

Non-Aqueous Solvation of n-Octanol and Ethanol
 Levering, Hayes, Callahan, Hadad*, Allen*

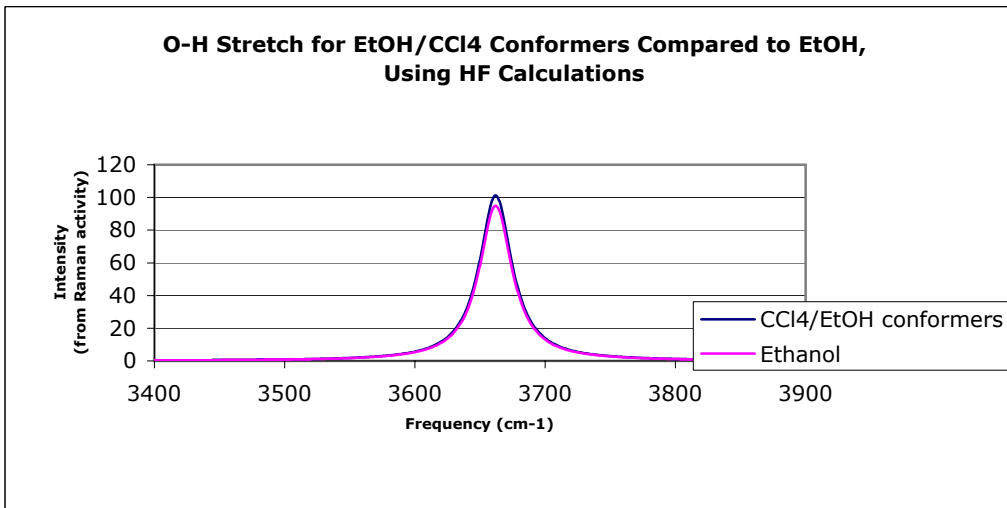
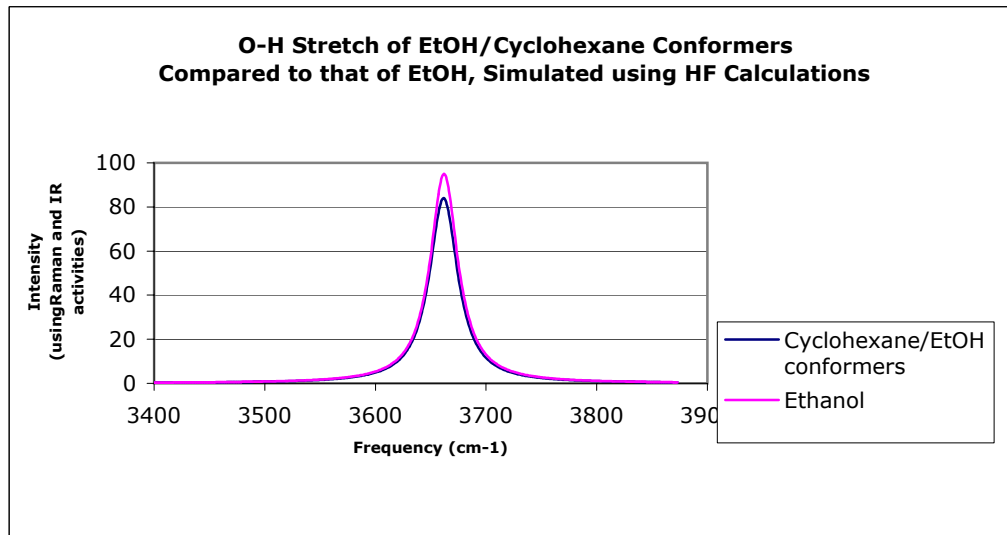
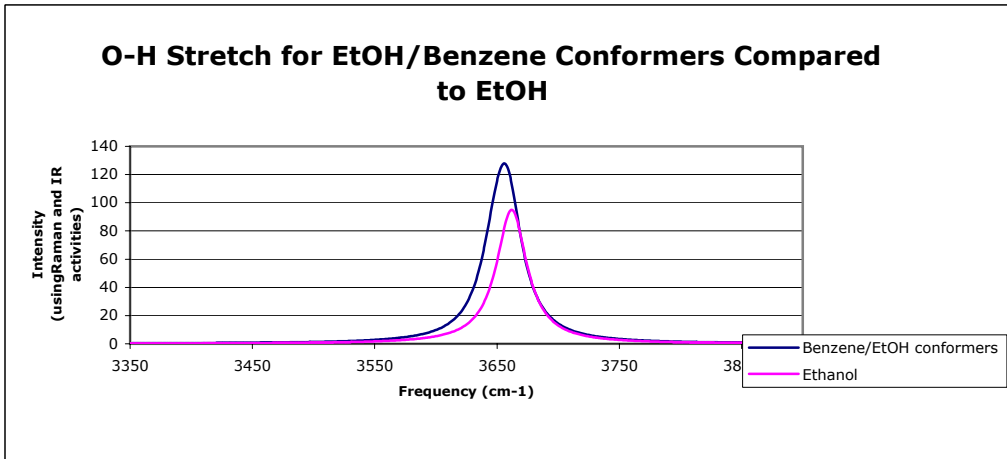
Binding Energies

	B3LYP/6-311+G(3df,2p)//MP2/6-31G*				B3LYP/6-31+G**//MP2/6-31G*			
*All values in kcal/mol	ΔE_{BW}	ΔH_0	ΔH_{298}	ΔG_{298}	ΔE_{BW}	ΔH_0	ΔH_{298}	ΔG_{298}
1	-0.61	-0.63	0.81	7.83	-0.55	-0.57	0.87	7.9
2	-0.73	-0.76	0.71	8.44	-0.77	-0.81	-0.27	8.4
3	-0.02	-0.06	1.44	9.02	-0.24	-0.27	1.23	8.81
4	0.68	0.66	2.05	8.32	0.54	0.51	1.91	8.18
6	0.86	0.84	2.23	9.46	0.85	0.82	2.22	9.45
8	0.32	0.32	1.5	5.87	0.46	0.45	1.63	5.87
9	-1.17	-1.19	0.06	5.01	-1.38	-1.4	-0.15	4.8
10	0.11	0.09	1.33	6.82	0.21	0.19	1.42	6.91

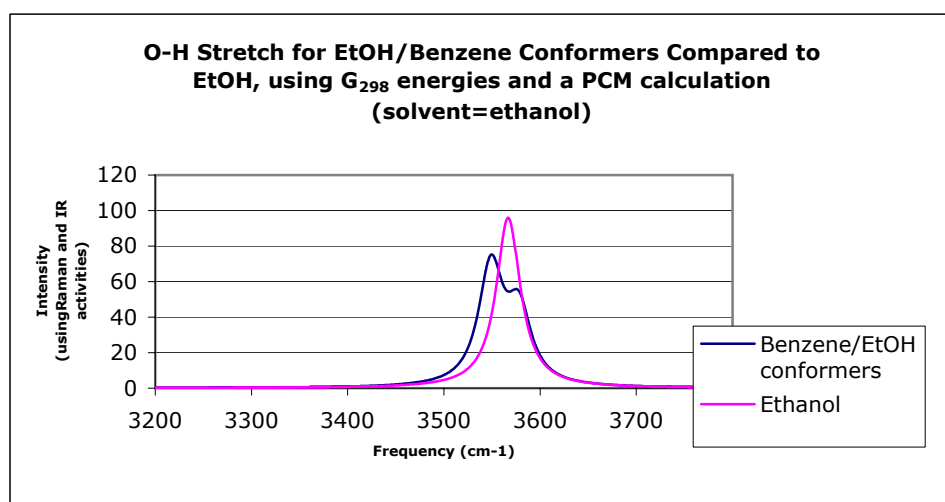
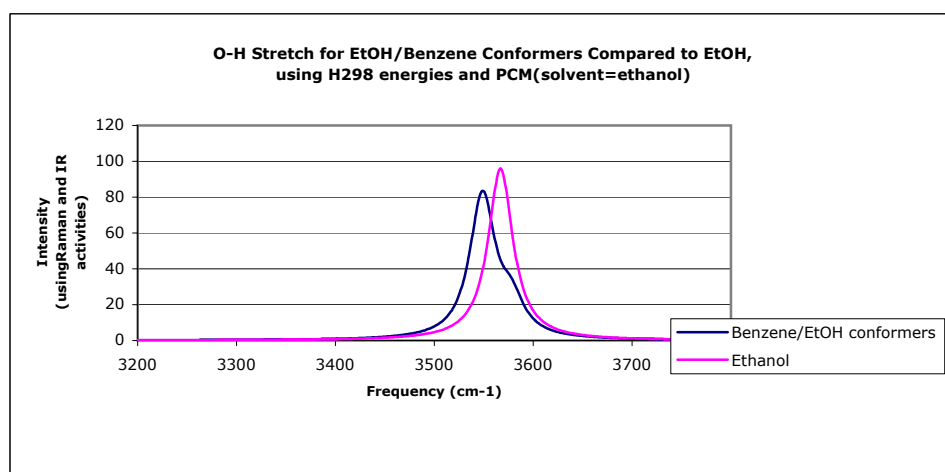
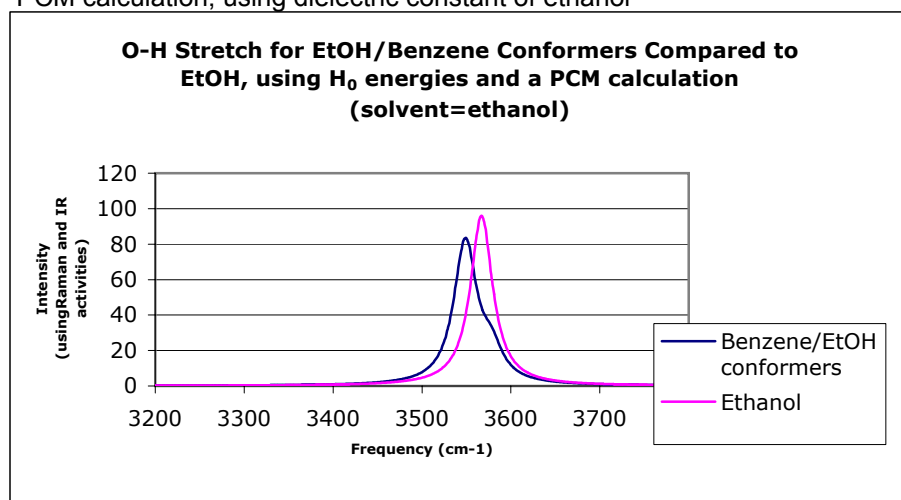
Binding energies compiled using two distinct basis sets.

Energy calculated relative to that of infinitely-separated ethanol and solvent.

