.401001	-0.161394	0.037069
6	6	0	1.204004	-0.006313	-0.654213
7	1	0	-0.911457	0.238165	2.008847
8	1	0	1.207908	-0.057986	3.220422
9	1	0	3.348691	-0.311743	1.973251
10	1	0	3.332234	-0.260031	-0.516514
11	1	0	1.199208	0.018355	-1.740497
12	6	0	-1.258001	0.315787	-0.717486
13	8	0	-1.189413	0.825581	-1.904982

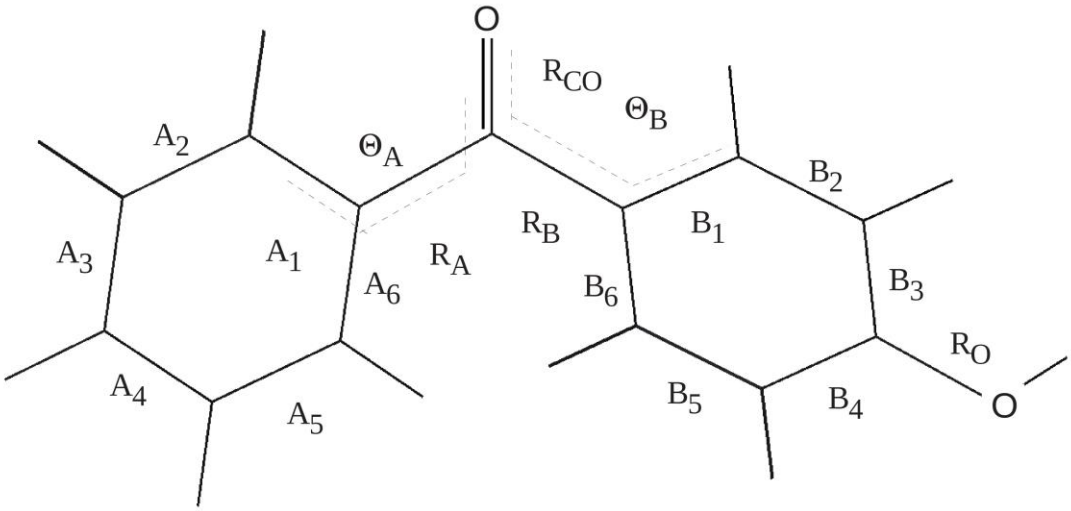
14	6	0	-2.565772	-0.097588	-0.308957
15	6	0	-2.804002	-1.153777	0.647163
16	6	0	-4.076436	-1.508001	1.000330
17	6	0	-5.199421	-0.871834	0.389698
18	6	0	-4.999741	0.109835	-0.608057
19	6	0	-3.727286	0.478719	-0.966139
20	1	0	-1.961232	-1.676614	1.087452
21	1	0	-4.254880	-2.291986	1.731873
22	8	0	-6.419619	-1.274420	0.794278
23	1	0	-5.861571	0.575714	-1.083120
24	1	0	-3.567640	1.238121	-1.723230
25	1	0	-7.111068	-0.798712	0.299534

Table 1.4b

4HOBP in ACN - T_1 - Vertical transitions:

Excited State 1:	3.021-A	0.9563 eV	1296.53 nm	f=0.0212
Excited State 2:	3.023-A	1.3579 eV	913.07 nm	f=0.0563
Excited State 3:	3.029-A	1.8418 eV	673.16 nm	f=0.0002
Excited State 4:	3.045-A	1.9819 eV	625.59 nm	f=0.0024
Excited State 5:	3.059-A	2.4907 eV	497.79 nm	f=0.2209
Excited State 6:	3.037-A	2.5830 eV	480.01 nm	f=0.0050
Excited State 7:	3.055-A	2.8428 eV	436.13 nm	f=0.0284
Excited State 8:	3.038-A	3.0508 eV	406.40 nm	f=0.0288
Excited State 9:	3.290-A	3.5969 eV	344.70 nm	f=0.0195
Excited State 10:	3.042-A	3.7267 eV	332.69 nm	f=0.0054
Excited State 11:	3.077-A	3.7599 eV	329.75 nm	f=0.0095
Excited State 12:	3.363-A	3.8860 eV	319.05 nm	f=0.1863
Excited State 13:	3.220-A	4.0226 eV	308.22 nm	f=0.0091
Excited State 14:	3.378-A	4.1501 eV	298.75 nm	f=0.0023
Excited State 15:	3.251-A	4.1529 eV	298.55 nm	f=0.0205
Excited State 16:	3.343-A	4.1901 eV	295.90 nm	f=0.0122
Excited State 17:	3.239-A	4.2728 eV	290.17 nm	f=0.0287
Excited State 18:	3.324-A	4.3564 eV	284.60 nm	f=0.0043
Excited State 19:	3.060-A	4.4047 eV	281.48 nm	f=0.0006
Excited State 20:	3.440-A	4.4735 eV	277.15 nm	f=0.0516
Excited State 21:	3.043-A	4.5161 eV	274.54 nm	f=0.0050
Excited State 22:	3.091-A	4.6037 eV	269.31 nm	f=0.0055
Excited State 23:	3.555-A	4.6893 eV	264.40 nm	f=0.0018
Excited State 24:	3.509-A	4.6996 eV	263.82 nm	f=0.0022
Excited State 25:	3.142-A	4.7365 eV	261.76 nm	f=0.1369
Excited State 26:	3.083-A	4.8823 eV	253.95 nm	f=0.0340
Excited State 27:	3.348-A	4.9177 eV	252.12 nm	f=0.0004
Excited State 28:	3.069-A	4.9658 eV	249.68 nm	f=0.0164
Excited State 29:	3.498-A	5.0007 eV	247.93 nm	f=0.0079
Excited State 30:	3.182-A	5.0223 eV	246.87 nm	f=0.0156
Excited State 31:	3.104-A	5.1145 eV	242.41 nm	f=0.0046
Excited State 32:	3.052-A	5.1844 eV	239.15 nm	f=0.0027
Excited State 33:	3.083-A	5.2038 eV	238.26 nm	f=0.0032
Excited State 34:	3.947-A	5.3020 eV	233.84 nm	f=0.0044
Excited State 35:	3.241-A	5.3602 eV	231.30 nm	f=0.0155
Excited State 36:	3.057-A	5.4988 eV	225.48 nm	f=0.0081

Figure 3: Structures of the S_0, S_1, S_2, and T_1 states of 4HOBP in 2-Propanol.



Coord	Values ----------				Deviations ----------		
	S_0	T_1	S_1	S_2	T_1	S_1	S_2
R_{CO}	1.234	1.285	1.298	1.283	0.01	0.01	0.01
R_A	1.492	1.477	1.409	1.449	0.00	**0.02**	0.01
R_B	1.479	1.432	1.478	1.485	0.01	0.00	0.00
R_O	1.353	1.346	1.328	1.328	0.00	0.00	0.00
A_1	1.402	1.406	1.426	1.428	0.00	0.00	0.00
A_2	1.391	1.391	1.385	1.383	0.00	0.00	0.00
A_3	1.397	1.396	1.402	1.403	0.00	0.00	0.00
A_4	1.395	1.396	1.404	1.402	0.00	0.00	0.00
A_5	1.393	1.393	1.385	1.386	0.00	0.00	0.00
A_6	1.401	1.405	1.426	1.426	0.00	0.00	0.00
B_1	1.404	1.463	1.420	1.431	0.01	0.00	0.00
B_2	1.386	1.367	1.374	1.374	0.00	0.00	0.00
B_3	1.401	1.419	1.414	1.416	0.00	0.00	0.00
B_4	1.398	1.436	1.414	1.420	0.01	0.00	0.00
B_5	1.387	1.363	1.373	1.374	0.00	0.00	0.00
B_6	1.404	1.451	1.420	1.424	0.01	0.00	0.00
Θ_A	-34.24	-29.19	0.57	-22.36	0.01	**0.37**	**0.04**
Θ_B	-23.46	-16.79	-84.98	-13.61	0.01	**1.15**	**0.03**
	Standard deviations from S_0 =				**0.062**	**0.296**	**0.076**

Tables 2.1-2.4: Energies, Cartesian coordinates and vertical transitions of the S_0, S_1, S_2 and T_1 states of 4HOBP in 2-Propanol.

Table 2.1a

****

4HOBP in 2-Propanol - S_0:

SCF Done: E(RPBE1PBE) = -651.149703095

Sum of electronic and thermal Free Energies= -650.991777

1	6	0	-0.004345	0.009665	0.000885
2	6	0	-0.005251	0.016421	1.402038
3	6	0	1.199115	0.005536	2.102915
4	6	0	2.410093	-0.035862	1.412468
5	6	0	2.417478	-0.047371	0.015987
6	6	0	1.217369	-0.010257	-0.686114
7	1	0	-0.944653	0.059205	1.947082
8	1	0	1.190939	0.028466	3.189952
9	1	0	3.348760	-0.056087	1.961326
10	1	0	3.360464	-0.081598	-0.524414
11	1	0	1.216228	-0.010036	-1.773212
12	6	0	-1.265592	0.097831	-0.790870
13	8	0	-1.277353	0.752098	-1.836643
14	6	0	-2.487087	-0.593520	-0.323605
15	6	0	-2.443825	-1.738642	0.488388
16	6	0	-3.608812	-2.395277	0.856170
17	6	0	-4.846467	-1.902605	0.430569
18	6	0	-4.909978	-0.761786	-0.380493
19	6	0	-3.737707	-0.126726	-0.758503
20	1	0	-1.489656	-2.143023	0.814300
21	1	0	-3.574682	-3.291156	1.470596
22	8	0	-5.951463	-2.571901	0.831686
23	1	0	-5.875828	-0.382185	-0.707371
24	1	0	-3.784471	0.756127	-1.390690
25	1	0	-6.750977	-2.149229	0.477676

Table 2.1b

4HOBP in 2-Propanol - S_0 - Vertical transitions:

Excited State	1:	Singlet-A	3.8637 eV	320.89 nm	f=0.0077
Excited State	2:	Singlet-A	4.2484 eV	291.84 nm	f=0.4416
Excited State	3:	Singlet-A	4.6358 eV	267.45 nm	f=0.0215
Excited State	4:	Singlet-A	4.7449 eV	261.30 nm	f=0.0051
Excited State	5:	Singlet-A	4.8685 eV	254.66 nm	f=0.1471
Excited State	6:	Singlet-A	5.3960 eV	229.77 nm	f=0.0980
Excited State	7:	Singlet-A	5.6684 eV	218.73 nm	f=0.0636
Excited State	8:	Singlet-A	5.7227 eV	216.65 nm	f=0.0283
Excited State	9:	Singlet-A	5.7856 eV	214.30 nm	f=0.0195
Excited State	10:	Singlet-A	5.9733 eV	207.57 nm	f=0.0058
Excited State	11:	Singlet-A	6.0114 eV	206.25 nm	f=0.0127
Excited State	12:	Singlet-A	6.1508 eV	201.57 nm	f=0.1388
Excited State	13:	Singlet-A	6.1852 eV	200.45 nm	f=0.0016
Excited State	14:	Singlet-A	6.2503 eV	198.36 nm	f=0.0347
Excited State	15:	Singlet-A	6.3900 eV	194.03 nm	f=0.3314

```
Excited State  16:      Singlet-A      6.3990 eV  193.76 nm  f=0.0188
Excited State  17:      Singlet-A      6.4490 eV  192.25 nm  f=0.0636
Excited State  18:      Singlet-A      6.5354 eV  189.71 nm  f=0.1097
Excited State  19:      Singlet-A      6.5631 eV  188.91 nm  f=0.0290
Excited State  20:      Singlet-A      6.6095 eV  187.58 nm  f=0.0187
Excited State  21:      Singlet-A      6.6248 eV  187.15 nm  f=0.0335
Excited State  22:      Singlet-A      6.7135 eV  184.68 nm  f=0.2713
Excited State  23:      Singlet-A      6.7649 eV  183.27 nm  f=0.2641
Excited State  24:      Singlet-A      6.8086 eV  182.10 nm  f=0.2447
Excited State  25:      Singlet-A      6.8369 eV  181.34 nm  f=0.3200
Excited State  26:      Singlet-A      6.9032 eV  179.60 nm  f=0.0669
Excited State  27:      Singlet-A      6.9409 eV  178.63 nm  f=0.0205
Excited State  28:      Singlet-A      6.9992 eV  177.14 nm  f=0.0164
Excited State  29:      Singlet-A      7.0146 eV  176.75 nm  f=0.0048
Excited State  30:      Singlet-A      7.0589 eV  175.64 nm  f=0.0309
Excited State  31:      Singlet-A      7.0976 eV  174.69 nm  f=0.0292
Excited State  32:      Singlet-A      7.1652 eV  173.04 nm  f=0.0128
Excited State  33:      Singlet-A      7.1765 eV  172.76 nm  f=0.0348
Excited State  34:      Singlet-A      7.2365 eV  171.33 nm  f=0.0041
Excited State  35:      Singlet-A      7.3415 eV  168.88 nm  f=0.0433
Excited State  36:      Singlet-A      7.3638 eV  168.37 nm  f=0.0004
-----------------------------------------------------------------------

Table 2.2
***********************************************************************
4HOBP in 2-Propanol - S_1:
Total Energy, E(TD-HF/TD-KS) =  -651.029413720
Energy, force constant and most relevant orbital transitions:
Excited State   1:      Singlet-A      2.4547 eV  505.08 nm  f=0.0011
MO: Occ  Virt         Coeff.
     49 -> 53         0.18244
     52 -> 53         0.67699
-----------------------------------------------------------------------
     1          6           0       -0.001280    0.011052   -0.003728
     2          6           0       -0.004402   -0.009508    1.421626
     3          6           0        1.184807   -0.027971    2.131009
     4          6           0        2.421904   -0.026724    1.467799
     5          6           0        2.439946   -0.006428    0.065632
     6          6           0        1.262722    0.012215   -0.664594
     7          1           0       -0.952817   -0.012227    1.955613
     8          1           0        1.155056   -0.044817    3.219002
     9          1           0        3.350700   -0.042118    2.031965
    10          1           0        3.392588   -0.005525   -0.461336
    11          1           0        1.292378    0.028134   -1.751466
    12          6           0       -1.201861    0.029100   -0.740342
    13          8           0       -1.348363    0.037914   -2.030218
    14          6           0       -2.586335    0.017183   -0.221753
    15          6           0       -3.257493   -1.214023    0.003021
    16          6           0       -4.537165   -1.228027    0.500137
    17          6           0       -5.207395   -0.002597    0.721222
    18          6           0       -4.583656    1.232046    0.430143
    19          6           0       -3.300616    1.233999   -0.062272
    20          1           0       -2.730416   -2.145790   -0.181687
    21          1           0       -5.052760   -2.156721    0.726601
    22          8           0       -6.444242   -0.077407    1.198791
```