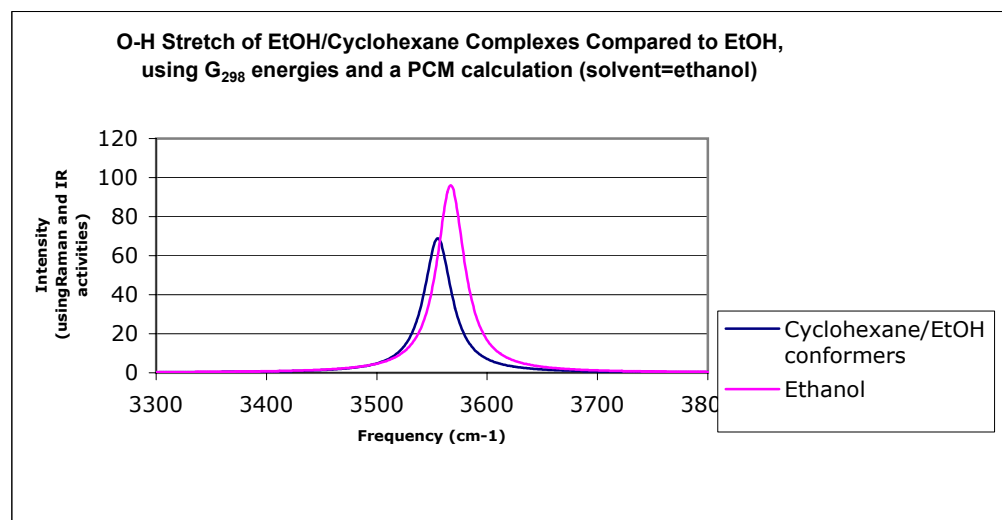
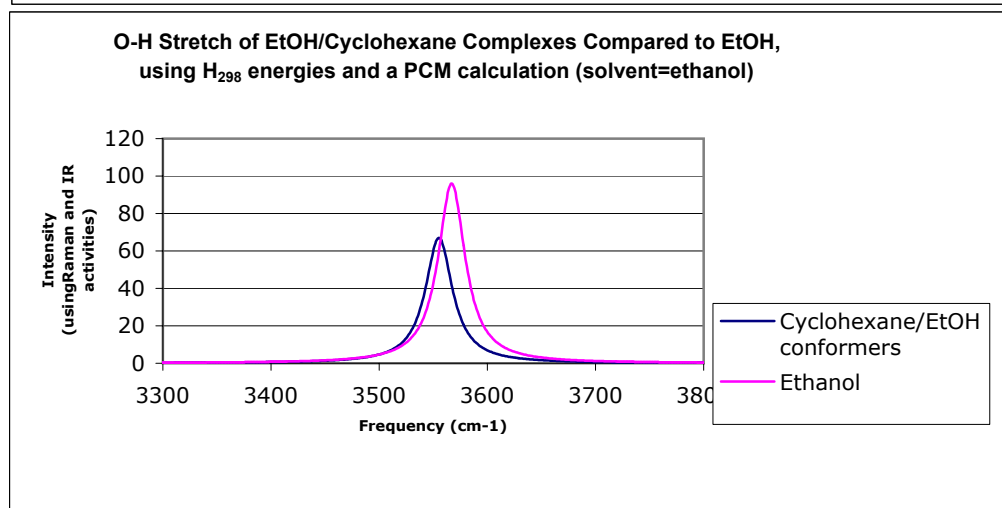
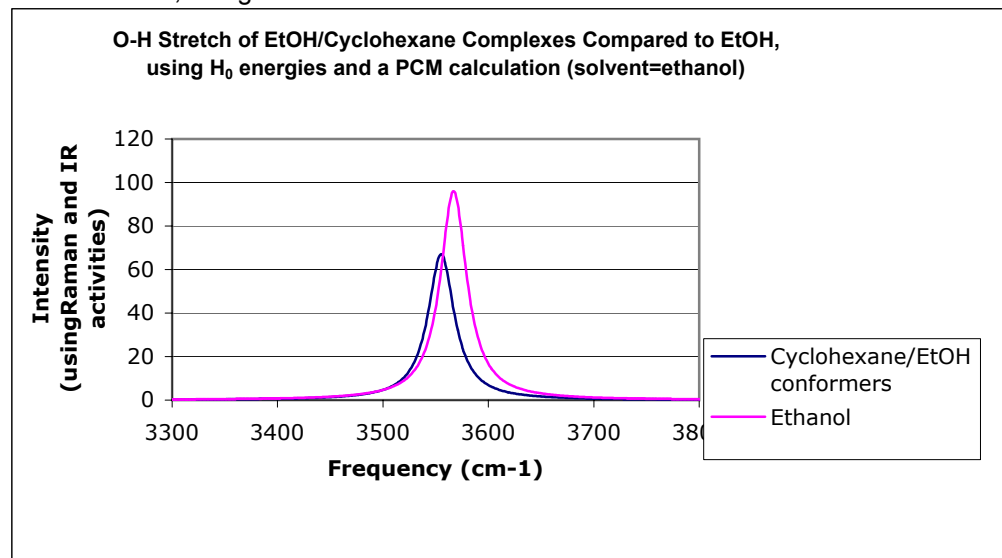
Simulated Raman spectra, using HF frequencies and G 298 energies



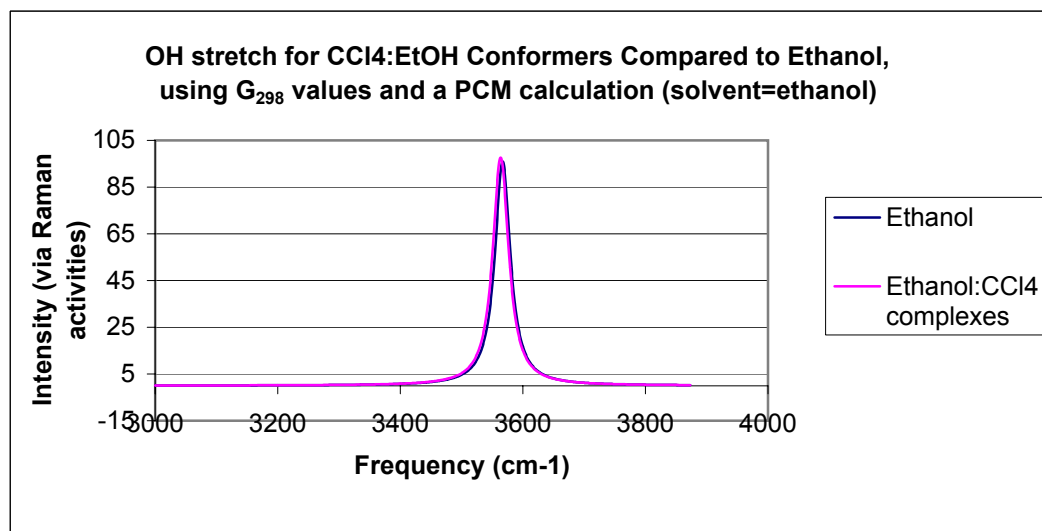
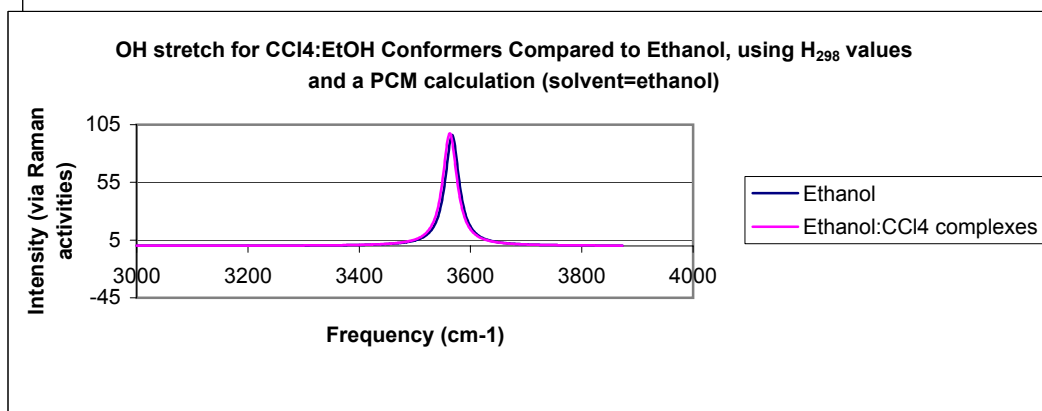
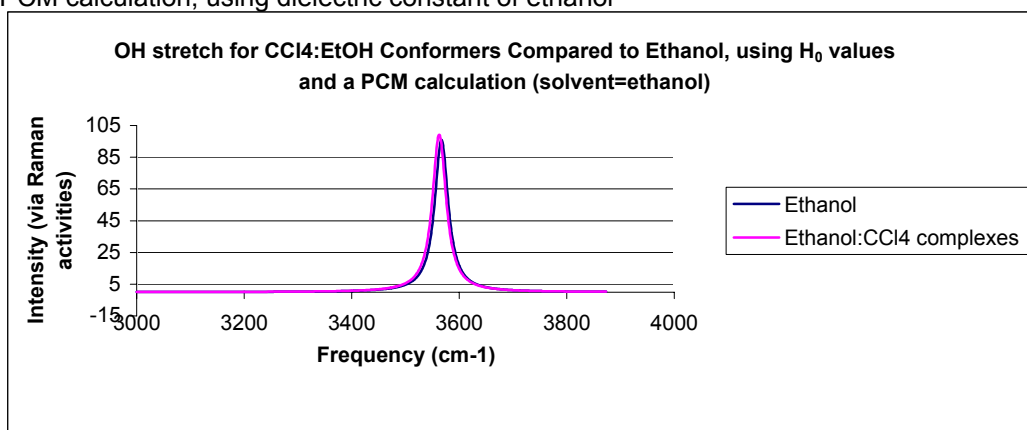
Simulated Raman spectra, using MP2 frequencies and B3LYP/6-31+G** energies
PCM calculation, using dielectric constant of ethanol



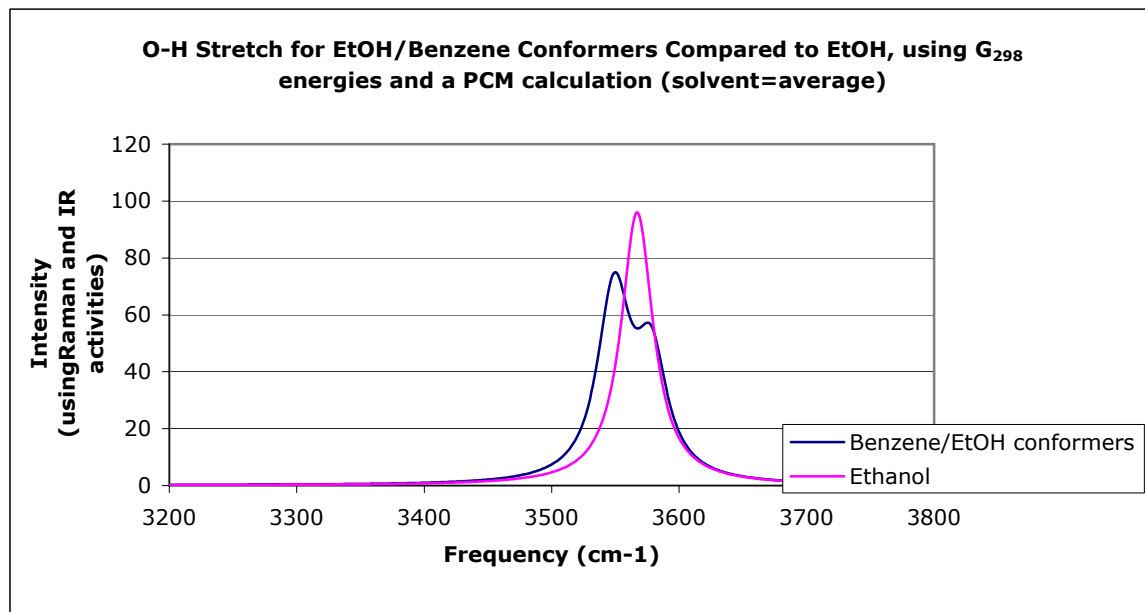
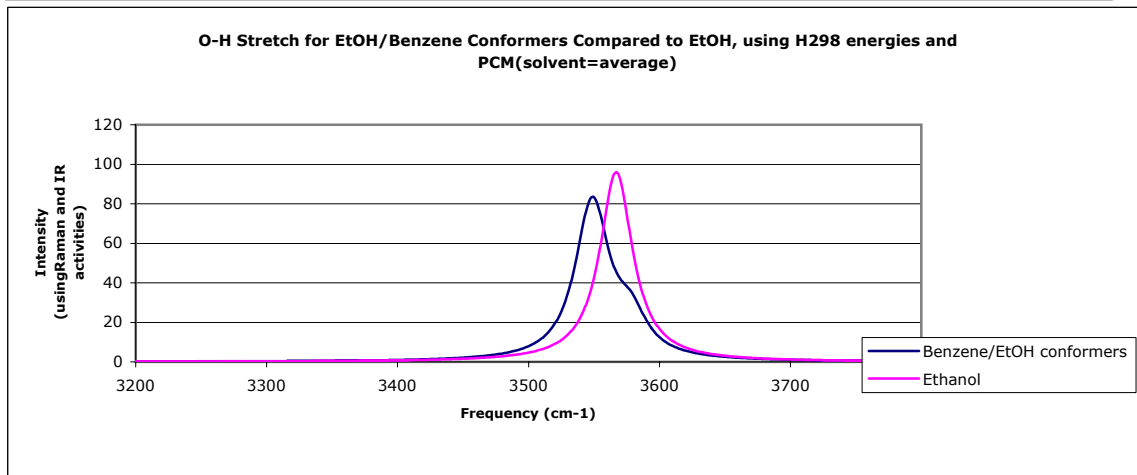
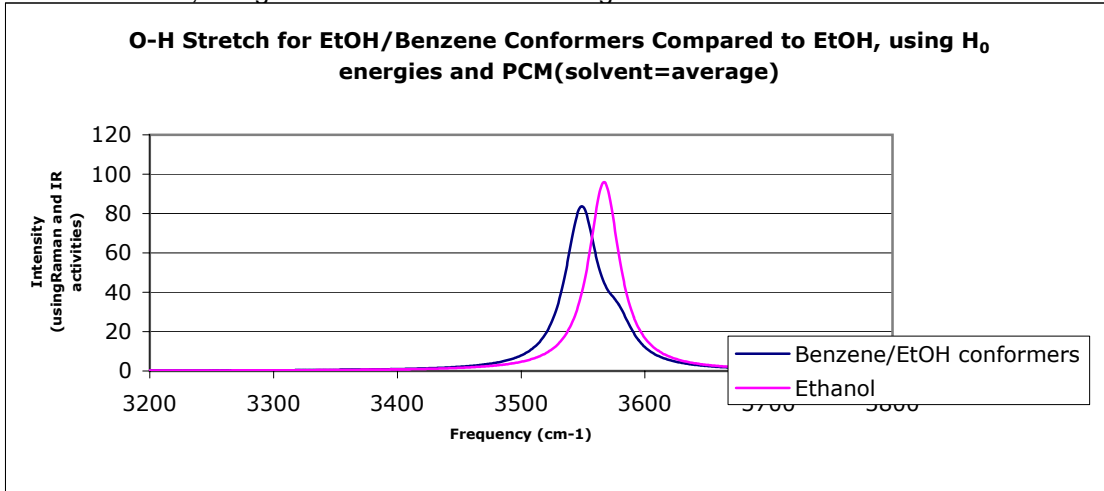
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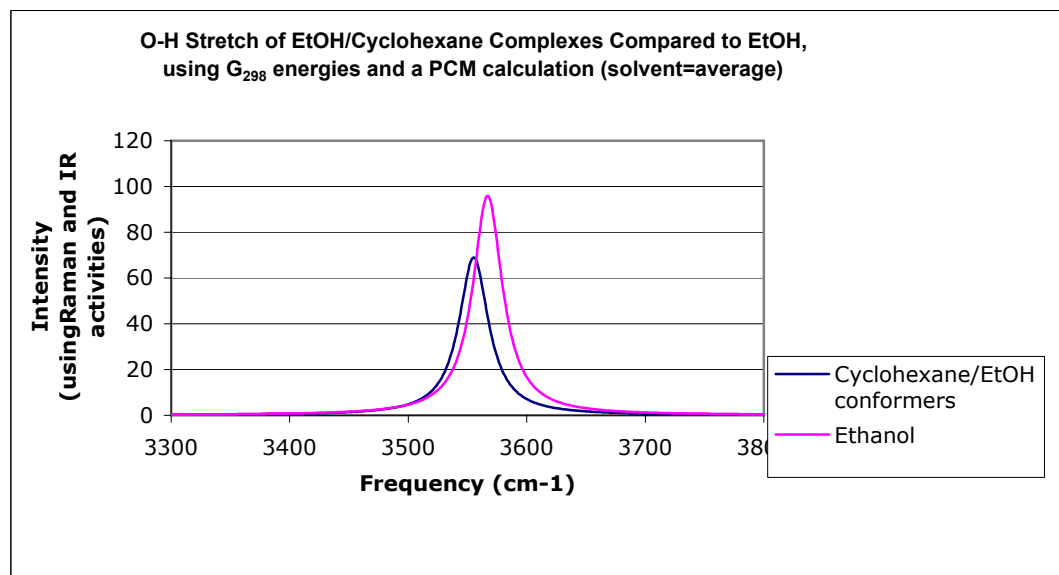
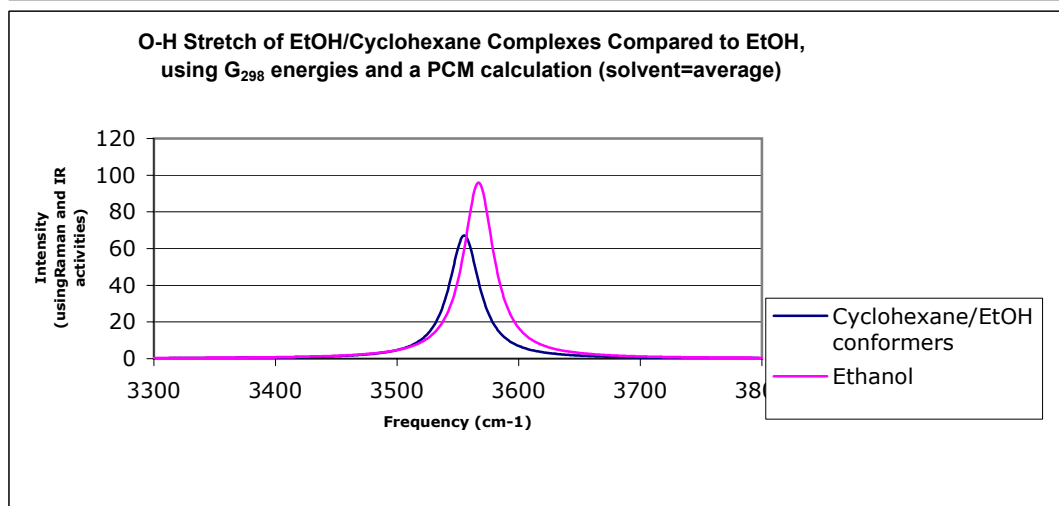
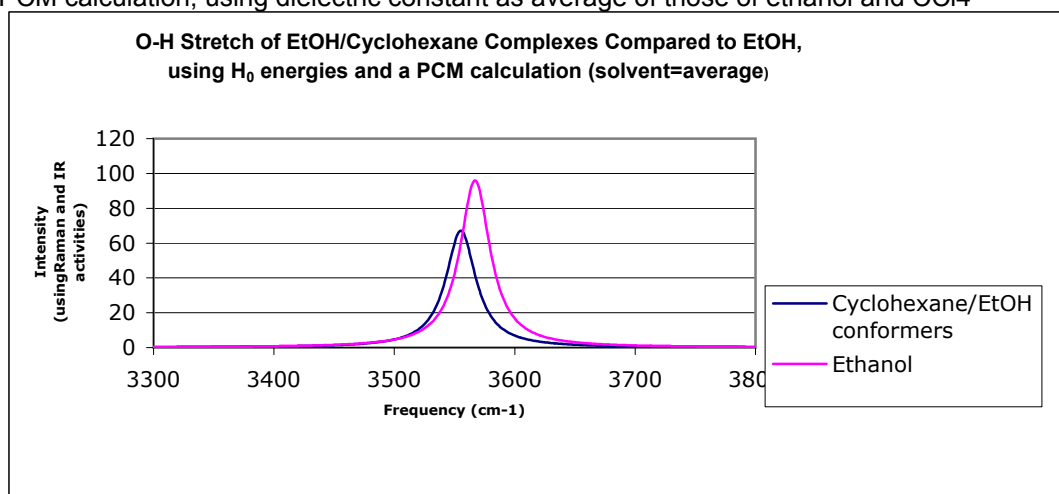
Simulated Raman spectra, using MP2 frequencies and B3LYP/6-31+G** energies
PCM calculation, using dielectric constant of ethanol



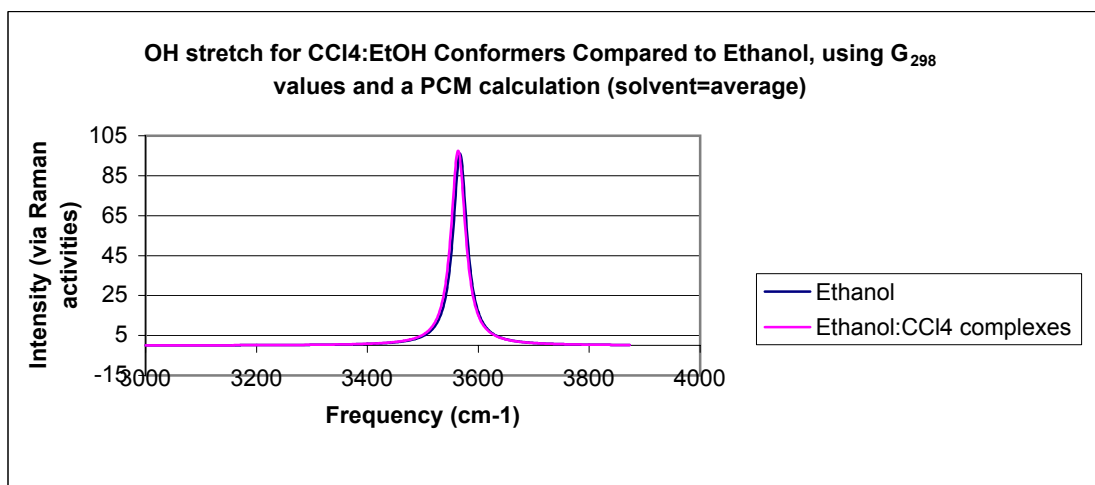
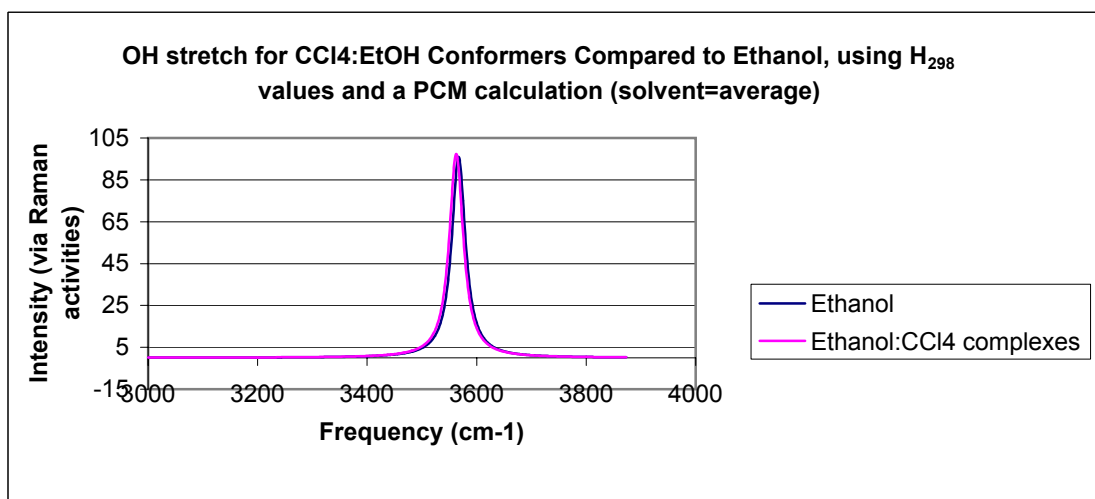
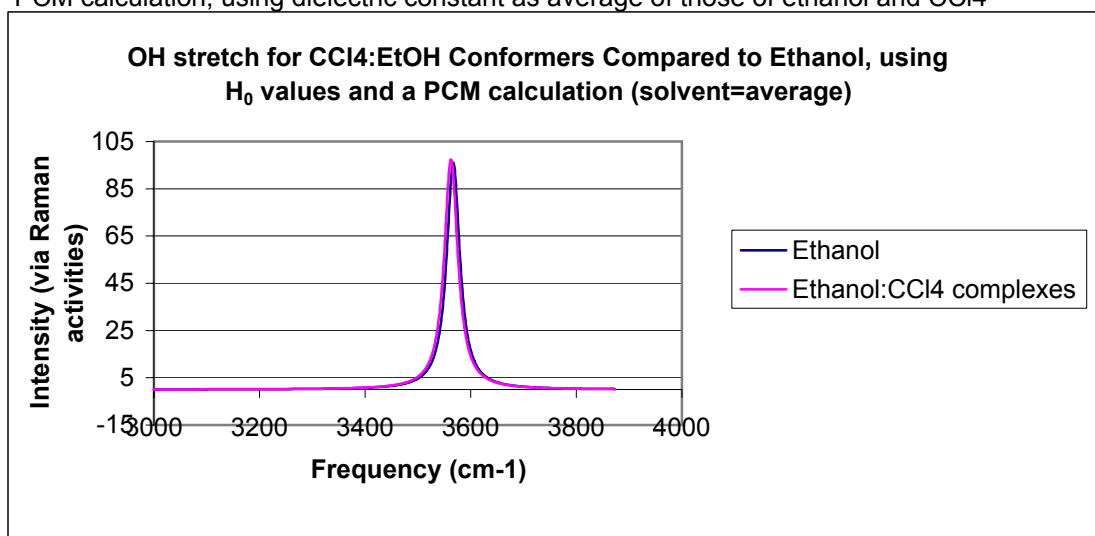
Simulated Raman spectra, using MP2 frequencies and B3LYP/6-31+G** energies
PCM calculation, using dielectric constant as average of those of ethanol and CCl4