23	1	0	-5.124447	2.160168	0.598129
24	1	0	-2.806162	2.172311	-0.297314
25	1	0	-6.836821	0.806807	1.312027

Table 2.3

4HOBP in 2-Propanol - S_2:
Total Energy, E(TD-HF/TD-KS) = -651.007060603
Energy, force constant and most relevant orbital transitions:
Excited State 2: Singlet-A 3.6292 eV 341.63 nm f=0.5999

MO: Occ	Virt	Coeff.
48	53	0.11232
49	53	-0.11506
51	53	0.29807
52	53	-0.61561

1	6	0	0.000262	0.083561	0.048589
2	6	0	0.042418	0.048092	1.473517
3	6	0	1.247876	-0.053193	2.150752
4	6	0	2.463593	-0.115038	1.456060
5	6	0	2.447906	-0.045083	0.054548
6	6	0	1.253807	0.070309	-0.634453
7	1	0	-0.869316	0.154056	2.052682
8	1	0	1.244776	-0.070443	3.238862
9	1	0	3.403411	-0.205663	1.994923
10	1	0	3.383574	-0.085657	-0.499862
11	1	0	1.253297	0.120086	-1.719757
12	6	0	-1.200687	0.234812	-0.747355
13	8	0	-1.121236	0.769107	-1.911314
14	6	0	-2.551684	-0.129690	-0.249880
15	6	0	-2.803532	-1.010302	0.840946
16	6	0	-4.086162	-1.356189	1.192610
17	6	0	-5.186461	-0.798995	0.489686
18	6	0	-4.965876	0.077178	-0.600297
19	6	0	-3.678420	0.401248	-0.953434
20	1	0	-1.978905	-1.471968	1.371881
21	1	0	-4.281666	-2.056028	2.000118
22	8	0	-6.400716	-1.160126	0.888373
23	1	0	-5.817192	0.464443	-1.155806
24	1	0	-3.491977	1.050069	-1.803120
25	1	0	-7.093136	-0.707584	0.371387

Table 2.4a

4HOBP in 2-Propanol - T_1:
Total Energy, E(TD-HF/TD-KS) = -651.049250074
Energy, force constant and most relevant orbital transitions:
Excited State 1: Triplet-?Sym 2.4301 eV 510.21 nm f=0.000

MO: Occ	Virt	Coeff.
51	53	-0.11937
52	53	-0.65711
52	54	0.16123

1	6	0	-0.010908	0.031934	0.005809
2	6	0	-0.011005	0.043047	1.411045
3	6	0	1.186171	0.009251	2.121667
4	6	0	2.406612	-0.033889	1.445247
5	6	0	2.419321	-0.029282	0.048818
6	6	0	1.224954	0.010902	-0.663893
7	1	0	-0.950951	0.108389	1.954465
8	1	0	1.165808	0.027376	3.209171
9	1	0	3.340504	-0.061632	2.001775
10	1	0	3.365402	-0.057836	-0.487424
11	1	0	1.238856	0.017532	-1.750881
12	6	0	-1.256767	0.124342	-0.782199
13	8	0	-1.236321	0.727088	-1.916471
14	6	0	-2.493157	-0.491670	-0.403147
15	6	0	-2.593569	-1.566852	0.565924
16	6	0	-3.804206	-2.099833	0.895032
17	6	0	-5.002800	-1.633490	0.256544
18	6	0	-4.926274	-0.644862	-0.758983
19	6	0	-3.718740	-0.101923	-1.100765
20	1	0	-1.691889	-1.957535	1.025590
21	1	0	-3.883987	-2.899156	1.627704
22	8	0	-6.157973	-2.202962	0.646740
23	1	0	-5.838862	-0.323213	-1.257468
24	1	0	-3.651781	0.657438	-1.871251
25	1	0	-6.906954	-1.834015	0.147016

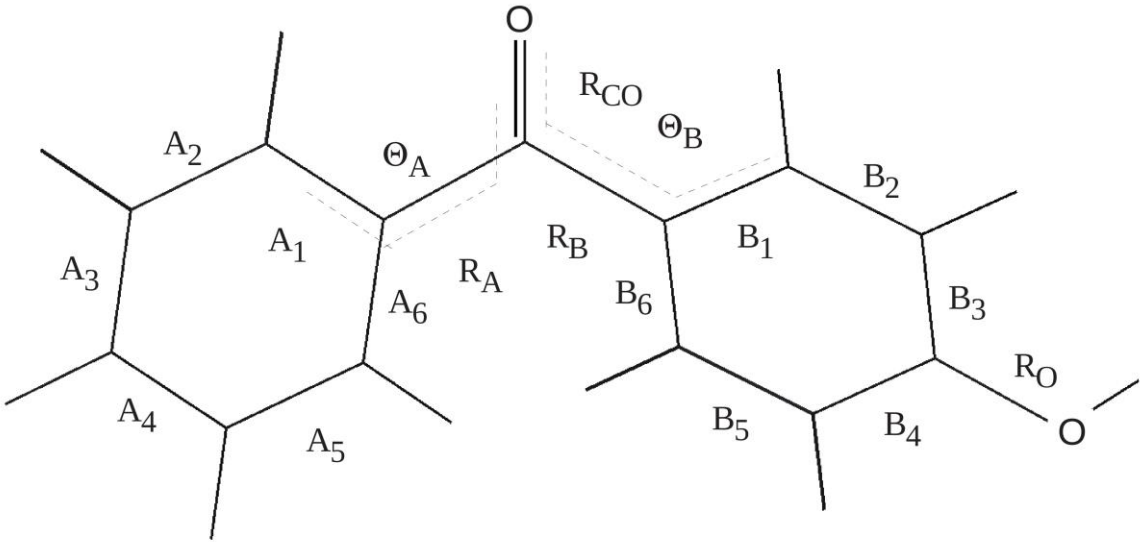
Table 2.4b

4HOBP in 2-Propanol - T_1 - Vertical transitions:

Excited State	1:	3.021-A	0.9677 eV	1281.22 nm	f=0.0288
Excited State	2:	3.021-A	1.3114 eV	945.42 nm	f=0.0585
Excited State	3:	3.028-A	1.7809 eV	696.18 nm	f=0.0002
Excited State	4:	3.044-A	1.9208 eV	645.49 nm	f=0.0025
Excited State	5:	3.052-A	2.4458 eV	506.93 nm	f=0.2312
Excited State	6:	3.034-A	2.5527 eV	485.70 nm	f=0.0020
Excited State	7:	3.056-A	2.8484 eV	435.28 nm	f=0.0267
Excited State	8:	3.039-A	3.0254 eV	409.80 nm	f=0.0377
Excited State	9:	3.269-A	3.5787 eV	346.45 nm	f=0.0236
Excited State	10:	3.043-A	3.7080 eV	334.37 nm	f=0.0052
Excited State	11:	3.072-A	3.7684 eV	329.01 nm	f=0.0131
Excited State	12:	3.300-A	3.9068 eV	317.36 nm	f=0.1658
Excited State	13:	3.198-A	3.9707 eV	312.24 nm	f=0.0015
Excited State	14:	3.328-A	4.0948 eV	302.78 nm	f=0.0001
Excited State	15:	3.512-A	4.1557 eV	298.35 nm	f=0.0466
Excited State	16:	3.095-A	4.2125 eV	294.33 nm	f=0.0013
Excited State	17:	3.223-A	4.2633 eV	290.82 nm	f=0.0292
Excited State	18:	3.363-A	4.3329 eV	286.15 nm	f=0.0031
Excited State	19:	3.064-A	4.4048 eV	281.47 nm	f=0.0006
Excited State	20:	3.464-A	4.4420 eV	279.12 nm	f=0.0483
Excited State	21:	3.052-A	4.5266 eV	273.90 nm	f=0.0028
Excited State	22:	3.112-A	4.6127 eV	268.79 nm	f=0.0143
Excited State	23:	3.070-A	4.6710 eV	265.43 nm	f=0.0032
Excited State	24:	3.202-A	4.7185 eV	262.76 nm	f=0.1363
Excited State	25:	3.853-A	4.7281 eV	262.23 nm	f=0.0183

```
Excited State  26:  3.073-A           4.8742 eV  254.37 nm  f=0.0311
Excited State  27:  3.324-A           4.9532 eV  250.31 nm  f=0.0031
Excited State  28:  3.196-A           4.9859 eV  248.67 nm  f=0.0172
Excited State  29:  3.276-A           5.0157 eV  247.19 nm  f=0.0049
Excited State  30:  3.133-A           5.0313 eV  246.43 nm  f=0.0147
Excited State  31:  3.309-A           5.0715 eV  244.47 nm  f=0.0092
Excited State  32:  3.067-A           5.1946 eV  238.68 nm  f=0.0020
Excited State  33:  3.069-A           5.2081 eV  238.06 nm  f=0.0041
Excited State  34:  3.934-A           5.3027 eV  233.81 nm  f=0.0052
Excited State  35:  3.263-A           5.3663 eV  231.04 nm  f=0.0138
Excited State  36:  3.054-A           5.4603 eV  227.06 nm  f=0.0079
-----------------------------------------------------------------------
```

Figure 4: Structures of the S_0, S_1, S_2, and T_1 states of 4HOBP in Water.



Coord	Values ----------				Deviations ----------		
	S_0	T_1	S_1	S_2	T_1	S_1	S_2
R_{CO}	1.237	1.286	1.305	1.292	0.01	**0.02**	0.01
R_A	1.490	1.478	1.410	1.450	0.00	**0.02**	0.01
R_B	1.477	1.434	1.477	1.476	0.01	0.00	0.00
R_O	1.359	1.349	1.328	1.332	0.00	0.00	0.00
A_1	1.402	1.405	1.426	1.427	0.00	0.00	0.00
A_2	1.391	1.392	1.386	1.384	0.00	0.00	0.00
A_3	1.397	1.396	1.402	1.402	0.00	0.00	0.00
A_4	1.395	1.396	1.403	1.401	0.00	0.00	0.00
A_5	1.393	1.393	1.385	1.387	0.00	0.00	0.00
A_6	1.401	1.405	1.425	1.424	0.00	0.00	0.00
B_1	1.405	1.464	1.421	1.433	0.01	0.00	0.00
B_2	1.385	1.366	1.372	1.374	0.00	0.00	0.00
B_3	1.401	1.421	1.415	1.415	0.00	0.00	0.00
B_4	1.398	1.437	1.415	1.420	0.01	0.00	0.00
B_5	1.387	1.362	1.373	1.374	0.00	0.00	0.00
B_6	1.405	1.451	1.421	1.427	0.01	0.00	0.00
Θ_A	-34.45	-29.11	0.80	-25.69	0.01	**0.38**	**0.02**
Θ_B	-23.20	-16.70	-84.96	-7.84	0.01	**1.16**	**0.07**
	Standard deviations from S_0 =				**0.061**	**0.297**	**0.084**

Tables 3.1-3.4: Energies, Cartesian coordinates and vertical transitions of the S_0, S_1, S_2 and T_1 states of 4HOBP in Water.