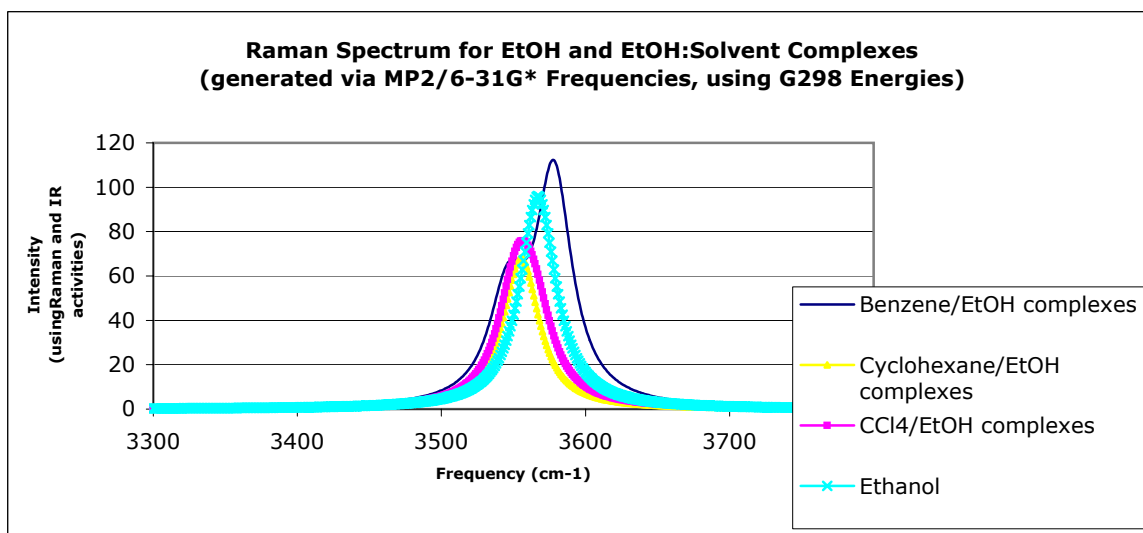
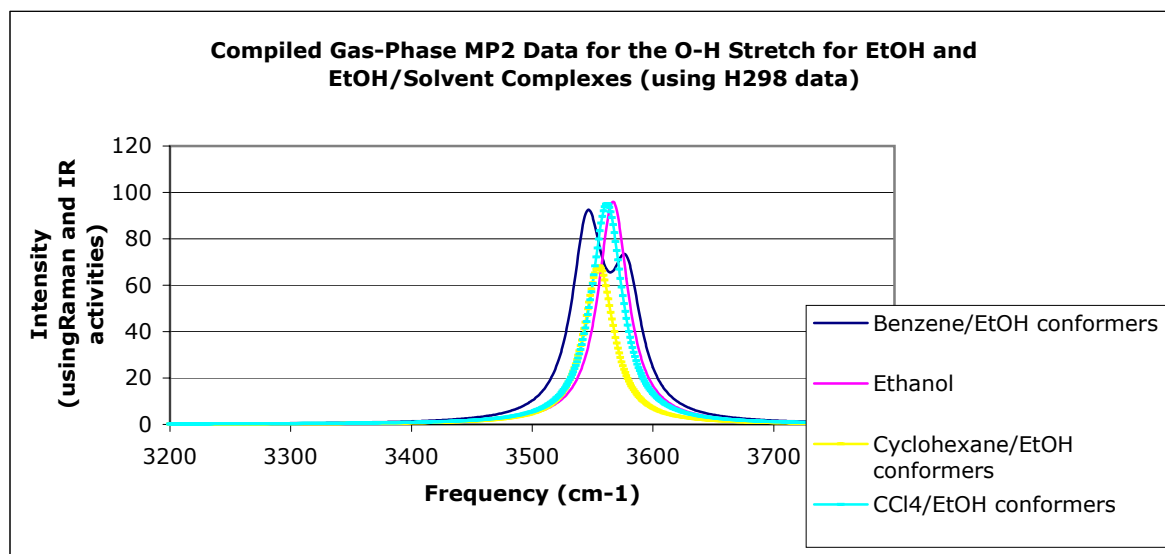
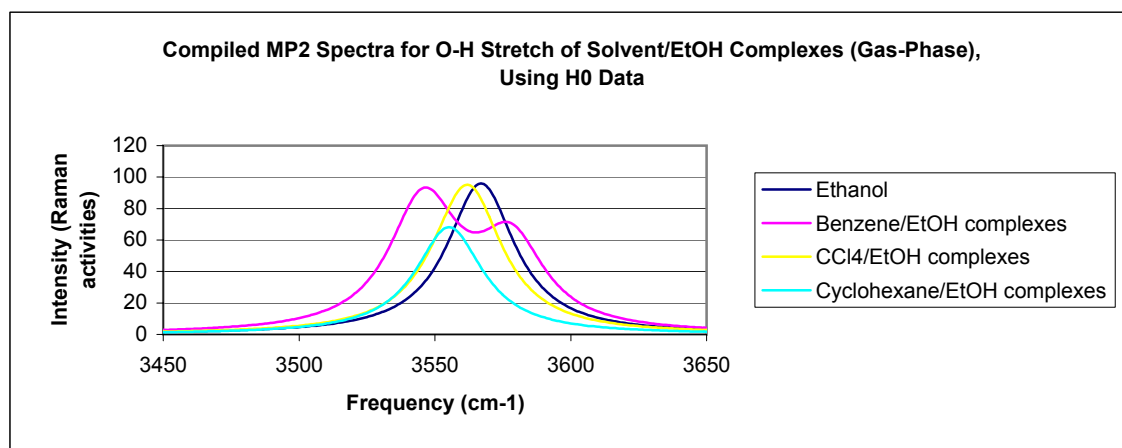
Simulated Raman spectra, using MP2 frequencies and B3LYP/6-31+G** energies
PCM calculation, using dielectric constant as average of those of ethanol and CCl₄



Simulated Raman spectra, using MP2 frequencies and B3LYP/6-31+G** energies
PCM calculation, using dielectric constant as average of those of ethanol and CCl₄



Simulated Raman spectra using MP2 frequencies and B3LYP/6-31+G** energies
Gas-phase calculations



Non-Aqueous Solvation of n-Octanol and Ethanol
 Levering, Hayes, Callahan, Hadad*, Allen*

	1	2	3	Benzene	Ethanol
<i>C</i>	6.25	6.24	6.25	6.25	
<i>C</i>	6.25	6.25	6.25	6.25	
<i>C</i>	6.25	6.24	6.25	6.25	
<i>C</i>	6.25	6.26	6.25	6.25	
<i>C</i>	6.25	6.26	6.25	6.25	
<i>C</i>	6.25	6.25	6.25	6.25	
<i>H</i>	0.75	0.75	0.76	0.75	
<i>H</i>	0.75	0.75	0.76	0.75	
<i>H</i>	0.75	0.75	0.76	0.75	
<i>H</i>	0.75	0.75	0.76	0.75	
<i>H</i>	0.75	0.74	0.73	0.75	
<i>H</i>	0.75	0.75	0.76	0.75	
<i>C</i>	6.12	6.13	6.13		6.12
<i>C</i>	6.72	6.73	6.72		6.72
<i>O</i>	8.79	8.78	8.78		8.79
<i>H</i>	0.81	0.76	0.75		0.80
<i>H</i>	0.81	0.80	0.77		0.80
<i>H</i>	0.76	0.78	0.80		0.75
<i>H</i>	0.76	0.76	0.75		0.75
<i>H</i>	0.76	0.77	0.77		0.76
<i>H</i>	0.50	0.51	0.51		0.51

Atomic charges for complexes **1-3** compared to their infinitely-separated component parts, as calculated at the NPA level via the B3LYP/6-31+G**//MP2/6-31G* level of theory

Non-Aqueous Solvation of n-Octanol and Ethanol
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	4	5	6	Cyclohexane	Ethanol
<i>C</i>	6.47	6.47	6.47	6.39	
<i>C</i>	6.48	6.47	6.47	6.39	
<i>C</i>	6.47	6.47	6.47	6.39	
<i>C</i>	6.48	6.47	6.47	6.39	
<i>C</i>	6.47	6.47	6.47	6.39	
<i>C</i>	6.48	6.47	6.49	6.39	
<i>H</i>	0.76	0.76	0.76	0.80	
<i>H</i>	0.77	0.77	0.77	0.81	
<i>H</i>	0.75	0.77	0.78	0.81	
<i>H</i>	0.76	0.76	0.76	0.80	
<i>H</i>	0.76	0.76	0.76	0.80	
<i>H</i>	0.77	0.77	0.77	0.81	
<i>H</i>	0.75	0.77	0.77	0.81	
<i>H</i>	0.76	0.76	0.76	0.80	
<i>H</i>	0.76	0.76	0.76	0.80	
<i>H</i>	0.77	0.77	0.77	0.81	
<i>H</i>	0.76	0.76	0.76	0.80	
<i>H</i>	0.76	0.77	0.75	0.81	
<i>C</i>	6.13	6.12	6.13		6.12
<i>C</i>	6.72	6.71	6.72		6.72
<i>O</i>	8.79	8.78	8.78		8.79
<i>H</i>	8.79	0.80	0.80		0.80
<i>H</i>	0.79	0.80	0.80		0.80
<i>H</i>	0.75	0.76	0.76		0.75
<i>H</i>	0.75	0.76	0.75		0.75
<i>H</i>	0.76	0.76	0.76		0.76
<i>H</i>	0.50	0.50	0.50		0.50

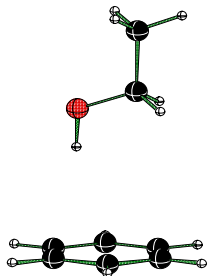
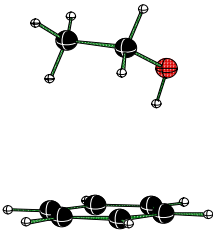
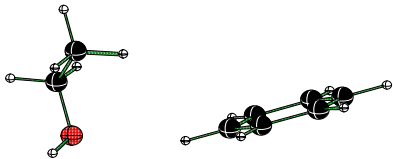
Atomic charges for complexes **4-6** compared to their infinitely-separated component parts, as calculated at the NPA level via the B3LYP/6-31+G**//MP2/6-31G* level of theory

	7	8	9	10	CCl4	Ethanol
C	6.32	6.32	6.32	6.32	6.32	
Cl	16.91	16.92	16.93	16.9	16.92	
Cl	16.92	16.92	16.93	16.91	16.92	
Cl	16.92	16.92	16.93	16.92	16.92	
Cl	16.92	16.92	16.9	16.93	16.92	
C	6.12	6.12	6.13	6.13		6.12
C	6.71	6.72	6.72	6.72		6.72
O	8.78	8.79	8.79	8.79		8.79
H	0.80	0.80	0.80	0.80		0.80
H	0.80	0.80	0.80	0.80		0.80
H	0.76	0.76	0.75	0.76		0.75
H	0.76	0.76	0.75	0.75		0.75
H	0.76	0.76	0.76	0.76		0.76
H	0.50	0.50	0.50	0.50		0.50

Atomic charges for complexes **7-10** compared to their infinitely-separated component parts, as calculated at the NPA level via the B3LYP/6-31+G**//MP2/6-31G* level of theory

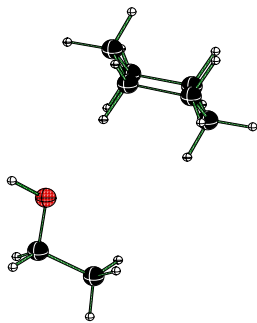
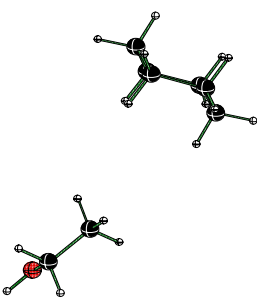
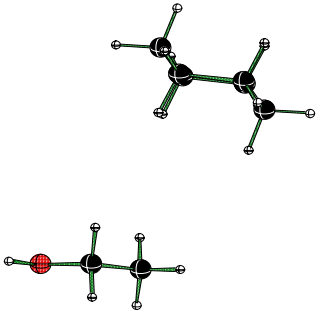
Non-Aqueous Solvation of n-Octanol and Ethanol Levering, Hayes, Callahan, Hadad*, Allen*

Ethanol/Benzene Complexes (HF)

1				2				3			
											
C	1.574194	1.286126	0.664523	C	-1.537781	1.053053	0.966937	C	-2.508785	1.253394	-0.192738
C	1.689336	0.108390	1.387130	C	-1.709958	1.328732	-0.381554	C	-3.262806	0.244886	0.386367
C	1.812212	-1.103564	0.723186	C	-1.738083	0.293247	-1.303015	C	-2.735264	-1.031686	0.505914
C	1.817694	-1.136885	-0.663930	C	-1.597175	-1.019217	-0.876129	C	-1.454835	-1.298637	0.047175
C	1.700125	0.041749	-1.386289	C	-1.425084	-1.295075	0.472962	C	-0.698010	-0.291227	-0.532689
C	1.579513	1.252805	-0.722041	C	-1.394341	-0.258039	1.394202	C	-1.228228	0.984865	-0.651414
H	1.480595	2.225610	1.179402	H	-1.516767	1.856600	1.681371	H	-2.917676	2.244016	-0.286758
H	1.683952	0.133792	2.462113	H	-1.822477	2.345824	-0.712281	H	-4.256615	0.452210	0.742131
H	1.902434	-2.017060	1.283244	H	-1.871180	0.506666	-2.348495	H	-3.320393	-1.815002	0.954648
H	1.912359	-2.076181	-1.178766	H	-1.622836	-1.823099	-1.590010	H	-1.046393	-2.289484	0.139546
H	1.703020	0.015447	-2.461258	H	-1.316201	-2.312380	0.803975	H	0.296817	-0.497182	-0.884532
H	1.490016	2.166425	-1.282196	H	-1.262024	-0.472234	2.439682	H	-0.644499	1.767891	-1.102721
C	-2.428404	0.332786	-0.000299	O	2.136433	-1.181953	-0.359099	O	2.959570	-0.591537	-0.942681
C	-3.937602	0.188311	-0.000700	C	2.773641	-0.193582	0.404089	C	3.420121	-0.412586	0.373607
O	-1.866832	-0.951756	-0.001151	C	2.753533	1.168320	-0.274474	C	3.156452	0.990695	0.897627
H	-2.106851	0.893046	-0.876491	H	1.209869	-0.988137	-0.410610	H	3.435740	-0.015441	-1.524688
H	-2.107181	0.891729	0.876854	H	2.325913	-0.125559	1.393972	H	2.889189	-1.141255	0.971434
H	-4.263723	-0.358380	0.877257	H	3.794404	-0.530046	0.535270	H	4.480179	-0.649223	0.438959
H	-4.263338	-0.357249	-0.879504	H	3.289132	1.904337	0.318754	H	2.096424	1.215446	0.863359
H	-4.417348	1.162576	-0.000179	H	1.733892	1.520183	-0.404184	H	3.681721	1.734342	0.302852
H	-0.921682	-0.884011	-0.000751	H	3.218308	1.108836	-1.252751	H	3.497074	1.087755	1.924122

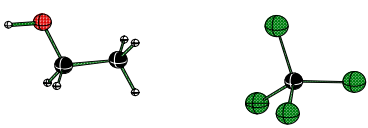
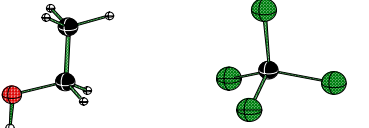
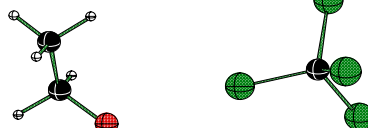
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Ethanol/Cyclohexane Complexes (HF)

4				5				6			
											
C	1.915729	0.778721	1.265410	C	2.424970	0.495518	1.394461	C	2.003895	1.551016	-0.032056
C	1.477030	-0.689196	1.265840	C	1.947789	-0.932073	1.109134	C	1.390195	0.821783	1.167272
C	1.949695	-1.412646	0.000543	C	2.391707	-1.404491	-0.278918	C	2.041152	-0.548024	1.383623
C	1.477200	-0.690092	-1.265335	C	1.937713	-0.432867	-1.372867	C	1.979092	-1.404721	0.115107
C	1.915882	0.777828	-1.265890	C	2.414738	0.994755	-1.087843	C	2.592774	-0.675431	-1.084221
C	1.444642	1.501522	-0.000523	C	1.971489	1.467167	0.300362	C	1.941746	0.694320	-1.300503
H	1.532036	1.283457	2.148351	H	2.059116	0.825782	2.363067	H	1.495206	2.497424	-0.194693
H	3.002287	0.830366	1.325477	H	3.512463	0.504462	1.453662	H	3.043280	1.790490	0.188238
H	0.391816	-0.736909	1.319428	H	0.860672	-0.964320	1.167730	H	0.322739	0.688327	0.996515
H	1.860736	-1.192979	2.149790	H	2.319939	-1.610715	1.872145	H	1.487544	1.428197	2.063966
H	1.590665	-2.439034	0.000881	H	2.003002	-2.399850	-0.477570	H	1.559068	-1.065631	2.208864
H	3.037862	-1.465468	0.000644	H	3.477623	-1.485522	-0.299287	H	3.082322	-0.408224	1.670885
H	0.392000	-0.737870	-1.319022	H	0.850250	-0.442120	-1.430953	H	0.939707	-1.644250	-0.105063
H	1.861044	-1.194505	-2.148868	H	2.302973	-0.763069	-2.341713	H	2.487583	-2.351353	0.277773
H	1.532289	1.281943	-2.149230	H	2.041415	1.673078	-1.850335	H	2.495000	-1.281864	-1.980688
H	3.002446	0.829436	-1.325865	H	3.501756	1.027799	-1.147577	H	3.660250	-0.542054	-0.914254
H	1.803233	2.527895	-0.000857	H	2.360884	2.462164	0.498913	H	2.424338	1.211833	-2.125271
H	0.357368	1.548029	-0.000611	H	0.885702	1.548953	0.320988	H	0.900643	0.555284	-1.588151
C	-3.570886	-0.415449	-0.000136	C	-4.322748	-0.462092	0.210343	C	-3.722871	-0.098516	0.471145
C	-3.506030	1.098530	0.000012	C	-2.878031	-0.456519	-0.248056	C	-3.059532	-1.164799	-0.377489
O	-2.254413	-0.908732	0.000101	O	-4.865062	0.807514	-0.047408	O	-4.254081	0.874862	-0.390709
H	-4.109364	-0.767091	0.877635	H	-4.879732	-1.231867	-0.320773	H	-4.509002	-0.541452	1.079985
H	-4.109004	-0.766931	-0.878192	H	-4.376820	-0.693426	1.272616	H	-2.995725	0.345520	1.148754
H	-2.978906	1.452978	-0.878699	H	-2.316847	0.301862	0.286645	H	-2.268578	-0.729315	-0.977987
H	-2.979397	1.452852	0.879068	H	-2.821632	-0.236740	-1.308307	H	-3.782885	-1.617697	-1.046205
H	-4.504864	1.523716	-0.000234	H	-2.415500	-1.422205	-0.068384	H	-2.632199	-1.941778	0.248946
H	-2.266515	-1.855331	-0.000018	H	-5.770533	0.829235	0.228697	H	-4.675342	1.553889	0.116779

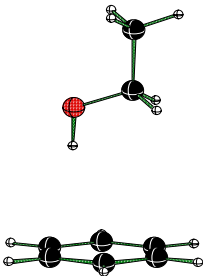
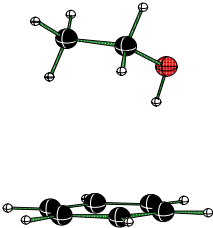

Non-Aqueous Solvation of n-Octanol and Ethanol
 Levering, Hayes, Callahan, Hadad*, Allen*

Ethanol/CCl4 Complexes (HF)