Table 3.1a

****

4HOBP in Water - S_0:

SCF Done: E(RPBE1PBE) = -651.143255699

Sum of electronic and thermal Free Energies= -650.984820

1	6	0	-0.020554	0.000292	-0.004286
2	6	0	-0.034812	-0.007686	1.396927
3	6	0	1.163091	-0.019235	2.108391
4	6	0	2.380388	-0.047191	1.428215
5	6	0	2.400823	-0.045884	0.031743
6	6	0	1.207215	-0.007247	-0.681102
7	1	0	-0.979470	0.024092	1.932889
8	1	0	1.144984	-0.006808	3.195008
9	1	0	3.313810	-0.068863	1.985050
10	1	0	3.348495	-0.071671	-0.499930
11	1	0	1.217051	0.000385	-1.767884
12	6	0	-1.274832	0.090246	-0.802687
13	8	0	-1.282067	0.760222	-1.843037
14	6	0	-2.493190	-0.615024	-0.356699
15	6	0	-2.444005	-1.767589	0.444864
16	6	0	-3.604688	-2.442115	0.792830
17	6	0	-4.841838	-1.958619	0.357235
18	6	0	-4.912666	-0.810155	-0.441448
19	6	0	-3.744742	-0.157105	-0.800079
20	1	0	-1.488597	-2.162896	0.777006
21	1	0	-3.566340	-3.343136	1.398572
22	8	0	-5.950452	-2.647187	0.735643
23	1	0	-5.880912	-0.440967	-0.771806
24	1	0	-3.796388	0.732181	-1.422177
25	1	0	-6.745743	-2.224083	0.372589

Table 3.1b

4HOBP in Water - S_0 - Vertical transitions:

Excited State	1:	Singlet-A	3.9142 eV	316.75 nm	f=0.0106
Excited State	2:	Singlet-A	4.2198 eV	293.82 nm	f=0.4528
Excited State	3:	Singlet-A	4.5844 eV	270.45 nm	f=0.0221
Excited State	4:	Singlet-A	4.7020 eV	263.68 nm	f=0.0053
Excited State	5:	Singlet-A	4.8287 eV	256.77 nm	f=0.1369
Excited State	6:	Singlet-A	5.4150 eV	228.97 nm	f=0.0929
Excited State	7:	Singlet-A	5.6950 eV	217.71 nm	f=0.0564
Excited State	8:	Singlet-A	5.7276 eV	216.47 nm	f=0.0218
Excited State	9:	Singlet-A	5.8223 eV	212.95 nm	f=0.0167
Excited State	10:	Singlet-A	6.0443 eV	205.12 nm	f=0.0032
Excited State	11:	Singlet-A	6.0763 eV	204.05 nm	f=0.0296
Excited State	12:	Singlet-A	6.1838 eV	200.50 nm	f=0.1534
Excited State	13:	Singlet-A	6.2662 eV	197.86 nm	f=0.0019
Excited State	14:	Singlet-A	6.3130 eV	196.39 nm	f=0.0294
Excited State	15:	Singlet-A	6.4106 eV	193.40 nm	f=0.3061

```
Excited State  16:      Singlet-A      6.4188 eV  193.16 nm  f=0.0151
Excited State  17:      Singlet-A      6.4977 eV  190.81 nm  f=0.0488
Excited State  18:      Singlet-A      6.5434 eV  189.48 nm  f=0.0857
Excited State  19:      Singlet-A      6.5585 eV  189.04 nm  f=0.0265
Excited State  20:      Singlet-A      6.5853 eV  188.28 nm  f=0.0815
Excited State  21:      Singlet-A      6.6389 eV  186.75 nm  f=0.0059
Excited State  22:      Singlet-A      6.7224 eV  184.43 nm  f=0.2525
Excited State  23:      Singlet-A      6.7918 eV  182.55 nm  f=0.3294
Excited State  24:      Singlet-A      6.8284 eV  181.57 nm  f=0.3138
Excited State  25:      Singlet-A      6.8783 eV  180.25 nm  f=0.1886
Excited State  26:      Singlet-A      6.9363 eV  178.75 nm  f=0.0413
Excited State  27:      Singlet-A      6.9723 eV  177.82 nm  f=0.0310
Excited State  28:      Singlet-A      6.9970 eV  177.20 nm  f=0.0188
Excited State  29:      Singlet-A      7.0424 eV  176.05 nm  f=0.0192
Excited State  30:      Singlet-A      7.0629 eV  175.54 nm  f=0.0067
Excited State  31:      Singlet-A      7.1498 eV  173.41 nm  f=0.0494
Excited State  32:      Singlet-A      7.2215 eV  171.69 nm  f=0.0140
Excited State  33:      Singlet-A      7.2730 eV  170.47 nm  f=0.0345
Excited State  34:      Singlet-A      7.3023 eV  169.79 nm  f=0.0068
Excited State  35:      Singlet-A      7.3926 eV  167.71 nm  f=0.0445
Excited State  36:      Singlet-A      7.4417 eV  166.61 nm  f=0.0050
--------------------------------------------------------------------------------
```

Table 3.2

```
********************************************************************************
4HOBP in Water - S_1:
Total Energy, E(TD-HF/TD-KS) =  -651.022471433
Energy, force constant and most relevant orbital transitions:
Excited State   1:      Singlet-A      2.4846 eV  499.02 nm  f=0.0013
MO: Occ  Virt         Coeff.
     48 -> 53         0.17382
     52 -> 53         0.67988
--------------------------------------------------------------------------------
     1          6          0        0.023987   -0.194206   -0.063875
     2          6          0       -0.084481    0.055160    1.334858
     3          6          0        1.035563    0.371389    2.086086
     4          6          0        2.303810    0.454404    1.491135
     5          6          0        2.425226    0.212401    0.115195
     6          6          0        1.318175   -0.105747   -0.655159
     7          1          0       -1.058899   -0.006036    1.815341
     8          1          0        0.925950    0.555607    3.152759
     9          1          0        3.177631    0.701569    2.087470
    10          1          0        3.402726    0.273637   -0.359011
    11          1          0        1.428234   -0.290619   -1.720757
    12          6          0       -1.107119   -0.520563   -0.839041
    13          8          0       -1.147310   -0.787754   -2.115574
    14          6          0       -2.502600   -0.665998   -0.378590
    15          6          0       -2.980584   -1.925711    0.074478
    16          6          0       -4.272075   -2.061673    0.516426
    17          6          0       -5.145648   -0.949949    0.449678
    18          6          0       -4.709218    0.294173   -0.063853
    19          6          0       -3.412505    0.419696   -0.496533
    20          1          0       -2.298002   -2.769670    0.106688
    21          1          0       -4.646829   -3.000709    0.911794
```

22	8	0	-6.389158	-1.140325	0.875788
23	1	0	-5.405366	1.127389	-0.108726
24	1	0	-3.058805	1.364181	-0.899256
25	1	0	-6.926335	-0.333405	0.776259

Table 3.3

4HOBP in Water - S_2:
Total Energy, E(TD-HF/TD-KS) = -651.002739736
Energy, force constant and most relevant orbital transitions:
Excited State 2: Singlet-?Sym 3.5572 eV 348.54 nm f=0.686

MO: Occ	Virt	Coeff.
48	53	-0.15775
51	53	0.26620
52	53	0.62899

1	6	0	-0.054038	0.066689	0.063734
2	6	0	0.038957	-0.094685	1.475558
3	6	0	1.270225	-0.233955	2.097794
4	6	0	2.459370	-0.206975	1.357017
5	6	0	2.393239	-0.012565	-0.030317
6	6	0	1.171596	0.136875	-0.662944
7	1	0	-0.852652	-0.058263	2.092284
8	1	0	1.308461	-0.351424	3.178354
9	1	0	3.419262	-0.326966	1.852247
10	1	0	3.308145	0.014128	-0.617920
11	1	0	1.130756	0.276977	-1.739194
12	6	0	-1.287542	0.266381	-0.672593
13	8	0	-1.249692	0.966073	-1.758581
14	6	0	-2.600213	-0.248449	-0.237259
15	6	0	-2.795630	-1.197883	0.809589
16	6	0	-4.047951	-1.673460	1.113753
17	6	0	-5.180566	-1.190197	0.407600
18	6	0	-5.018805	-0.249236	-0.636732
19	6	0	-3.759874	0.203390	-0.948163
20	1	0	-1.947204	-1.608826	1.342946
21	1	0	-4.193072	-2.423580	1.885441
22	8	0	-6.367777	-1.682490	0.757975
23	1	0	-5.892247	0.082121	-1.193672
24	1	0	-3.624187	0.903810	-1.765082
25	1	0	-7.084765	-1.287203	0.228279

Table 3.4a

4HOBP in Water - T_1:
Total Energy, E(TD-HF/TD-KS) = -651.042787905
Energy, force constant and most relevant orbital transitions:
Excited State 1: Triplet-?Sym 2.4453 eV 507.03 nm f=0.000

MO: Occ	Virt	Coeff.
51	53	0.10320
52	53	-0.66036

52 -> 54	0.16632				
1	6	0	0.001197	-0.009512	-0.006415
2	6	0	-0.004861	-0.013866	1.398641
3	6	0	1.189981	-0.005078	2.113993
4	6	0	2.413532	0.008665	1.442293
5	6	0	2.431583	0.026653	0.046085
6	6	0	1.239031	0.025237	-0.671077
7	1	0	-0.948119	0.005811	1.939026
8	1	0	1.164430	0.001229	3.200998
9	1	0	3.345084	0.013510	2.002537
10	1	0	3.379460	0.041609	-0.486513
11	1	0	1.257636	0.042426	-1.757627
12	6	0	-1.244425	0.048195	-0.799057
13	8	0	-1.241248	0.667253	-1.926244
14	6	0	-2.461576	-0.608325	-0.420683
15	6	0	-2.524754	-1.689769	0.545350
16	6	0	-3.716061	-2.261956	0.875639
17	6	0	-4.930958	-1.826393	0.244122
18	6	0	-4.890416	-0.827009	-0.765056
19	6	0	-3.702186	-0.247485	-1.108650
20	1	0	-1.609818	-2.053727	0.999581
21	1	0	-3.768752	-3.068332	1.602222
22	8	0	-6.071248	-2.434176	0.631270
23	1	0	-5.815918	-0.530998	-1.254517
24	1	0	-3.662792	0.519125	-1.873408
25	1	0	-6.829415	-2.077308	0.136292

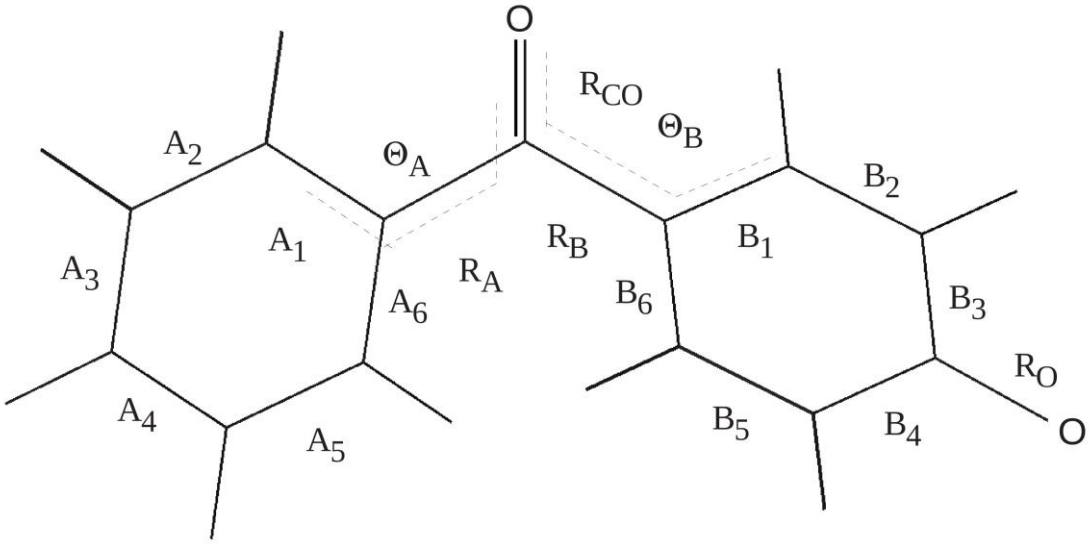
Table 3.4b

4HOBP in Water - T_1 - Vertical transitions:

Excited State	1:	3.020-A	0.9896 eV	1252.87 nm	f=0.0340
Excited State	2:	3.019-A	1.2931 eV	958.78 nm	f=0.0564
Excited State	3:	3.028-A	1.7466 eV	709.84 nm	f=0.0004
Excited State	4:	3.043-A	1.8588 eV	667.01 nm	f=0.0024
Excited State	5:	3.046-A	2.4174 eV	512.88 nm	f=0.2235
Excited State	6:	3.033-A	2.5457 eV	487.03 nm	f=0.0018
Excited State	7:	3.056-A	2.8507 eV	434.92 nm	f=0.0254
Excited State	8:	3.041-A	3.0096 eV	411.96 nm	f=0.0454
Excited State	9:	3.254-A	3.5641 eV	347.87 nm	f=0.0235
Excited State	10:	3.046-A	3.6831 eV	336.63 nm	f=0.0054
Excited State	11:	3.069-A	3.7873 eV	327.36 nm	f=0.0155
Excited State	12:	3.110-A	3.9054 eV	317.47 nm	f=0.0688
Excited State	13:	3.264-A	3.9345 eV	315.12 nm	f=0.0661
Excited State	14:	3.321-A	4.0395 eV	306.93 nm	f=0.0061
Excited State	15:	3.570-A	4.1537 eV	298.49 nm	f=0.0574
Excited State	16:	3.207-A	4.2630 eV	290.84 nm	f=0.0262
Excited State	17:	3.042-A	4.2712 eV	290.28 nm	f=0.0006
Excited State	18:	3.401-A	4.3136 eV	287.43 nm	f=0.0019
Excited State	19:	3.520-A	4.4159 eV	280.77 nm	f=0.0385
Excited State	20:	3.035-A	4.4337 eV	279.64 nm	f=0.0026
Excited State	21:	3.068-A	4.5623 eV	271.76 nm	f=0.0012
Excited State	22:	3.128-A	4.6340 eV	267.55 nm	f=0.0309
Excited State	23:	3.054-A	4.6494 eV	266.66 nm	f=0.0044

```
Excited State  24:  3.156-A           4.7244 eV  262.44 nm  f=0.1650
Excited State  25:  3.848-A           4.7721 eV  259.81 nm  f=0.0058
Excited State  26:  3.068-A           4.9009 eV  252.98 nm  f=0.0169
Excited State  27:  3.308-A           4.9739 eV  249.27 nm  f=0.0053
Excited State  28:  3.178-A           5.0069 eV  247.63 nm  f=0.0237
Excited State  29:  3.179-A           5.0193 eV  247.02 nm  f=0.0013
Excited State  30:  3.130-A           5.0532 eV  245.36 nm  f=0.0010
Excited State  31:  3.455-A           5.0747 eV  244.32 nm  f=0.0212
Excited State  32:  3.119-A           5.2288 eV  237.12 nm  f=0.0024
Excited State  33:  3.072-A           5.2420 eV  236.52 nm  f=0.0043
Excited State  34:  3.876-A           5.3067 eV  233.64 nm  f=0.0051
Excited State  35:  3.301-A           5.3778 eV  230.55 nm  f=0.0093
Excited State  36:  3.055-A           5.4191 eV  228.79 nm  f=0.0065
-----------------------------------------------------------------------
```

Figure 5: Structures of the S_0 and S_1 states of 4OBP Anion in Water.



Coord	Values ----------		Deviations ----------
	S_0	S_1	S_1
R_{CO}	1.250	1.303	0.01
R_A	1.496	1.421	**0.02**
R_B	1.452	1.486	0.00
R_O	1.285	1.260	0.00
A_1	1.416	1.429	0.00
A_2	1.376	1.385	0.00
A_3	1.436	1.404	0.00
A_4	1.433	1.404	0.00
A_5	1.379	1.386	0.00
A_6	1.415	1.428	0.00
B_1	1.403	1.422	0.00
B_2	1.386	1.368	0.00
B_3	1.401	1.449	0.01
B_4	1.398	1.449	0.01
B_5	1.388	1.368	0.00
B_6	1.404	1.422	0.00
Θ_A	-41.97	0.08	**0.54**
Θ_B	-13.55	-87.86	**1.68**
	Standard deviations from S_0 =		**0.357**

Tables 4.1-4.2: Energies, Cartesian coordinates and vertical transitions of the S_0 and S_1 states of 4OBP Anion in Water.

Table 4.1a

****

4OBP Anion in Water - S_0:

SCF Done: E(RPBE1PBE) = -650.681535156

Sum of electronic and thermal Free Energies= -650.536616

1	6	0	-0.019363	0.043007	0.048300
2	6	0	0.033662	0.052904	1.447963
3	6	0	1.261558	-0.005760	2.105392
4	6	0	2.444781	-0.095656	1.372594
5	6	0	2.399209	-0.107962	-0.022907
6	6	0	1.175395	-0.023205	-0.680813
7	1	0	-0.883850	0.132419	2.024992
8	1	0	1.292819	0.018985	3.191749
9	1	0	3.400909	-0.152535	1.886922
10	1	0	3.318941	-0.178965	-0.598199
11	1	0	1.137727	-0.021718	-1.767374
12	6	0	-1.309269	0.187156	-0.696483
13	8	0	-1.334182	0.979375	-1.662798
14	6	0	-2.478739	-0.573899	-0.296205
15	6	0	-2.413612	-1.704463	0.553025
16	6	0	-3.540272	-2.430672	0.875493
17	6	0	-4.838032	-2.071492	0.385232
18	6	0	-4.884871	-0.928895	-0.483627
19	6	0	-3.750358	-0.223148	-0.811926
20	1	0	-1.452149	-2.031436	0.941182
21	1	0	-3.461416	-3.305823	1.517971
22	8	0	-5.895244	-2.730993	0.701052
23	1	0	-5.853748	-0.627247	-0.877877
24	1	0	-3.825899	0.639149	-1.470890

Table 4.1b

4OBP Anion in Water - S_0 - Vertical transitions:

Excited State	1:	Singlet-A	3.5844 eV	345.90 nm	f=0.5361
Excited State	2:	Singlet-A	4.0415 eV	306.77 nm	f=0.0147
Excited State	3:	Singlet-A	4.2350 eV	292.76 nm	f=0.0032
Excited State	4:	Singlet-A	4.5098 eV	274.92 nm	f=0.0219
Excited State	5:	Singlet-A	4.7158 eV	262.91 nm	f=0.0016
Excited State	6:	Singlet-A	4.8204 eV	257.21 nm	f=0.2195
Excited State	7:	Singlet-A	4.8640 eV	254.90 nm	f=0.0416
Excited State	8:	Singlet-A	4.9507 eV	250.44 nm	f=0.0199
Excited State	9:	Singlet-A	5.1009 eV	243.06 nm	f=0.1417
Excited State	10:	Singlet-A	5.2429 eV	236.48 nm	f=0.0037
Excited State	11:	Singlet-A	5.4748 eV	226.47 nm	f=0.0009
Excited State	12:	Singlet-A	5.7060 eV	217.29 nm	f=0.0000
Excited State	13:	Singlet-A	5.7387 eV	216.05 nm	f=0.0309
Excited State	14:	Singlet-A	5.8095 eV	213.42 nm	f=0.0056
Excited State	15:	Singlet-A	5.8848 eV	210.69 nm	f=0.0021
Excited State	16:	Singlet-A	5.9896 eV	207.00 nm	f=0.0113

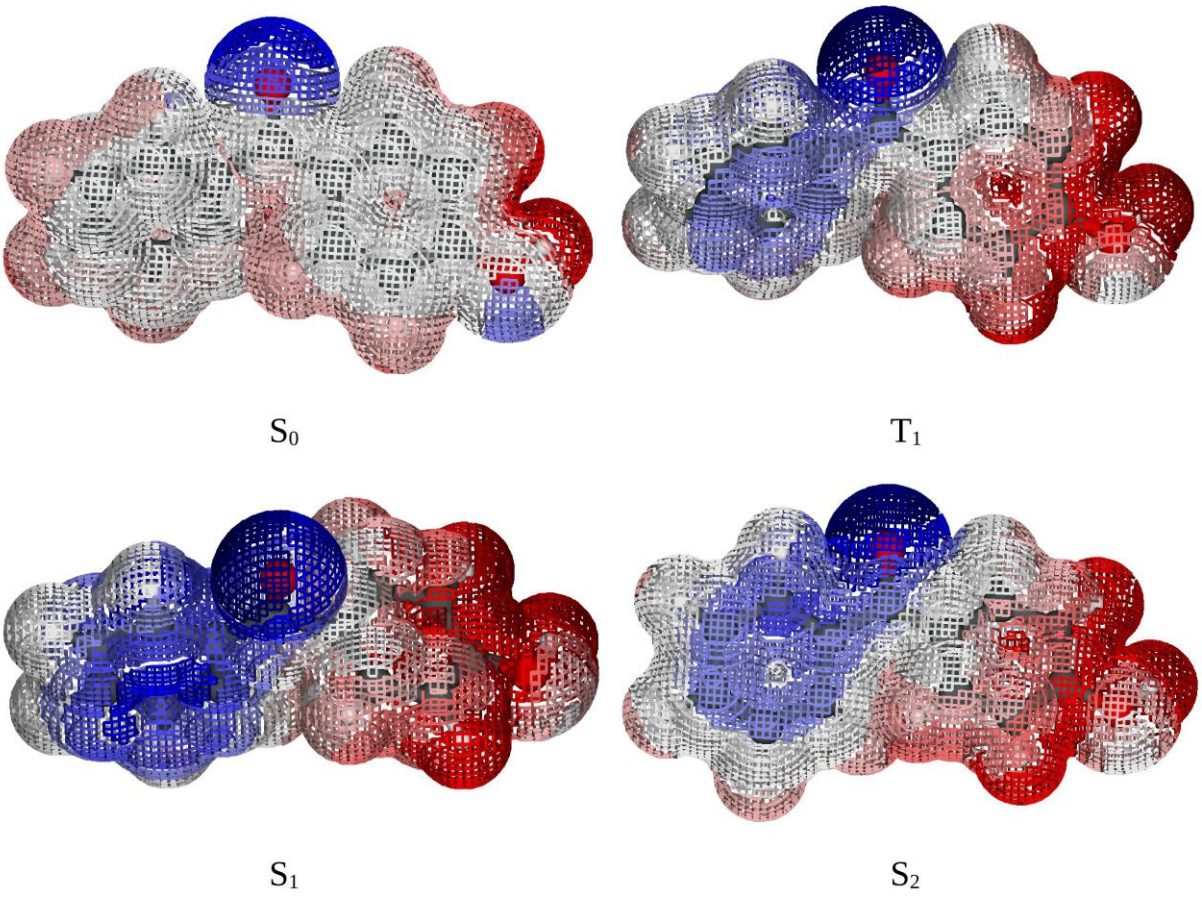
```
Excited State  17:      Singlet-A      6.0219 eV  205.89 nm  f=0.0430
Excited State  18:      Singlet-A      6.0543 eV  204.79 nm  f=0.0164
Excited State  19:      Singlet-A      6.0962 eV  203.38 nm  f=0.0325
Excited State  20:      Singlet-A      6.1736 eV  200.83 nm  f=0.0601
Excited State  21:      Singlet-A      6.1766 eV  200.73 nm  f=0.0847
Excited State  22:      Singlet-A      6.2473 eV  198.46 nm  f=0.0038
Excited State  23:      Singlet-A      6.3008 eV  196.78 nm  f=0.0378
Excited State  24:      Singlet-A      6.3289 eV  195.90 nm  f=0.0278
Excited State  25:      Singlet-A      6.3663 eV  194.75 nm  f=0.0012
Excited State  26:      Singlet-A      6.3936 eV  193.92 nm  f=0.0593
Excited State  27:      Singlet-A      6.4243 eV  192.99 nm  f=0.0049
Excited State  28:      Singlet-A      6.4421 eV  192.46 nm  f=0.0455
Excited State  29:      Singlet-A      6.5325 eV  189.80 nm  f=0.0032
Excited State  30:      Singlet-A      6.6424 eV  186.66 nm  f=0.0753
Excited State  31:      Singlet-A      6.6696 eV  185.89 nm  f=0.1882
Excited State  32:      Singlet-A      6.6882 eV  185.38 nm  f=0.0456
Excited State  33:      Singlet-A      6.7023 eV  184.99 nm  f=0.0318
Excited State  34:      Singlet-A      6.7065 eV  184.87 nm  f=0.1816
Excited State  35:      Singlet-A      6.7583 eV  183.45 nm  f=0.0563
Excited State  36:      Singlet-A      6.7913 eV  182.56 nm  f=0.1366
-----------------------------------------------------------------------
```

Table 4.2

```
**********************************************************************
4OBP Anion in Water - S_1:
Total Energy, E(TD-HF/TD-KS) =  -650.587126029
Energy, force constant and most relevant orbital transitions:
Excited State   1:      Singlet-?Sym    1.7982 eV  689.48 nm  f=0.000
MO: Occ  Virt         Coeff.
      52 -> 53         0.70023
----------------------------------------------------------------------
     1          6          0        0.115300   -0.340743   -0.197365
     2          6          0       -0.077480   -0.194482    1.210382
     3          6          0        0.929797    0.297577    2.025691
     4          6          0        2.175282    0.668228    1.495274
     5          6          0        2.384749    0.529137    0.113621
     6          6          0        1.390399    0.039493   -0.717313
     7          1          0       -1.031602   -0.474239    1.652326
     8          1          0        0.746979    0.396018    3.094197
     9          1          0        2.960336    1.053774    2.139803
    10          1          0        3.344927    0.810451   -0.315631
    11          1          0        1.575075   -0.060149   -1.783809
    12          6          0       -0.906084   -0.838612   -1.050398
    13          8          0       -0.793965   -0.996018   -2.338577
    14          6          0       -2.237841   -1.235686   -0.523866
    15          6          0       -2.489958   -2.580494   -0.136960
    16          6          0       -3.722325   -2.968144    0.313887
    17          6          0       -4.816839   -2.020890    0.388729
    18          6          0       -4.548933   -0.661989   -0.038381
    19          6          0       -3.307476   -0.299837   -0.485275
    20          1          0       -1.674978   -3.298700   -0.187861
    21          1          0       -3.916283   -3.989631    0.630089
    22          8          0       -5.955341   -2.365414    0.804992
    23          1          0       -5.365211    0.053502    0.013609
```

24	1	0	-3.117152	0.723144	-0.801107

Figure 6: Electrostatic potential V on the Van der Waals surfaces of the S_0, T_1, S_1, and S_2 states in 2-Propanol.