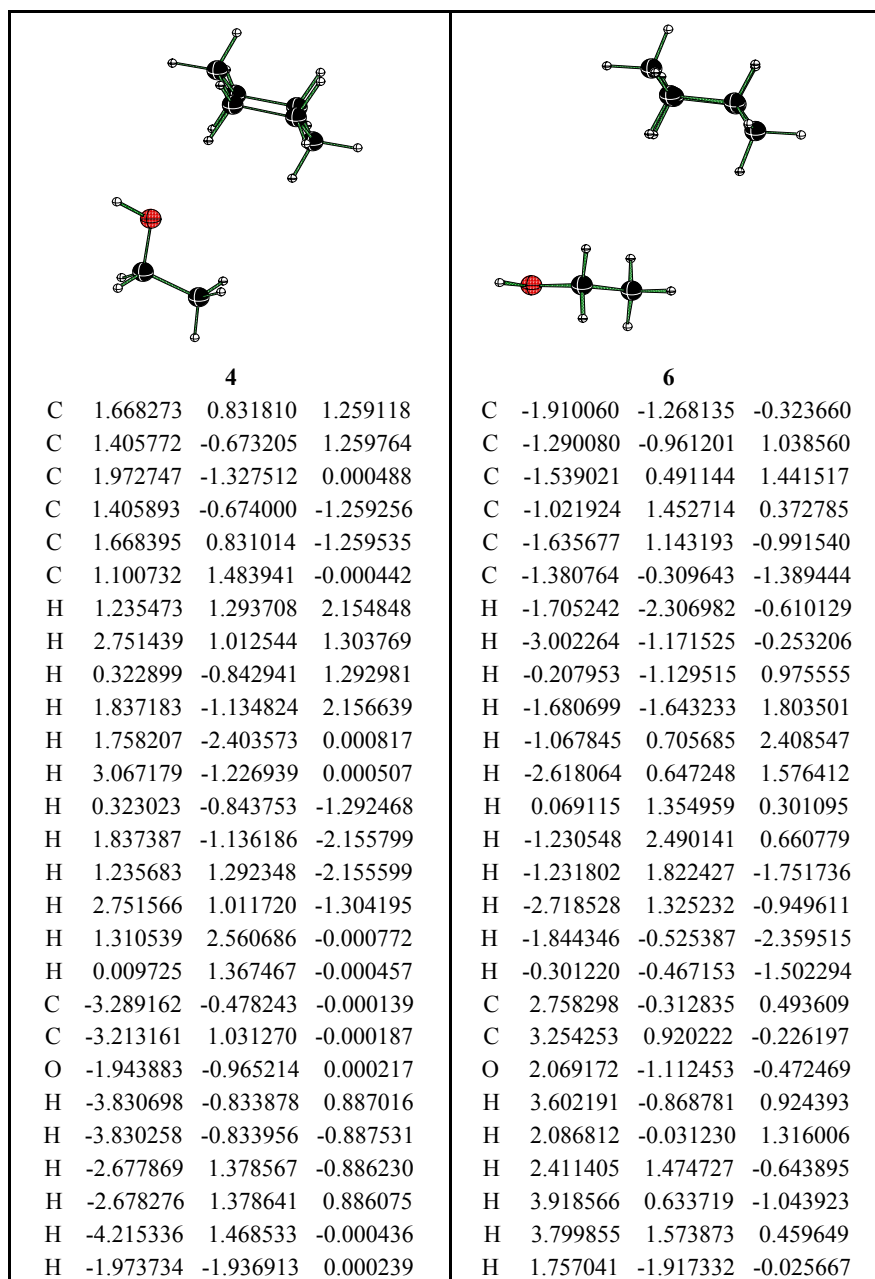
											
7		8		9							
C	-1.647189	0.012885	0.002588	C	-1.488052	-0.023645	0.003306	C	-1.419885	-0.022147	-0.004857
Cl	-0.838644	1.575896	-0.141027	Cl	-0.692254	-0.729587	-1.407793	Cl	-2.104171	-0.517783	1.548627
Cl	-1.199852	-1.010260	-1.366542	Cl	-0.791321	-0.708867	1.475088	Cl	0.309465	0.255895	0.168319
Cl	-3.397332	0.252521	0.010515	Cl	-3.215637	-0.383999	-0.053879	Cl	-2.212398	1.465930	-0.542456
Cl	-1.153876	-0.770005	1.507591	Cl	-1.249755	1.726341	-0.001392	Cl	-1.702975	-1.295941	-1.199692
C	4.914115	-0.535355	0.033932	C	3.827233	-0.280162	-0.140003	C	4.382128	0.323023	-0.347716
C	3.456862	-0.133387	-0.074882	C	3.798650	1.226992	0.016954	C	4.413427	-1.118263	0.119130
O	5.691080	0.634678	0.014337	O	5.137121	-0.719521	0.114109	O	3.335801	0.979726	0.326005
H	5.080691	-1.090212	0.955532	H	3.126987	-0.741184	0.554129	H	5.332258	0.806806	-0.131653
H	5.184289	-1.188292	-0.794105	H	3.519187	-0.556588	-1.146750	H	4.227803	0.366125	-1.423761
H	3.284205	0.410109	-0.997012	H	4.486496	1.691157	-0.680935	H	3.474122	-1.610211	-0.107157
H	3.180389	0.508098	0.754307	H	4.094548	1.506213	1.021979	H	4.572073	-1.163531	1.190655
H	2.816064	-1.009643	-0.063799	H	2.801144	1.612123	-0.170652	H	5.214703	-1.660323	-0.373297
H	6.607959	0.409083	0.081424	H	5.180132	-1.660778	0.023395	H	3.309952	1.889940	0.066272

Non-Aqueous Solvation of n-Octanol and Ethanol Levering, Hayes, Callahan, Hadad*, Allen*

Ethanol/Benzene Complexes (MP2)

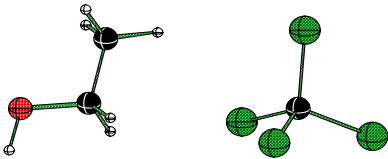
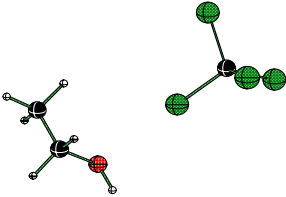
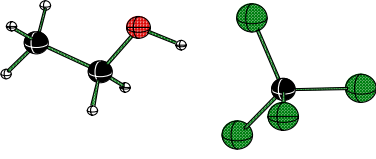
1				2				3			
											
C	1.844581	-1.042492	-0.697715	C	-1.278337	1.095271	0.956629	C	-2.361990	1.188496	-0.133225
C	1.522285	0.123147	-1.396295	C	-1.568263	1.314022	-0.391576	C	-2.939973	0.097713	0.517331
C	1.204387	1.289978	-0.698893	C	-1.673751	0.232615	-1.267621	C	-2.289864	-1.137106	0.520021
C	1.204084	1.290654	0.697648	C	-1.493492	-1.068965	-0.794811	C	-1.059909	-1.278717	-0.123754
C	1.521737	0.124513	1.396316	C	-1.202718	-1.288345	0.554604	C	-0.478645	-0.189704	-0.776596
C	1.844269	-1.041819	0.699005	C	-1.093261	-0.204899	1.429384	C	-1.131813	1.044538	-0.776329
H	2.089702	-1.951468	-1.240651	H	-1.197048	1.937947	1.638555	H	-2.869407	2.150161	-0.136953
H	1.518277	0.120929	-2.483126	H	-1.713527	2.326839	-0.758792	H	-3.898331	0.208915	1.018648
H	0.956851	2.197834	-1.243036	H	-1.899645	0.402475	-2.317148	H	-2.741315	-1.987484	1.025335
H	0.956403	2.199055	1.240812	H	-1.581670	-1.912423	-1.475048	H	-0.554844	-2.241869	-0.126870
H	1.517203	0.123328	2.483147	H	-1.060390	-2.301267	0.922198	H	0.486962	-0.301135	-1.262231
H	2.089199	-1.950254	1.242931	H	-0.870197	-0.376073	2.479393	H	-0.684180	1.894024	-1.287302
C	-2.200382	0.292844	0.000160	O	1.923300	-1.217580	-0.395684	O	2.842055	-0.594340	-0.869645
C	-3.681965	-0.012368	-0.000163	C	2.477477	-0.148372	0.365249	C	2.781730	-0.383275	0.544172
O	-1.512239	-0.952648	-0.000029	C	2.391827	1.179850	-0.365878	C	2.594269	1.079194	0.901694
H	-1.934368	0.889620	-0.884544	H	0.968916	-1.042831	-0.468619	H	3.597437	-0.081531	-1.203765
H	-1.934679	0.889181	0.885257	H	1.988158	-0.073041	1.347005	H	1.924053	-0.968847	0.880102
H	-3.942528	-0.596566	0.884834	H	3.520708	-0.424673	0.537928	H	3.677933	-0.791187	1.031725
H	-3.942314	-0.595891	-0.885667	H	2.868297	1.979340	0.210516	H	1.674499	1.457933	0.452152
H	-4.270237	0.909547	0.000124	H	1.345995	1.454639	-0.530028	H	3.435786	1.679610	0.540237
H	-0.559579	-0.760881	-0.000236	H	2.887101	1.102655	-1.336354	H	2.532139	1.209297	1.986201

Ethanol/Cyclohexane Complexes (MP2)



Non-Aqueous Solvation of n-Octanol and Ethanol
 Levering, Hayes, Callahan, Hadad*, Allen*

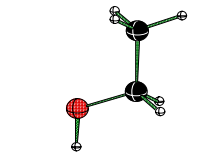
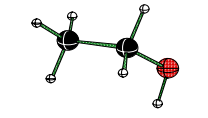
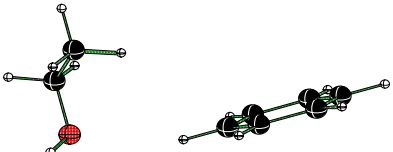
Ethanol/CCl4 Complexes (MP2)

											
8		9		10							
C	-1.275334	-0.031008	0.005487	C	1.293083	0.020560	0.002374	C	1.180171	0.040981	0.017250
Cl	-0.430666	-0.865525	-1.309779	Cl	1.531674	1.766082	-0.201717	Cl	0.270872	-0.216500	1.508093
Cl	-0.510323	-0.438116	1.549593	Cl	1.772171	-0.444598	1.646992	Cl	2.902419	-0.241433	0.304571
Cl	-2.970207	-0.540093	0.033547	Cl	2.303791	-0.848357	-1.166741	Cl	0.937888	1.699959	-0.551196
Cl	-1.187204	1.717864	-0.254539	Cl	-0.405181	-0.382675	-0.259451	Cl	0.603441	-1.092547	-1.226758
C	3.276475	-0.317592	-0.172219	C	-3.860197	-0.214412	0.503439	C	-3.054534	0.087999	-0.457569
C	3.014213	1.162315	0.004214	C	-4.019927	1.117270	-0.196476	C	-4.247852	0.705471	0.239023
O	4.651787	-0.540854	0.147707	O	-3.189586	-1.092945	-0.410287	O	-2.790000	-1.158780	0.188840
H	2.619424	-0.900401	0.488475	H	-3.275711	-0.095619	1.425874	H	-3.272275	-0.062786	-1.524758
H	3.059755	-0.621216	-1.206506	H	-4.842190	-0.623797	0.776587	H	-2.185611	0.757102	-0.387658
H	3.662817	1.738191	-0.659659	H	-4.597017	0.989605	-1.114762	H	-4.021471	0.864591	1.295566
H	3.224519	1.457706	1.034525	H	-3.040930	1.526002	-0.455336	H	-5.109144	0.037736	0.166949
H	1.972128	1.400295	-0.225190	H	-4.538687	1.830673	0.450041	H	-4.507073	1.666025	-0.215247
H	4.827733	-1.490250	0.041841	H	-3.108275	-1.961473	0.019462	H	-1.999680	-1.540266	-0.227862

Non-Aqueous Solvation of n-Octanol and Ethanol Levering, Hayes, Callahan, Hadad*, Allen*

Frequencies (cm-1)

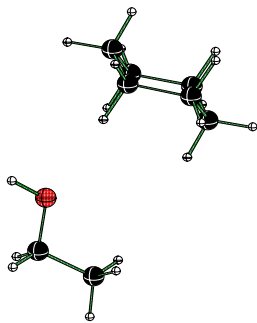
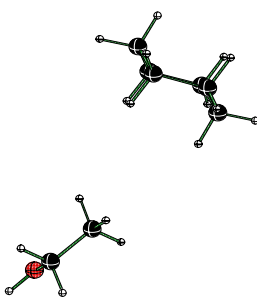
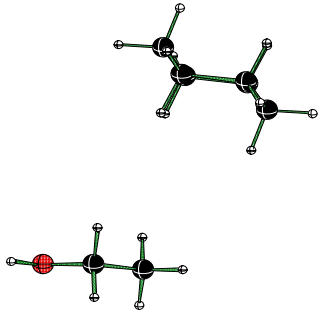
Ethanol/Benzene Complexes (HF)

 1			 2			 3		
1.8600	24.9088	26.9070	8.1957	27.9747	29.3956	9.8515	16.5290	19.1662
35.3415	41.4505	60.4454	47.4654	55.0425	71.0126	38.1181	56.7528	67.8645
275.5199	368.8027	451.1668	285.3429	388.2838	453.9644	284.2949	331.4849	453.9814
453.9202	455.4131	665.0753	454.2767	457.3174	664.9285	454.3060	457.2026	664.2691
665.1611	770.3563	776.1280	665.0063	770.3355	776.4943	666.5838	772.3132	778.7482
884.6649	965.8738	966.2695	869.4218	965.5299	966.0003	869.2850	962.6802	965.0516
978.5181	1081.7701	1097.7533	967.0717	1081.5550	1097.3049	973.8518	1083.0036	1096.1700
1104.9785	1105.3604	1136.9431	1104.8462	1105.2901	1139.4271	1100.2935	1111.4083	1141.4248
1138.5721	1140.9785	1141.0955	1140.2914	1141.0144	1159.1001	1143.8984	1149.2108	1150.5389
1198.2825	1225.0876	1294.2172	1198.2084	1200.5501	1248.0528	1194.5858	1198.3657	1244.3349
1294.4260	1299.5266	1352.0821	1294.2433	1294.3676	1352.5748	1293.4748	1298.9839	1354.4279
1405.7256	1421.3752	1508.2523	1406.3495	1508.3804	1518.8397	1399.6793	1506.9744	1510.8823
1548.5860	1614.8367	1628.9522	1546.4753	1577.5290	1634.5657	1546.6768	1578.5032	1634.3092
1646.0256	1650.2603	1650.5579	1641.8786	1650.1169	1650.8471	1641.1445	1651.4808	1655.0826
1686.4250	1794.1319	1794.7718	1671.4917	1793.7292	1794.8018	1671.7851	1796.5419	1796.8887
3174.6062	3198.2267	3209.4079	3183.9525	3200.8560	3251.8348	3188.8294	3199.3537	3251.1261
3272.4934	3285.4390	3354.1627	3269.1147	3282.2886	3353.7074	3280.6377	3291.0921	3347.3549
3364.7415	3365.1181	3382.3589	3364.2793	3364.6749	3381.9018	3356.3927	3362.3286	3375.2497
3382.8765	3393.8141	4109.8576	3382.4429	3393.3388	4098.5269	3381.3860	3392.2402	4103.3028

Non-Aqueous Solvation of n-Octanol and Ethanol Levering, Hayes, Callahan, Hadad*, Allen*