S_0 T_1

S_1 S_2

Figure 7: Deprotonation equilibrium of 4HOBP in 2-Propanol.

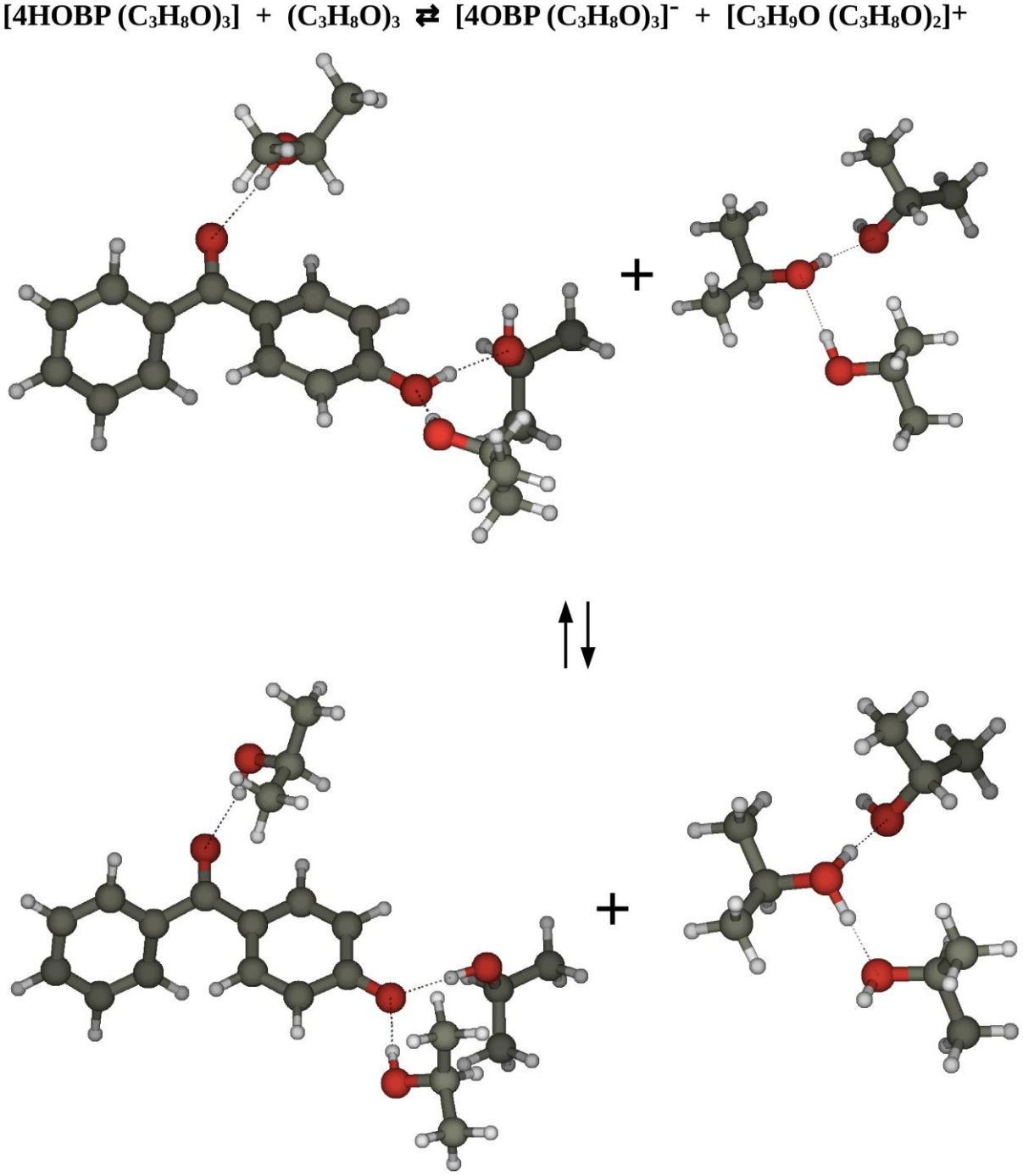


Table 5: Total and relative energies for the deprotonation equilibrium of of the S_0, S_1, and T_1 states of 4HOBP in 2-Propanol.

	E / au	G / au	SP E / au	G / au	Kcal / mol
Deprotonations of Ground State					
Cpl S_0 * 3 Pol	-1233.595213	0.454927	-1233.900693	-1233.445766	
Pol * 2 Pol	-582.439544	0.280013	-582.603099	-582.323086	
(S_0) AH * 3 Pol + Pol * 2 Pol				-1815.768852	**0.00**
Cpl (S_0) DeH^+ * 2 Pol	-1233.132632	0.441501	-1233.432996	-1232.991495	
Cpl $PolH^+$ * 2 Pol	-582.876819	0.294202	-583.045427	-582.751225	
(S_0) A^- * 3 Pol + $PolH_3^+$ * 2 Pol				-1815.742720	**16.40**
		K =	***9.6E-13***	**pK_a =**	**12.0**
Deprotonations of First Singlet Excited State					
Cpl S_1 * 3 Pol	-1233.477520	*0.453301*	-1233.782696	-1233.329395	
(S_1) AH * 3 Pol + Pol * 2 Pol				-1815.652481	**0.00**
Cpl (S_1) DeH^+ * 3 Pol	-1233.038963	*0.439092*	-1233.339015	-1232.899923	
(S_1) A^- * 3 Pol + $PolH_3^+$ * 2 Pol				-1815.651148	**0.84**
		K =	***2.4E-1***	**pK_a =**	**0.6**
Deprotonations of Triplet State					
Cpl T_1 * 3 Pol	-1233.490598	0.453301	-1233.795828	-1233.342527	
(T_1) AH * 3 Pol + Pol * 2 Pol				-1815.665613	**0.00**
Cpl (T_1) DeH^+ * 3 Pol	-1233.049376	0.439092	-1233.349540	-1232.910448	
(T_1) A^- * 3 Pol + $PolH_3^+$ * 2 Pol				-1815.661673	**2.47**
		K =	***1.5E-2***	**pK_a =**	**1.8**

Tables 6.1-6.8: Cartesian coordinates for structures as in Table 5.

Table 6.1

Cpl [2-Propanol * 2 2-Propanol] in 2-Propanol

1	8	0	0.297839	0.253296	-0.261555
2	1	0	0.124471	0.166592	0.704641
3	6	0	1.696934	0.050301	-0.499681
4	1	0	-0.693053	-1.081260	-0.966163
5	8	0	-0.345822	-0.088021	2.414939
6	1	0	0.431436	-0.159529	2.992470
7	6	0	-1.239651	0.886922	2.981938

8	8	0	-1.191041	-1.856934	-1.312815
9	6	0	-2.433089	-1.946383	-0.615434
10	6	0	1.913366	0.121942	-1.997984
11	6	0	2.526427	1.077824	0.252618
12	1	0	1.966548	-0.957180	-0.146244
13	1	0	2.964248	-0.071746	-2.241111
14	1	0	1.300257	-0.621703	-2.520264
15	1	0	1.650135	1.116801	-2.379223
16	1	0	3.596031	0.909047	0.077349
17	1	0	2.278484	2.093747	-0.079938
18	1	0	2.351557	1.016266	1.333637
19	6	0	-3.051622	-3.286322	-0.964048
20	1	0	-2.234038	-1.919289	0.468139
21	6	0	-3.345488	-0.782593	-0.974428
22	1	0	-4.000478	-3.425189	-0.433158
23	1	0	-3.249180	-3.350779	-2.041967
24	1	0	-2.381766	-4.108862	-0.686724
25	1	0	-4.291032	-0.841482	-0.420694
26	1	0	-2.872602	0.177251	-0.732504
27	1	0	-3.573616	-0.791247	-2.048126
28	1	0	-2.066449	0.933325	2.263852
29	6	0	-1.761917	0.403250	4.322787
30	6	0	-0.568807	2.246228	3.068720
31	1	0	-2.507059	1.102112	4.721054
32	1	0	-2.234102	-0.580971	4.225448
33	1	0	-0.945354	0.326621	5.052935
34	1	0	-1.276525	3.000833	3.432289
35	1	0	0.280612	2.217121	3.764311
36	1	0	-0.202476	2.567159	2.086938

Table 6.2

Cpl [2-Propanol_H(+) * 2 2-Propanol] in 2-Propanol

1	8	0	0.278701	0.207769	-0.187452
2	1	0	0.076944	0.138404	0.830765
3	6	0	1.717265	-0.011461	-0.471616
4	1	0	-0.309008	-0.511150	-0.655235
5	8	0	-0.306325	-0.045749	2.276217
6	1	0	0.487176	-0.106027	2.835179
7	6	0	-1.206647	0.939937	2.843805
8	8	0	-1.131221	-1.611459	-1.281490
9	6	0	-2.483258	-1.778017	-0.783971
10	6	0	1.897890	0.087711	-1.967197
11	6	0	2.490032	1.024624	0.307640
12	1	0	1.947748	-1.021182	-0.116275
13	1	0	2.950072	-0.094315	-2.210662
14	1	0	1.297491	-0.660264	-2.496608
15	1	0	1.627025	1.085973	-2.328895
16	1	0	3.560598	0.876954	0.129741
17	1	0	2.223957	2.037485	-0.014836
18	1	0	2.314113	0.934766	1.385127
19	6	0	-3.024508	-3.116198	-1.244621

20	1	0	-2.357857	-1.783745	0.303908
21	6	0	-3.349325	-0.605861	-1.201038
22	1	0	-4.017246	-3.293245	-0.815261
23	1	0	-3.118912	-3.142349	-2.337925
24	1	0	-2.365347	-3.933265	-0.931128
25	1	0	-4.348854	-0.697582	-0.760873
26	1	0	-2.916264	0.344408	-0.868575
27	1	0	-3.461305	-0.574361	-2.292765
28	1	0	-2.056376	0.937975	2.153121
29	6	0	-1.660242	0.476813	4.213294
30	6	0	-0.556182	2.309301	2.858392
31	1	0	-2.403008	1.172445	4.620266
32	1	0	-2.116038	-0.518009	4.159278
33	1	0	-0.814884	0.436985	4.912361
34	1	0	-1.263244	3.058350	3.233332
35	1	0	0.323223	2.316527	3.515147
36	1	0	-0.244739	2.609878	1.851826
37	1	0	-1.161962	-1.513747	-2.248408

Table 6.3

Cpl [4-hydroxybenzophenone * 3 2-Propanol] in 2-Propanol

1	6	0	-4.062430	-1.196801	-0.572016
2	6	0	-3.725917	-2.376652	-1.249539
3	6	0	-4.640182	-3.425507	-1.322385
4	6	0	-5.884511	-3.313912	-0.702644
5	6	0	-6.224058	-2.142312	-0.022530
6	6	0	-5.323387	-1.084332	0.031067
7	1	0	-2.763792	-2.466433	-1.746903
8	1	0	-4.379934	-4.330970	-1.865119
9	1	0	-6.592480	-4.138001	-0.752073
10	1	0	-7.192937	-2.054037	0.462964
11	1	0	-5.583516	-0.166492	0.552234
12	6	0	-3.149601	-0.021704	-0.529203
13	8	0	-3.639591	1.114967	-0.556201
14	6	0	-1.688769	-0.209379	-0.456953
15	6	0	-1.102004	-1.341135	0.134658
16	6	0	0.275322	-1.454846	0.240665
17	6	0	1.102011	-0.443566	-0.265809
18	6	0	0.531421	0.690217	-0.864771
19	6	0	-0.846707	0.804024	-0.944194
20	1	0	-1.727056	-2.128176	0.547405
21	1	0	0.727090	-2.322196	0.715088
22	8	0	2.433603	-0.609819	-0.156448
23	1	0	1.172175	1.471629	-1.265598
24	1	0	-1.284931	1.682870	-1.409971
25	1	0	3.722427	2.200388	-0.639958
26	1	0	2.952429	0.163947	-0.519710
27	8	0	4.020197	1.354156	-1.010743
28	6	0	4.208027	1.511354	-2.433609
29	1	0	-2.990981	2.750625	0.064234
30	8	0	-2.768153	3.660177	0.349578

31	6	0	-2.060436	3.592364	1.588505
32	1	0	3.243107	-1.495283	1.337204
33	8	0	3.597040	-1.943920	2.128495
34	6	0	5.024221	-1.857263	2.101133
35	6	0	-1.655859	5.008435	1.948285
36	6	0	-2.909448	2.944128	2.671702
37	1	0	-1.149982	2.988413	1.443433
38	1	0	-1.077330	5.020831	2.879063
39	1	0	-1.039867	5.452699	1.157468
40	1	0	-2.543804	5.638337	2.087986
41	1	0	-2.350318	2.876213	3.613300
42	1	0	-3.819268	3.530955	2.852122
43	1	0	-3.206579	1.927932	2.384515
44	6	0	5.530480	-2.481069	3.386148
45	6	0	5.589059	-2.540725	0.865645
46	1	0	5.313319	-0.794133	2.083758
47	1	0	6.623043	-2.415826	3.442270
48	1	0	5.112411	-1.968956	4.260721
49	1	0	5.247367	-3.540208	3.437968
50	1	0	6.682034	-2.450297	0.837532
51	1	0	5.331234	-3.607596	0.862856
52	1	0	5.192097	-2.087605	-0.051196
53	6	0	5.112884	2.695600	-2.713011
54	6	0	4.772442	0.202982	-2.943662
55	1	0	3.223368	1.687440	-2.889938
56	1	0	5.240092	2.829652	-3.793500
57	1	0	4.686370	3.622608	-2.309680
58	1	0	6.102100	2.543884	-2.263952
59	1	0	4.898314	0.246852	-4.031104
60	1	0	5.751224	0.000482	-2.491732
61	1	0	4.102453	-0.633436	-2.714018

Table 6.4

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Cpl [DeProtonated 4-hydroxybenzophenone * 3 2-Propanol] in 2-Propan

1	6	0	-3.959036	-1.348296	-0.543989
2	6	0	-3.611891	-2.554053	-1.167004
3	6	0	-4.478881	-3.644497	-1.118529
4	6	0	-5.688369	-3.547999	-0.430907
5	6	0	-6.040108	-2.349617	0.193466
6	6	0	-5.187240	-1.252251	0.124389
7	1	0	-2.676049	-2.633566	-1.714277
8	1	0	-4.208461	-4.570824	-1.619969
9	1	0	-6.359038	-4.403065	-0.385488
10	1	0	-6.982413	-2.269732	0.730541
11	1	0	-5.462037	-0.313567	0.599416
12	6	0	-3.097193	-0.130134	-0.633495
13	8	0	-3.664067	0.963238	-0.831750
14	6	0	-1.653525	-0.233132	-0.495680
15	6	0	-1.014273	-1.331502	0.124104
16	6	0	0.354770	-1.367212	0.291704
17	6	0	1.192678	-0.307142	-0.170575

18	6	0	0.534682	0.798839	-0.796043
19	6	0	-0.834606	0.832512	-0.937510
20	1	0	-1.609922	-2.154652	0.511676
21	1	0	0.822903	-2.214237	0.789547
22	8	0	2.474543	-0.343829	-0.030581
23	1	0	1.145690	1.622346	-1.161096
24	1	0	-1.304292	1.686906	-1.420523
25	1	0	3.563117	0.807741	-0.698042
26	8	0	4.228633	1.453502	-1.051338
27	6	0	4.559636	1.082260	-2.386407
28	1	0	-3.424639	2.642533	-0.100170
29	8	0	-3.524724	3.555008	0.243132
30	6	0	-2.413355	3.864079	1.084758
31	1	0	3.273875	-1.560955	0.888946
32	8	0	3.790584	-2.246190	1.387321
33	6	0	4.956981	-1.631541	1.928400
34	1	0	-1.486939	3.788248	0.493206
35	6	0	-2.584294	5.300369	1.539034
36	6	0	-2.325217	2.898088	2.256082
37	1	0	-1.734998	5.612706	2.157387
38	1	0	-2.647224	5.977768	0.679086
39	1	0	-3.500897	5.410770	2.132968
40	1	0	-1.456718	3.129344	2.885383
41	1	0	-3.228430	2.960644	2.876737
42	1	0	-2.218540	1.863924	1.906636
43	1	0	5.498257	-1.118699	1.116303
44	6	0	4.594249	-0.605371	2.992666
45	6	0	5.839471	-2.735300	2.479702
46	1	0	5.494131	-0.117808	3.388783
47	1	0	3.943821	0.174900	2.579117
48	1	0	4.066575	-1.085993	3.826914
49	1	0	6.771221	-2.323155	2.884561
50	1	0	5.324015	-3.273728	3.285805
51	1	0	6.097569	-3.456709	1.695225
52	1	0	3.629482	0.991212	-2.971769
53	6	0	5.397002	2.200733	-2.977933
54	6	0	5.287097	-0.254688	-2.423622
55	1	0	5.658874	1.980802	-4.019491
56	1	0	4.850582	3.151238	-2.956689
57	1	0	6.327914	2.325461	-2.409435
58	1	0	5.511856	-0.547673	-3.457150
59	1	0	6.233113	-0.194072	-1.869941
60	1	0	4.676392	-1.046808	-1.974129

Table 6.5

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Cpl [4-hydroxybenzophenone S_1 * 3 2-Propanol] in 2-Propanol

1	6	0	-0.212119	0.476978	0.028774
2	6	0	-0.425779	0.450482	1.438053
3	6	0	0.527908	0.948646	2.310890
4	6	0	1.730000	1.492432	1.833420
5	6	0	1.955161	1.524716	0.449073

6	6	0	1.014620	1.032195	-0.440951
7	1	0	-1.350808	0.034400	1.833253
8	1	0	0.337016	0.916146	3.382077
9	1	0	2.473389	1.881644	2.524055
10	1	0	2.883798	1.942673	0.063949
11	1	0	1.205006	1.063181	-1.510948
12	6	0	-1.174478	-0.024715	-0.874372
13	8	0	-1.089005	-0.045767	-2.172353
14	6	0	-2.473950	-0.631196	-0.513066
15	6	0	-2.590202	-2.040289	-0.351285
16	6	0	-3.793520	-2.608110	-0.028599
17	6	0	-4.948183	-1.784982	0.087992
18	6	0	-4.860017	-0.382002	-0.129702
19	6	0	-3.648325	0.170401	-0.452569
20	1	0	-1.701441	-2.657137	-0.449789
21	1	0	-3.896207	-3.675795	0.142317
22	8	0	-6.078246	-2.377595	0.387381
23	1	0	-5.753493	0.229245	-0.040617
24	1	0	-3.565357	1.238490	-0.632896
25	1	0	-8.472154	-0.639344	-0.309992
26	1	0	-6.886797	-1.751826	0.452636
27	8	0	-8.256763	-1.014325	0.559906
28	6	0	-8.388665	0.023248	1.561558
29	1	0	-2.282843	-0.686510	-3.392622
30	8	0	-2.922327	-0.987401	-4.074547
31	6	0	-2.615305	-2.337069	-4.424480
32	1	0	-6.376810	-4.373899	0.350040
33	8	0	-6.420748	-5.339109	0.241106
34	6	0	-7.779590	-5.754561	0.415777
35	6	0	-3.716031	-2.824817	-5.345813
36	6	0	-1.240475	-2.438662	-5.068246
37	1	0	-2.623889	-2.950735	-3.508926
38	1	0	-3.553986	-3.873683	-5.619382
39	1	0	-4.696001	-2.746729	-4.860119
40	1	0	-3.740750	-2.229762	-6.268065
41	1	0	-1.001486	-3.481338	-5.312605
42	1	0	-1.203696	-1.850149	-5.994160
43	1	0	-0.461873	-2.064216	-4.392519
44	6	0	-7.827318	-7.240640	0.124188
45	6	0	-8.274270	-5.421606	1.814084
46	1	0	-8.406032	-5.226667	-0.320454
47	1	0	-8.854430	-7.614706	0.201310
48	1	0	-7.462087	-7.451868	-0.887709
49	1	0	-7.205294	-7.794870	0.838617
50	1	0	-9.320639	-5.726283	1.938760
51	1	0	-7.671468	-5.940248	2.570489
52	1	0	-8.215186	-4.342875	2.005961
53	6	0	-9.760166	0.658567	1.460664
54	6	0	-8.133978	-0.629714	2.902233
55	1	0	-7.616122	0.779838	1.365965
56	1	0	-9.857001	1.464663	2.196991
57	1	0	-9.921588	1.093650	0.466488
58	1	0	-10.547243	-0.081053	1.650596
59	1	0	-8.174245	0.124325	3.695846
60	1	0	-8.892324	-1.393415	3.113097

61	1	0	-7.145027	-1.101150	2.934537

Table 6.6

Cpl [DeProtonated 4-hydroxybenzophenone S_1 * 3 2-Propanol] in 2-P

1	6	0	-0.024513	0.416791	-0.013471
2	6	0	-0.400502	0.508476	1.360976
3	6	0	0.402573	1.162426	2.282429
4	6	0	1.613608	1.756626	1.895756
5	6	0	2.000428	1.675810	0.548223
6	6	0	1.211528	1.026972	-0.387148
7	1	0	-1.333755	0.058693	1.694590
8	1	0	0.083953	1.212735	3.322454
9	1	0	2.238449	2.267962	2.623369
10	1	0	2.937212	2.130562	0.229004
11	1	0	1.528003	0.975265	-1.425843
12	6	0	-0.830036	-0.247097	-0.977505
13	8	0	-0.528522	-0.364939	-2.235134
14	6	0	-2.118680	-0.892442	-0.606913
15	6	0	-2.155134	-2.261950	-0.228615
16	6	0	-3.338395	-2.884543	0.063689
17	6	0	-4.588775	-2.164944	-0.027956
18	6	0	-4.539799	-0.779481	-0.437418
19	6	0	-3.342931	-0.180183	-0.722870
20	1	0	-1.218203	-2.809652	-0.158255
21	1	0	-3.371964	-3.926592	0.370611
22	8	0	-5.688337	-2.729447	0.238623
23	1	0	-5.478844	-0.237579	-0.512252
24	1	0	-3.313581	0.861524	-1.033379
25	1	0	-7.291800	-1.852807	0.319321
26	8	0	-8.162419	-1.402730	0.361243
27	6	0	-8.387028	-0.973910	1.704839
28	1	0	-1.685515	-0.678442	-3.482939
29	8	0	-2.304520	-0.772634	-4.251560
30	6	0	-2.876799	-2.077044	-4.229172
31	1	0	-5.862935	-4.504890	0.649348
32	8	0	-6.019160	-5.436155	0.914471
33	6	0	-7.163671	-5.919684	0.210227
34	1	0	-3.355576	-2.240149	-3.249565
35	6	0	-3.946639	-2.124476	-5.303997
36	6	0	-1.814162	-3.147388	-4.433788
37	1	0	-4.451349	-3.097601	-5.307152
38	1	0	-4.703323	-1.348645	-5.136754
39	1	0	-3.504097	-1.964832	-6.295998
40	1	0	-2.256142	-4.150874	-4.389185
41	1	0	-1.328264	-3.026874	-5.410949
42	1	0	-1.041718	-3.086247	-3.657316
43	1	0	-8.010696	-5.242345	0.404752
44	6	0	-6.905051	-5.962206	-1.288360
45	6	0	-7.492801	-7.288424	0.773186
46	1	0	-7.796146	-6.307920	-1.827051
47	1	0	-6.646187	-4.967408	-1.671231

48	1	0	-6.077162	-6.645859	-1.517117
49	1	0	-8.387152	-7.699938	0.291280
50	1	0	-6.660891	-7.984272	0.603741
51	1	0	-7.681138	-7.232870	1.851935
52	1	0	-7.524151	-0.371944	2.033124
53	6	0	-9.619957	-0.091707	1.694858
54	6	0	-8.538301	-2.163244	2.641662
55	1	0	-9.826954	0.295164	2.699290
56	1	0	-9.482701	0.762588	1.021473
57	1	0	-10.497560	-0.658585	1.358089
58	1	0	-8.686904	-1.827365	3.675648
59	1	0	-9.400976	-2.776806	2.351241
60	1	0	-7.643387	-2.797233	2.620898

Table 6.7

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Cpl [4-hydroxybenzophenone T_1 * 3 2-Propanol] in 2-Propanol