Frequencies (cm-1)

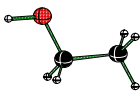
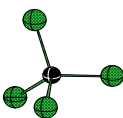
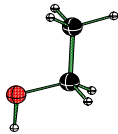
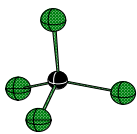
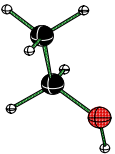
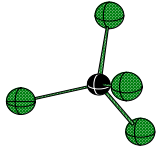
Ethanol/Cyclohexane Complexes (HF)

4			5			6		
								
8.9123	14.0558	16.5171	4.4974	9.8374	10.0730	2.6548	4.6897	8.8186
22.1236	45.3891	46.3695	11.2941	14.2857	16.1286	10.9616	15.5685	21.3557
248.9742	250.3156	272.5114	247.6232	247.6870	271.7915	247.5210	247.5550	270.8566
320.5262	404.8471	448.2585	323.0648	403.2215	448.1258	317.0250	403.1365	447.6581
458.9592	459.5916	565.7819	458.8190	458.8434	563.6771	458.8020	458.8533	563.6339
853.9672	865.2663	866.9690	853.8030	863.2652	863.3873	853.8116	863.1587	863.3466
886.7767	924.5882	924.8203	887.1750	924.7180	924.8144	886.5259	924.7530	924.8268
977.0445	1001.0074	1001.1560	978.1921	997.2929	997.3219	978.0012	997.0858	997.3008
1108.3163	1108.7351	1133.3415	1108.7273	1108.7920	1133.3305	1108.7294	1108.8472	1132.8149
1135.2941	1164.2938	1179.6240	1133.7136	1160.0155	1179.2006	1133.6712	1159.8488	1179.2242
1213.9890	1238.8920	1298.0072	1217.6781	1240.0278	1297.8255	1217.5862	1240.0712	1297.7446
1300.6005	1392.9690	1402.3735	1298.6915	1396.2059	1400.3748	1298.4324	1395.4549	1400.1420
1403.4656	1411.3575	1413.8825	1400.5055	1410.1474	1410.1822	1400.4925	1410.0441	1410.2242
1423.9779	1480.0347	1522.8824	1423.8059	1479.8323	1521.3798	1423.7839	1479.8188	1521.1939
1523.5513	1524.7470	1532.1243	1523.5047	1523.5399	1529.9126	1523.4668	1523.5591	1529.6997
1534.1874	1549.2775	1611.4739	1530.0536	1548.8007	1613.0672	1530.0427	1549.0525	1613.2098
1628.7184	1630.6629	1631.8081	1628.1297	1630.4225	1630.4500	1627.9939	1630.3715	1630.4436
1641.6129	1643.4081	1643.4318	1641.2625	1641.3177	1641.6029	1641.1707	1641.2890	1641.3558
1645.2050	1664.3837	1685.1200	1645.4626	1662.5156	1685.8867	1645.6099	1662.5189	1685.6096
3175.8819	3176.3050	3178.9204	3175.6364	3178.8078	3179.4184	3174.9376	3178.5251	3179.5550
3179.4532	3188.9640	3194.0526	3182.0969	3182.7127	3183.7923	3181.9670	3182.6350	3183.9881
3194.2852	3205.7139	3212.4178	3184.7750	3200.6690	3211.0705	3184.8446	3199.9283	3211.5116
3217.8467	3220.9107	3226.1607	3224.7682	3225.1410	3227.5255	3224.7115	3225.2177	3227.5523
3227.9844	3232.0756	3244.0108	3227.7018	3231.5805	3239.2554	3227.9791	3231.7529	3239.2894
3277.2911	3288.5176	4115.6271	3275.2457	3287.2846	4110.7813	3275.7091	3287.9569	4114.5751

Non-Aqueous Solvation of n-Octanol and Ethanol Levering, Hayes, Callahan, Hadad*, Allen*

Frequencies (cm-1)

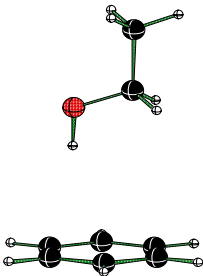
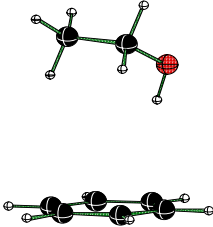

Ethanol/CCl4 Complexes (HF)

																	
7			8			9											
1.1305	3.5148	6.0172	2.1618	4.7462	8.3178	1.7626	17.0917	20.3474									
6.5119	6.8725	13.6069	9.9094	12.3913	15.0841	42.6536	47.0456	71.8476									
243.7005	243.7413	270.1193	243.7031	243.8244	270.4490	245.3892	246.1900	274.3165									
316.8484	348.2511	348.2541	316.7384	348.2075	348.2133	336.4228	348.8168	350.7880									
348.3096	447.5263	503.1259	348.4777	447.5587	503.0993	352.5185	450.1016	502.4588									
886.6168	901.3054	901.6962	886.7609	900.6964	902.1370	886.9924	896.1801	897.8991									
903.5730	977.9694	1132.7746	903.7302	978.1239	1132.9034	918.2982	976.2531	1134.6445									
217.3065	1298.6501	1395.4496	217.0868	1298.5947	1395.4450	212.5210	1298.3817	1395.6533									
423.8163	1549.3910	1613.1867	424.2408	1549.5320	1613.3693	424.6252	1550.3143	1611.7353									
628.3640	1645.7279	1685.8933	628.7348	1645.7821	1685.5644	629.1489	1645.4418	1684.7058									
175.1402	3199.9654	3212.5269	176.2274	3201.2171	3212.3262	182.4834	3209.6891	3213.3942									
277.0116	3289.1113	4114.5466	277.1279	3288.4910	4114.6245	278.2884	3290.3989	4113.0692									

Non-Aqueous Solvation of n-Octanol and Ethanol Levering, Hayes, Callahan, Hadad*, Allen*

Frequencies (cm-1)

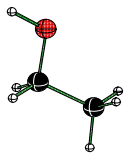
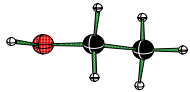
Ethanol/Benzene Complexes (MP2)

1			2			3		
								
6.7588	40.2279	50.1295	18.2882	18.8760	50.0301	21.3937	27.2628	31.0507
56.4366	62.5528	98.4307	73.7101	84.5532	117.0418	75.8009	95.2258	103.0530
271.4597	339.2001	396.6248	294.8806	389.8999	398.3117	293.2577	328.5586	400.6214
400.2427	433.1503	550.2497	412.1997	436.7389	510.6680	406.4129	433.0895	531.3591
620.9668	621.1743	694.7963	620.7647	620.9738	694.5113	620.2838	622.8263	700.0849
844.6429	854.4528	854.6310	829.3955	851.8215	853.7045	829.2726	851.8219	861.8799
907.1282	909.0893	913.5774	901.8488	904.9071	906.1462	903.4743	905.0160	921.2408
938.2727	1026.9090	1028.3098	924.2674	1026.2784	1026.4985	947.1918	1024.5717	1028.0919
1080.0324	1083.4924	1085.4729	1082.5647	1083.5535	1115.7771	1083.6371	1087.7465	1096.2452
1153.9310	1211.9056	1225.0233	1121.3309	1176.5820	1212.2997	1118.3146	1176.6985	1213.7530
1231.2165	1231.6818	1314.6971	1231.3881	1231.6439	1334.6143	1230.0678	1240.9709	1327.3662
1331.1468	1392.1468	1453.1059	1392.7545	1430.3327	1452.7288	1396.2258	1410.5358	1451.7262
1466.3994	1507.7337	1538.8935	1468.1118	1474.6200	1538.4902	1468.1103	1477.8168	1540.1061
1538.9442	1549.5119	1566.3388	1539.5699	1555.2580	1562.3465	1545.3297	1555.6353	1560.7558
1598.0164	1669.3178	1669.9207	1580.6082	1668.8134	1670.2802	1581.4970	1672.5132	1672.7815
3052.6206	3092.7003	3115.7950	3071.0166	3104.9626	3166.1785	3080.9573	3103.2248	3179.8080
3206.9710	3217.6924	3222.8869	3193.8925	3211.2502	3221.2498	3195.0330	3215.2172	3218.7174
3232.4360	3232.6329	3245.9310	3230.2854	3231.1129	3244.1162	3222.1973	3227.8921	3237.5213
3246.6407	3254.7827	3796.2628	3245.1911	3253.0056	3761.8963	3244.4368	3252.6275	3766.1525

Non-Aqueous Solvation of n-Octanol and Ethanol Levering, Hayes, Callahan, Hadad*, Allen*

Frequencies (cm-1)

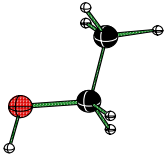
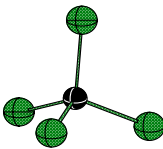
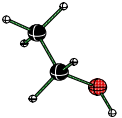
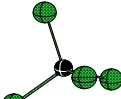
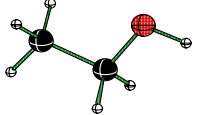
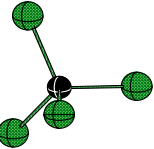
Ethanol/Cyclohexane Complexes (MP2)

4			6		
					
12.2024	23.1608	26.5777	11.6423	31.8981	48.9079
35.5718	67.0556	71.9744	56.2991	67.6617	87.7242
247.9150	250.3767	268.6602	246.6977	249.1274	267.6836
322.5890	401.7962	427.5473	334.9894	401.7815	427.7286
436.7933	437.8651	540.5038	436.1111	437.4590	539.5160
823.5471	826.1414	840.7562	821.3325	824.4899	840.5406
847.4560	904.4866	905.2267	846.1576	904.5242	904.7396
934.3516	953.7727	954.4402	934.1442	950.1740	952.7534
1074.6814	1076.5136	1079.1231	1073.9145	1077.1212	1078.9810
1080.7270	1110.0595	1138.4731	1080.5259	1106.3431	1139.5967
1151.0461	1168.4554	1220.7464	1150.8272	1168.3422	1222.3982
1230.8781	1303.5534	1328.1840	1229.7750	1307.5072	1326.3591
1328.4736	1336.2560	1338.6308	1328.8823	1334.3173	1337.9932
1342.3385	1384.4154	1426.6618	1340.7328	1383.8654	1425.8726
1426.9652	1430.2664	1436.7646	1426.2919	1427.1874	1430.0277
1439.5200	1454.5012	1504.5357	1440.1355	1454.8062	1506.4723
1544.6326	1545.9284	1548.7482	1542.0208	1545.0347	1548.3184
1551.9578	1553.5708	1559.6467	1550.7509	1551.6810	1559.5718
1563.5887	1574.7649	1596.2004	1564.7265	1573.7372	1594.9975
3066.9516	3075.8430	3076.8788	3066.6048	3079.5720	3080.2128
3077.9983	3091.6769	3093.5309	3081.4710	3090.4402	3095.3678
3093.5461	3111.6182	3117.4259	3096.1421	3111.3563	3118.2219
3127.5248	3131.3520	3131.5450	3131.9903	3132.4296	3135.0306
3146.9507	3150.8256	3156.6075	3145.2294	3150.6821	3156.8521
3209.3310	3219.5699	3770.4624	3210.4242	3219.7567	3772.5204

Non-Aqueous Solvation of n-Octanol and Ethanol Levering, Hayes, Callahan, Hadad*, Allen*

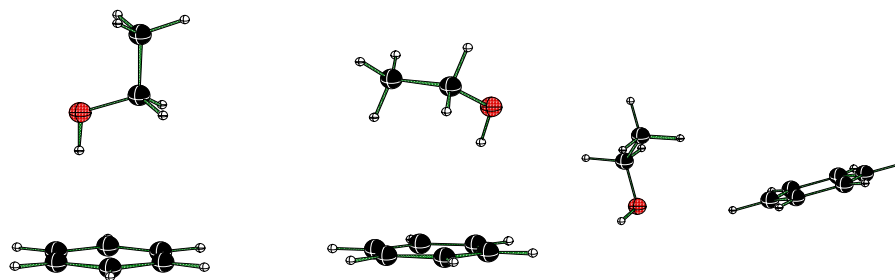
Frequencies (cm-1)