1	6	0	-0.074643	-0.083092	-0.083686
2	6	0	-0.019468	-0.242439	1.315841
3	6	0	1.198057	-0.403389	1.969855
4	6	0	2.394888	-0.409007	1.249380
5	6	0	2.357744	-0.234928	-0.136417
6	6	0	1.143578	-0.066963	-0.793277
7	1	0	-0.931843	-0.204324	1.905927
8	1	0	1.213277	-0.513615	3.052176
9	1	0	3.344831	-0.537379	1.762997
10	1	0	3.283121	-0.230466	-0.708855
11	1	0	1.123406	0.072834	-1.870896
12	6	0	-1.326407	0.151167	-0.813708
13	8	0	-1.299655	0.781680	-1.938687
14	6	0	-2.613840	-0.340721	-0.380374
15	6	0	-2.791385	-1.462356	0.510505
16	6	0	-4.036782	-1.885823	0.862494
17	6	0	-5.206590	-1.242500	0.328996
18	6	0	-5.058829	-0.172863	-0.598332
19	6	0	-3.811933	0.253304	-0.953452
20	1	0	-1.922619	-1.990397	0.888426
21	1	0	-4.174609	-2.729355	1.534280
22	8	0	-6.381173	-1.710295	0.720070
23	1	0	-5.946619	0.299883	-1.011403
24	1	0	-3.691004	1.071801	-1.654090
25	1	0	-8.475997	-0.838118	-1.312242
26	1	0	-7.177363	-1.254309	0.278444
27	8	0	-8.535260	-0.725640	-0.349113
28	6	0	-8.882903	0.649439	-0.060843
29	1	0	-2.132434	0.409994	-3.502362
30	8	0	-2.544652	0.282264	-4.385201
31	6	0	-2.729530	-1.115117	-4.607572
32	1	0	-6.680325	-3.491785	1.547736
33	8	0	-6.739499	-4.388719	1.921208
34	6	0	-8.111880	-4.669418	2.214757
35	6	0	-3.500308	-1.264671	-5.904825

36	6	0	-1.396327	-1.847075	-4.645288
37	1	0	-3.336915	-1.527949	-3.785230
38	1	0	-3.706850	-2.320821	-6.112645
39	1	0	-4.457767	-0.732676	-5.854703
40	1	0	-2.923300	-0.856266	-6.744506
41	1	0	-1.547567	-2.922880	-4.799366
42	1	0	-0.771112	-1.466393	-5.463139
43	1	0	-0.848167	-1.716046	-3.704216
44	6	0	-8.167861	-6.086639	2.747739
45	6	0	-8.676047	-3.658345	3.199887
46	1	0	-8.689957	-4.617351	1.278368
47	1	0	-9.203544	-6.379049	2.954626
48	1	0	-7.751789	-6.794807	2.021551
49	1	0	-7.594531	-6.170808	3.679963
50	1	0	-9.731913	-3.869160	3.409582
51	1	0	-8.122286	-3.692472	4.146892
52	1	0	-8.611090	-2.638932	2.799309
53	6	0	-10.113466	1.046959	-0.850779
54	6	0	-9.082793	0.743713	1.435955
55	1	0	-8.034571	1.281085	-0.359152
56	1	0	-10.367450	2.094083	-0.649895
57	1	0	-9.939769	0.946297	-1.929440
58	1	0	-10.972038	0.422613	-0.575421
59	1	0	-9.299814	1.779812	1.717785
60	1	0	-9.923276	0.116429	1.756777
61	1	0	-8.183898	0.428018	1.977801

Table 6.8

Cpl [DeProtonated 4-hydroxybenzophenone T_1 * 3 2-Propanol] in 2-P

1	6	0	0.092687	-0.084977	-0.056626
2	6	0	0.062681	0.024915	1.364776
3	6	0	1.229574	0.012511	2.113677
4	6	0	2.485183	-0.109352	1.497655
5	6	0	2.538290	-0.205672	0.099834
6	6	0	1.379728	-0.189728	-0.662433
7	1	0	-0.888426	0.141535	1.879357
8	1	0	1.165415	0.104963	3.196826
9	1	0	3.396353	-0.121757	2.090982
10	1	0	3.502229	-0.294573	-0.399474
11	1	0	1.440465	-0.262702	-1.745139
12	6	0	-1.076524	-0.040189	-0.883939
13	8	0	-1.005394	0.024506	-2.179076
14	6	0	-2.453969	-0.079987	-0.332805
15	6	0	-2.864104	-1.049800	0.622369
16	6	0	-4.159127	-1.099229	1.075403
17	6	0	-5.152049	-0.179945	0.575943
18	6	0	-4.734025	0.777071	-0.418502
19	6	0	-3.435273	0.810604	-0.854864
20	1	0	-2.136942	-1.767377	0.993285
21	1	0	-4.471024	-1.836914	1.811007
22	8	0	-6.353141	-0.221519	0.990598

23	1	0	-5.479172	1.466290	-0.808860
24	1	0	-3.131691	1.532779	-1.608200
25	1	0	-7.625215	1.016471	0.514842
26	8	0	-8.312909	1.669446	0.263264
27	6	0	-8.325656	2.712380	1.239366
28	1	0	-2.164800	-0.607884	-3.312056
29	8	0	-2.744302	-0.922792	-4.051228
30	6	0	-3.475327	-2.065913	-3.616672
31	1	0	-6.975809	-1.525158	2.132759
32	8	0	-7.322264	-2.191366	2.764081
33	6	0	-8.664367	-2.513671	2.396210
34	1	0	-4.045646	-1.802294	-2.710601
35	6	0	-4.455931	-2.423222	-4.717391
36	6	0	-2.544258	-3.224023	-3.285629
37	1	0	-5.078120	-3.276156	-4.421842
38	1	0	-5.119192	-1.578905	-4.939880
39	1	0	-3.921373	-2.692163	-5.637741
40	1	0	-3.112880	-4.092662	-2.930086
41	1	0	-1.974197	-3.525784	-4.174060
42	1	0	-1.831238	-2.944575	-2.500532
43	1	0	-9.266261	-1.590634	2.408897
44	6	0	-8.720741	-3.114814	0.999951
45	6	0	-9.202335	-3.460807	3.450499
46	1	0	-9.755897	-3.343245	0.716917
47	1	0	-8.315533	-2.418895	0.255132
48	1	0	-8.138089	-4.044191	0.955978
49	1	0	-10.247223	-3.717426	3.241591
50	1	0	-8.617628	-4.389820	3.469298
51	1	0	-9.154886	-3.005067	4.446557
52	1	0	-7.306785	3.121703	1.333133
53	6	0	-9.243381	3.802028	0.719955
54	6	0	-8.768598	2.186244	2.596341
55	1	0	-9.274078	4.647297	1.416918
56	1	0	-8.898514	4.172826	-0.252504
57	1	0	-10.265294	3.419576	0.599555
58	1	0	-8.753689	2.985559	3.347934
59	1	0	-9.789148	1.785789	2.539887
60	1	0	-8.104220	1.386071	2.944871

Figure 8: Deprotonation equilibrium of 4HOBP in Water.

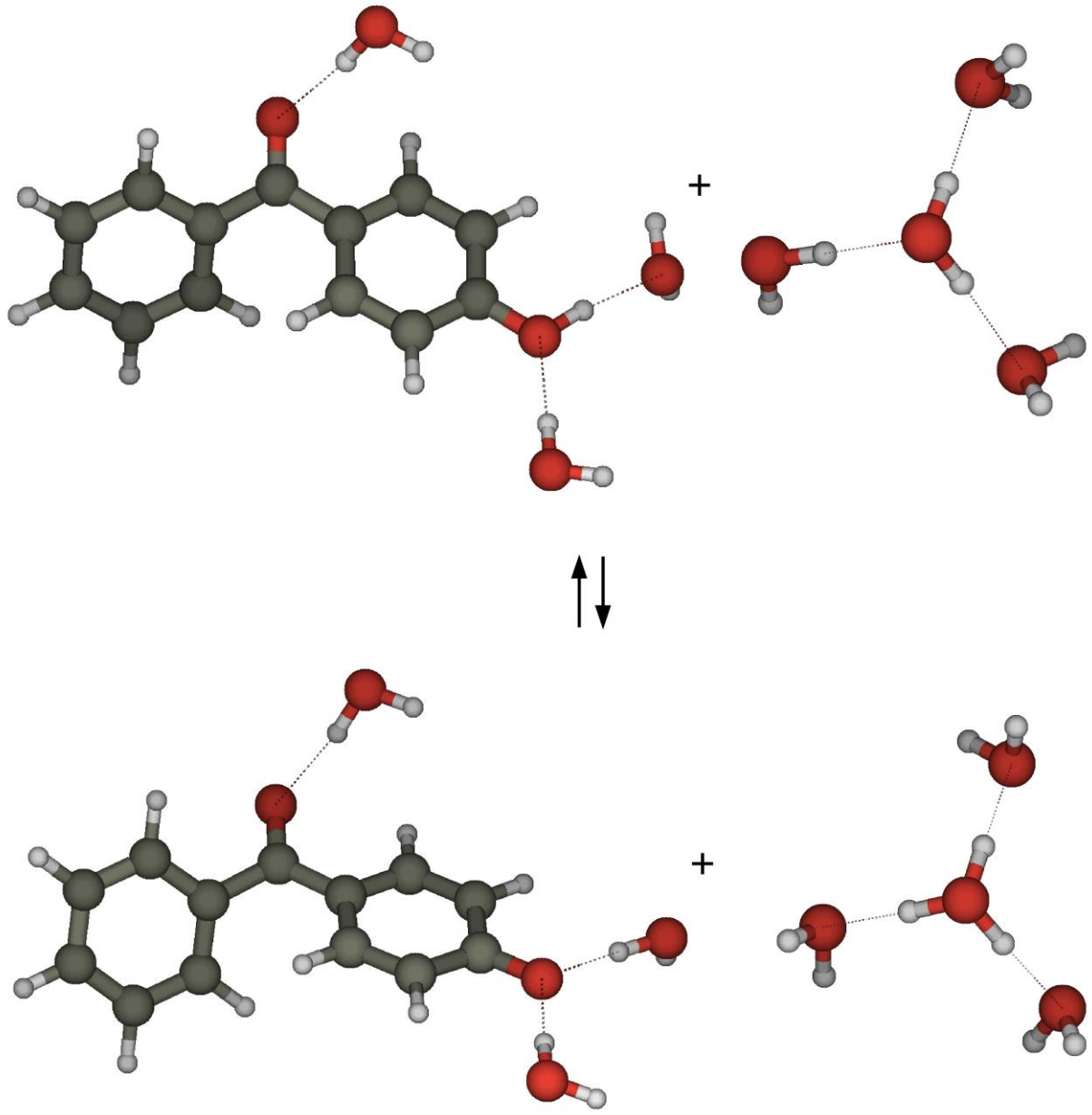

Table 7: Total and relative energies for the deprotonation equilibrium of of the S_0, S_1, and T_1 states of 4HOBP in Water.

	E / au	ΔG / au	SP E / au	G / au	Kcal / mol
Deprotonations of Ground State					
Cpl S_0 * 3 H_2O	-880.219434	0.215210	-880.459360	-880.244150	
H_2O * 3 H_2O	-305.427112	0.058350	-305.558233	-305.499883	
(S_0) AH * 3 H_2O + H O_2 * 3 H O_2				-1185.744033	**0.00**
Cpl (S_0) DeH^+ * 3 H_2O	-879.763298	0.201805	-879.998584	-879.796779	
Cpl H_3O^+ * 3 H_2O	-305.867755	0.074462	-305.999877	-305.925415	
(S_0) A^- * 3 H_2O + H_3O^+ * 3 H_2O				-1185.722194	**13.70**
		***K* =**	***9.0E-11***	**pK_a =**	**8.3**
Deprotonations of First Singlet Excited State					
Cpl S_1 * 3 H_2O	-880.101545	*0.211027*	-880.340984	-880.129957	
(S_1) AH * 3 H_2O + H O_2 * 3 H O_2				-1185.629841	**0.00**
Cpl (S_1) DeH^+ * 3 H_2O	-879.666802	*0.198832*	-879.901453	-879.702621	
(S_1) A^- * 3 H_2O + H_3O^+ * 3 H_2O				-1185.628036	**1.13**
		***K* =**	***1.5E-1***	**pK_a =**	**-0.9**
Deprotonations of Triplet State					
Cpl T_1 * 3 H_2O	-880.115899	0.211027	-880.355698	-880.144671	
(T_1) AH * 3 H_2O + H O_2 * 3 H O_2				-1185.644554	**0.00**
Cpl (T_1) DeH^+ * 3 H_2O	-879.680221	0.198832	-879.915132	-879.716300	
(T_1) A^- * 3 H_2O + H O_3^+ * 3 H O_2				-1185.641715	**1.78**
		***K* =**	***4.9E-2***	**pK_a =**	**-0.4**

Tables 8.1-8.8: Cartesian coordinates for structures as in Table 7.

Table 8.1

Cpl [H2O * 3 H2O] in Water

1	8	0	0.000215	0.081546	0.025351
2	1	0	0.011331	0.033046	1.007865
3	1	0	0.944058	0.033528	-0.248297
4	1	0	-0.717077	-1.433378	-0.492078
5	8	0	-0.074815	-0.086337	2.810296
6	1	0	0.803784	0.148966	3.145271

7	1	0	-0.642750	0.644650	3.098235
8	8	0	2.646578	-0.070261	-0.848252
9	1	0	3.185765	-0.286603	-0.072486
10	1	0	2.913131	0.832936	-1.077776
11	8	0	-1.133649	-2.261829	-0.836677
12	1	0	-1.214584	-2.837026	-0.062659

Table 8.2

Cpl [H3O(+) * 3 H2O] in Water

1	8	0	-0.001308	-0.004717	-0.001302
2	1	0	-0.004186	-0.004604	1.021177
3	1	0	0.973901	-0.002265	-0.311455
4	1	0	-0.430207	-0.880328	-0.313377
5	8	0	-0.037556	-0.019750	2.589533
6	1	0	0.879385	0.013599	2.905281
7	1	0	-0.429151	0.814573	2.893298
8	8	0	2.449513	0.005692	-0.829551
9	1	0	3.036799	-0.111446	-0.065928
10	1	0	2.650752	0.897165	-1.155812
11	8	0	-1.097144	-2.198329	-0.824084
12	1	0	-1.377746	-2.709542	-0.048272
13	1	0	-1.925069	-1.960226	-1.270767

Table 8.3

Cpl [4-hydroxybenzophenone * 3 H2O] in Water

1	6	0	-0.030614	0.055459	0.055594
2	6	0	-0.002168	-0.062023	1.452175
3	6	0	1.215835	-0.065875	2.128156
4	6	0	2.411372	0.026403	1.416084
5	6	0	2.389994	0.136895	0.023837
6	6	0	1.175404	0.165270	-0.652015
7	1	0	-0.930122	-0.118380	2.014249
8	1	0	1.230306	-0.138882	3.212378
9	1	0	3.360888	0.013778	1.945310
10	1	0	3.321358	0.204775	-0.532290
11	1	0	1.151403	0.257502	-1.734460
12	6	0	-1.308165	0.144697	-0.699003
13	8	0	-1.354179	0.856702	-1.715164
14	6	0	-2.500208	-0.593466	-0.248342
15	6	0	-2.411267	-1.808297	0.452974
16	6	0	-3.552594	-2.512295	0.802846
17	6	0	-4.815347	-2.000537	0.478728
18	6	0	-4.922336	-0.784986	-0.214108
19	6	0	-3.774386	-0.102518	-0.580197
20	1	0	-1.439779	-2.227102	0.698786
21	1	0	-3.481490	-3.461279	1.327078
22	8	0	-5.898532	-2.712573	0.851657

23	1	0	-5.903423	-0.386534	-0.458937
24	1	0	-3.861211	0.840511	-1.112809
25	1	0	-8.186610	-1.092298	-0.516120
26	1	0	-6.755820	-2.271771	0.587982
27	8	0	-8.289749	-1.693538	0.238108
28	1	0	-8.542515	-1.112665	0.972441
29	1	0	-2.490258	0.595342	-3.117606
30	8	0	-2.996194	0.471765	-3.949374
31	1	0	-3.820649	0.051094	-3.665515
32	1	0	-5.869214	-4.412289	1.646707
33	8	0	-5.841066	-5.294427	2.065786
34	1	0	-6.757269	-5.605344	2.040676

Table 8.4

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Cpl [DeProtonated 4-hydroxybenzophenone * 3 H2O] in Water

1	6	0	-0.063609	0.073208	0.062328
2	6	0	-0.023633	-0.174119	1.440897
3	6	0	1.197063	-0.208289	2.112177
4	6	0	2.387234	-0.017306	1.410786
5	6	0	2.354936	0.225809	0.036074
6	6	0	1.135678	0.286367	-0.631529
7	1	0	-0.948121	-0.311776	1.995089
8	1	0	1.217423	-0.382615	3.184890
9	1	0	3.339217	-0.053935	1.934574
10	1	0	3.281066	0.373537	-0.513613
11	1	0	1.105507	0.483903	-1.699924
12	6	0	-1.352272	0.196472	-0.678729
13	8	0	-1.441879	1.099228	-1.540086
14	6	0	-2.458590	-0.703146	-0.397634
15	6	0	-2.282285	-1.966792	0.210251
16	6	0	-3.345687	-2.822994	0.410942
17	6	0	-4.672901	-2.462468	0.035232
18	6	0	-4.841613	-1.181241	-0.573506
19	6	0	-3.769093	-0.344481	-0.789918
20	1	0	-1.286029	-2.294179	0.496064
21	1	0	-3.181997	-3.799776	0.860426
22	8	0	-5.676959	-3.257948	0.234237
23	1	0	-5.844569	-0.874252	-0.861803
24	1	0	-3.932797	0.628181	-1.248054
25	1	0	-7.254244	-2.801967	-0.226152
26	8	0	-8.197917	-2.631170	-0.490842
27	1	0	-8.485094	-1.905414	0.081369
28	1	0	-2.377786	0.917047	-3.067542
29	8	0	-2.778270	0.850734	-3.963111
30	1	0	-3.584926	0.333385	-3.825800
31	1	0	-5.414365	-4.742361	1.035067
32	8	0	-5.288748	-5.611301	1.503511
33	1	0	-6.184999	-5.912761	1.708617

Table 8.5

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Cpl [4-hydroxybenzophenone S_1 * 3 H2O] in Water

1	6	0	-0.055360	0.056712	-0.024833
2	6	0	-0.030865	-0.036304	1.396909
3	6	0	1.170965	-0.082350	2.085292
4	6	0	2.395156	-0.039259	1.401992
5	6	0	2.387306	0.051186	0.002354
6	6	0	1.196474	0.099193	-0.704695
7	1	0	-0.968738	-0.072192	1.947758
8	1	0	1.159853	-0.152835	3.170971
9	1	0	3.333541	-0.075617	1.948225
10	1	0	3.329655	0.084508	-0.540850
11	1	0	1.208409	0.169214	-1.789315
12	6	0	-1.275022	0.108568	-0.735170
13	8	0	-1.422835	0.206459	-2.030895
14	6	0	-2.624247	0.070193	-0.134137
15	6	0	-3.307170	-1.169276	0.020776
16	6	0	-4.553365	-1.211190	0.584837
17	6	0	-5.188955	0.002916	0.968318
18	6	0	-4.548008	1.255876	0.757882
19	6	0	-3.300346	1.279845	0.193176
20	1	0	-2.807603	-2.087333	-0.274352
21	1	0	-5.075552	-2.147232	0.757394
22	8	0	-6.379577	-0.087927	1.508160
23	1	0	-5.057076	2.168596	1.052018
24	1	0	-2.795758	2.226186	0.021578
25	1	0	-7.416207	2.770016	1.471261
26	1	0	-6.796404	0.812656	1.754345
27	8	0	-7.570259	2.107990	2.164518
28	1	0	-7.122441	2.469948	2.945737
29	1	0	-2.355264	-1.037200	-2.918867
30	8	0	-2.833738	-1.703586	-3.464220
31	1	0	-3.474389	-2.094098	-2.851889
32	1	0	-7.328406	-1.780110	1.770968
33	8	0	-7.808292	-2.617879	1.895206
34	1	0	-8.573284	-2.379239	2.438332

Table 8.6

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Cpl [DeProtonated 4-hydroxybenzophenone S_1 * 3 H2O] in Water

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1	6	0	0.093007	-0.054765	-0.139348
2	6	0	-0.071447	-0.076853	1.277991
3	6	0	0.930518	0.375391	2.122810
4	6	0	2.140100	0.868202	1.611236
5	6	0	2.320200	0.896174	0.219300
6	6	0	1.330355	0.449590	-0.640917
7	1	0	-0.998982	-0.453075	1.704624
8	1	0	0.770966	0.345375	3.198977
9	1	0	2.921488	1.221057	2.278522
10	1	0	3.253235	1.274168	-0.194908

11	1	0	1.490793	0.478798	-1.715332
12	6	0	-0.922304	-0.511657	-1.020504
13	8	0	-0.826715	-0.509049	-2.324348
14	6	0	-2.209012	-1.057844	-0.519939
15	6	0	-2.357195	-2.454396	-0.296198
16	6	0	-3.556090	-2.984768	0.093387
17	6	0	-4.712894	-2.134563	0.264376
18	6	0	-4.554072	-0.718953	0.016005
19	6	0	-3.343154	-0.213016	-0.368985
20	1	0	-1.491821	-3.098631	-0.429562
21	1	0	-3.673786	-4.048261	0.280883
22	8	0	-5.829078	-2.613872	0.617351
23	1	0	-5.423015	-0.079682	0.145137
24	1	0	-3.229603	0.851562	-0.557740
25	1	0	-7.288809	-1.566511	0.725440
26	8	0	-8.147583	-1.094758	0.806259
27	1	0	-7.914773	-0.156983	0.745313
28	1	0	-2.198050	-0.996643	-3.234475
29	8	0	-2.963384	-1.268890	-3.807794
30	1	0	-3.648724	-1.528838	-3.174768
31	1	0	-6.021564	-4.370088	0.989365
32	8	0	-6.157572	-5.317231	1.213943
33	1	0	-7.083900	-5.372385	1.488384

Table 8.7

Cpl [4-hydroxybenzophenone T_1 * 3 H2O] in Water

1	6	0	-0.008837	0.015277	0.028445
2	6	0	0.092275	-0.240310	1.413095
3	6	0	1.329404	-0.260241	2.048286
4	6	0	2.503471	-0.025628	1.327416
5	6	0	2.419529	0.244025	-0.041241
6	6	0	1.185069	0.271927	-0.679841
7	1	0	-0.804572	-0.389893	2.008461
8	1	0	1.376758	-0.448898	3.118365
9	1	0	3.468770	-0.044791	1.826924
10	1	0	3.324187	0.433428	-0.614734
11	1	0	1.130642	0.483988	-1.743964
12	6	0	-1.285996	0.114522	-0.678165
13	8	0	-1.359283	0.785672	-1.783676
14	6	0	-2.503723	-0.541208	-0.242372
15	6	0	-2.525598	-1.731895	0.568363
16	6	0	-3.704847	-2.311231	0.930332
17	6	0	-4.953391	-1.757820	0.486550
18	6	0	-4.955870	-0.616016	-0.364908
19	6	0	-3.774389	-0.037901	-0.727840
20	1	0	-1.591374	-2.187450	0.877282
21	1	0	-3.728319	-3.208841	1.542149
22	8	0	-6.058671	-2.365271	0.878956
23	1	0	-5.904247	-0.213934	-0.710678
24	1	0	-3.770069	0.837684	-1.367047
25	1	0	-8.183884	-0.878452	-0.746779

26	1	0	-6.911708	-1.930659	0.529399
27	8	0	-8.322790	-1.390731	0.065891
28	1	0	-8.606373	-0.732593	0.720284
29	1	0	-2.276080	0.236782	-3.193113
30	8	0	-2.711983	-0.055410	-4.028233
31	1	0	-3.575289	-0.385064	-3.738740
32	1	0	-6.127051	-3.993475	1.932539
33	8	0	-6.152056	-4.801649	2.475790
34	1	0	-7.080715	-5.074356	2.461717

Table 8.8

Cpl [DeProtonated 4-hydroxybenzophenone T_1 * 3 H2O] in Water

1	6	0	0.061440	-0.045836	-0.085270
2	6	0	0.073674	-0.331297	1.311945
3	6	0	1.203526	-0.106201	2.083149
4	6	0	2.377258	0.412994	1.514453
5	6	0	2.382964	0.712914	0.145035
6	6	0	1.259077	0.496518	-0.638745
7	1	0	-0.820614	-0.719800	1.792833
8	1	0	1.172465	-0.333340	3.147108
9	1	0	3.260458	0.583736	2.124461
10	1	0	3.280703	1.122856	-0.314463
11	1	0	1.284358	0.739638	-1.697479
12	6	0	-1.086390	-0.229391	-0.918967
13	8	0	-1.110587	0.161273	-2.164556
14	6	0	-2.331752	-0.880130	-0.439259
15	6	0	-2.326715	-2.149595	0.198326
16	6	0	-3.496154	-2.749852	0.594907
17	6	0	-4.768611	-2.117810	0.349319
18	6	0	-4.764713	-0.846245	-0.331071
19	6	0	-3.584756	-0.260676	-0.708254
20	1	0	-1.378014	-2.650750	0.370228
21	1	0	-3.493688	-3.716301	1.092328
22	8	0	-5.857215	-2.667284	0.712491
23	1	0	-5.721529	-0.368085	-0.525218
24	1	0	-3.592520	0.700704	-1.214647
25	1	0	-7.442590	-1.852215	0.350964
26	8	0	-8.333032	-1.471212	0.186031
27	1	0	-8.154740	-0.647988	-0.291835
28	1	0	-2.260206	-0.397618	-3.298592
29	8	0	-2.856594	-0.694417	-4.036940
30	1	0	-3.704967	-0.866864	-3.603597
31	1	0	-5.867718	-4.283904	1.544858
32	8	0	-5.914817	-5.155717	1.995429
33	1	0	-6.860868	-5.309502	2.129518