Ethanol/CCl4 Complexes (MP2)

8			9			10		
								
17.5105	18.5164	21.1922	2.0497	25.2890	33.8340	16.4702	20.5341	29.7179
31.2646	36.7803	43.9442	62.1310	67.7523	108.8801	43.7838	54.3039	77.5094
232.9613	233.3204	265.6074	235.7295	236.7505	272.2732	232.6673	234.7012	270.3649
313.7379	334.5940	334.6893	334.3891	336.6803	338.8744	333.4613	334.1034	334.9877
334.9782	426.3232	479.6011	366.1830	428.8957	477.8593	347.1576	427.1153	479.4143
829.4334	831.4701	832.8697	827.6907	830.2159	844.0800	818.9640	833.4660	840.8547
846.3129	935.1143	1077.3016	846.0126	931.8873	1077.9441	845.5789	935.2961	1079.3081
143.6797	1221.2248	1310.4272	1135.9083	1220.9719	1308.4956	1144.0492	1222.0504	1315.2019
335.2673	1453.9423	1507.7975	1336.1792	1454.3602	1505.1120	1336.0466	1453.8038	1508.5999
549.3572	1564.6790	1596.0282	1548.9913	1565.4142	1593.9739	1548.9574	1565.4904	1596.8267
061.8827	3105.2305	3119.7319	3070.9303	3116.7629	3118.9413	3062.7817	3106.6547	3117.0845
213.7956	3218.0821	3778.7502	3210.3823	3221.7696	3768.1204	3208.5971	3218.8148	3784.8309

Non-Aqueous Solvation of n-Octanol and Ethanol Levering, Hayes, Callahan, Hadad*, Allen*

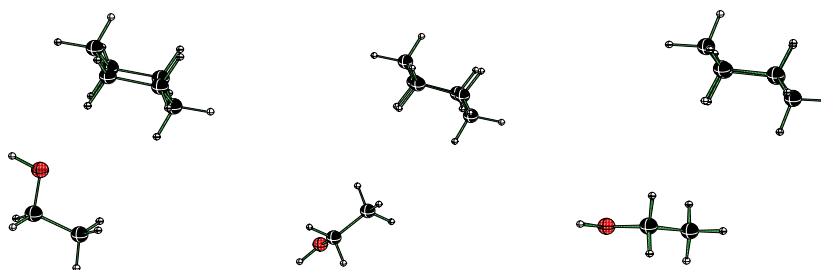
Ethanol/Benzene Complexes (HF)



	1	2	3
E B3LYP/6-311+G(3df,2p)	-387.4403518	-387.4402099	-387.4390081
E B3LYP/6-31+g**	-387.3266224	-387.3264624	-387.325234
E HF/6-31g*	-384.7825546	-384.7825618	-384.7811297
ZPE (raw)	0.194377	0.19456	0.194377
Therm Corr to H (raw)	0.205886	0.205935	0.20588
Therm Corr to G (raw)	0.150606	0.153069	0.151722
H (raw)	-384.576668	-384.576627	-384.57525
G (raw)	-384.631948	-384.629492	-384.629408
ZPE (scaled)	0.17756339	0.17773056	0.17756339
Electronic State			
s2 6-31g*	0	0	0
Symmetry	C1	C1	C1
N Imag	0	0	0
Rotational Con. (GHz)	2.55216	2.19292	3.15292
Rotational Con. (GHz)	0.72801	0.85508	0.55942
Rotational Con. (GHz)	0.71101	0.80236	0.52544

Non-Aqueous Solvation of n-Octanol and Ethanol Levering, Hayes, Callahan, Hadad*, Allen*

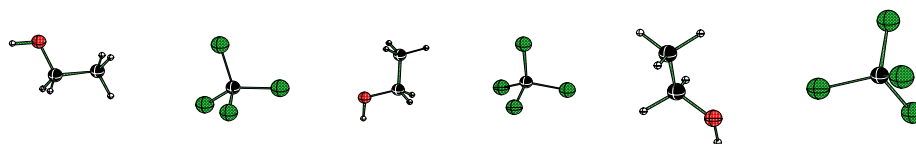
Ethanol/Cyclohexane Complexes (HF)



	4	5	6
E B3LYP/6-311+G(3df,2p)	-391.0692485	-391.0689559	-391.0690551
E B3LYP/6-31+g**	-390.9583406	-390.9579678	-390.9580287
E HF/6-31g*	-388.2853103	-388.2838896	-388.2839059
ZPE (raw)	0.268967	0.268604	0.268582
Therm Corr to H (raw)	0.281895	0.281733	0.281725
Therm Corr to G (raw)	0.223937	0.219191	0.218279
H (raw)	-388.003416	-388.002157	-388.00218
G (raw)	-388.061373	-388.064698	-388.065627
ZPE (scaled)	0.245701355	0.245369754	0.245349657
Electronic State	0	0	0
s2 6-31g*			
Symmetry	C1	C1	C1
N Imag	0	0	0
Rotational Con. (GHz)	2.02747	2.19209	2.02395
Rotational Con. (GHz)	0.6151	0.38273	0.4551
Rotational Con. (GHz)	0.58795	0.3783	0.4435

Non-Aqueous Solvation of n-Octanol and Ethanol Levering, Hayes, Callahan, Hadad*, Allen*

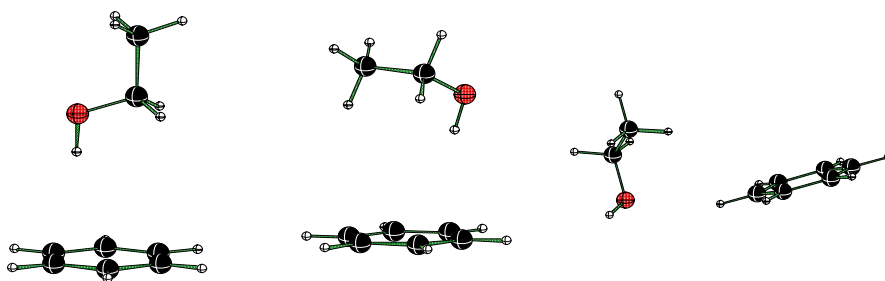
Ethanol/CCl4 Complexes (HF)



	7	8	9
E B3LYP/6-311+G(3df,2p)	-2034.121123	-2034.12118	-2034.123222
E B3LYP/6-31+g**	-2033.91523	-2033.915196	-2033.917525
E HF/6-31g*	-2029.820671	-2029.820761	-2029.823388
ZPE (raw)	0.096908	0.096949	0.09741
Therm Corr to H (raw)	0.110026	0.110033	0.110129
Therm Corr to G (raw)	0.042226	0.044607	0.050833
H (raw)	-2029.710645	-2029.710728	-2029.713259
G (raw)	-2029.778445	-2029.776153	-2029.772555
ZPE (scaled)	0.088525458	0.088562912	0.088984035
Electronic State	0	0	0
s2 6-31g*			
Symmetry	C1	C1	C1
N Imag	0	0	0
Rotational Con. (GHz)	1.63833	1.51599	1.48351
Rotational Con. (GHz)	0.28416	0.33875	0.37081
Rotational Con. (GHz)	0.2824	0.33096	0.3613

Non-Aqueous Solvation of n-Octanol and Ethanol Levering, Hayes, Callahan, Hadad*, Allen*

Ethanol/Benzene Complexes (MP2)

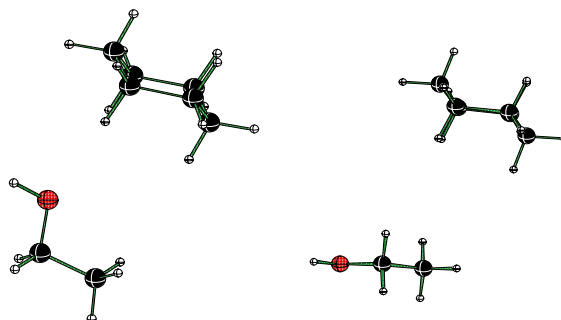


	1	2	3
PCM (solvent=ethanol)	-387.3375119	-387.3379022	-387.3394381
PCM (solvent=benzene)	-387.3315683	-387.3320853	-387.3317843
PCM (solvent=average*)	-387.3369284	-387.3373121	-387.338795
E B3LYP/6-311+G(3df,2p)	-387.4403518	-387.4395187	-387.4383925
E B3LYP/6-31+g**	-387.3270246	-387.3273776	-387.3265284
E MP2/6-31G*	-384.7779756	-384.7783809	-384.777999
ZPE (raw)	0.183929	0.184131	0.184109
Therm Corr to H (raw)	0.195718	0.195763	0.195807
Therm Corr to G (raw)	0.143343	0.144518	0.144313
H (raw)	-385.829062	-385.829631	-385.826533
G (raw)	-385.881437	-385.880876	-385.878028
ZPE (scaled)	0.177417913	0.177612763	0.177591541
Electronic State			
s2 6-31g*	0	0	0
Symmetry	C1	C1	C1
N Imag	0	0	0
Rotational Con. (GHz)	2.59154	2.16475	2.93157
Rotational Con. (GHz)	0.85094	1.03769	0.71047
Rotational Con. (GHz)	0.83546	0.95608	0.66141

* "solvent=average": ϵ = average of ϵ of benzene and ϵ of ethanol

Non-Aqueous Solvation of n-Octanol and Ethanol Levering, Hayes, Callahan, Hadad*, Allen*

Ethanol/Cyclohexane Complexes (MP2)

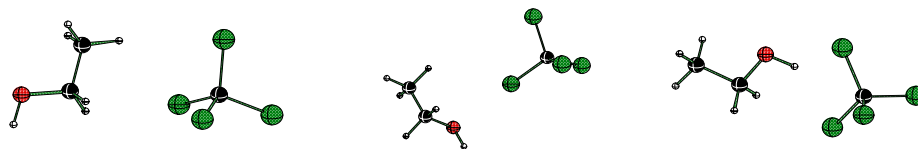


	4	6
PCM (solvent=ethanol)	-390.9664386	-390.9667954
PCM (solvent=cyclohexane)	-390.9617034	-390.9613211
PCM (solvent=average)	-390.9661379	-390.9663716
E B3LYP/6-311+G(3df,2p)	-391.068544	-391.0682489
E B3LYP/6-31+g**	-390.9589402	-390.9584423
E HF/6-31g*	-388.2818851	-388.2812679
ZPE (raw)	0.258028	0.258179
Therm Corr to H (raw)	0.271006	0.27101
Therm Corr to G (raw)	0.215327	0.216855
H (raw)	-389.284821	-389.285097
G (raw)	-389.3405	-389.339252
ZPE (scaled)	0.248893809	0.249039463
Electronic State		0
s2 6-31g*	0	
Symmetry	C1	C1
N Imag	0	0
Rotational Con. (GHz)	2.04387	1.9847
Rotational Con. (GHz)	0.71874	0.7701
Rotational Con. (GHz)	0.68278	0.7375

* "solvent=average": ϵ = average of ϵ of cyclohexane and ϵ of ethanol

Non-Aqueous Solvation of n-Octanol and Ethanol Levering, Hayes, Callahan, Hadad*, Allen*

Ethanol/CCl4 Complexes (MP2)



	8	9	10
PCM (solvent=ethanol)	-2033.92739	-2033.928987	-2033.923311
PCM (solvent=CCl4)	-2033.920659	-2033.922947	-2033.91927
PCM (solvent=average)	-2033.926787	-2033.928465	-2033.923383
E B3LYP/6-311+G(3df,2p)	-2034.121079	-2034.123465	-2034.121421
E B3LYP/6-31+g**	-2033.915809	-2033.91874	-2033.916208
E HF/6-31g*	-2029.817859	-2029.822254	-2029.817566
ZPE (raw)	0.092624	0.09309	0.092903
Therm Corr to H (raw)	0.105668	0.105781	0.105747
Therm Corr to G (raw)	0.047354	0.048394	0.049218
H (raw)	-2030.820313	-2030.824392	-2030.821662
G (raw)	-2030.878628	-2030.881779	-2030.878192
ZPE (scaled)	0.08934511	0.089794614	0.089614234
Electronic State			
s2 6-31g*	0	0	0
Symmetry	C1	C1	C1
N Imag	0	0	0
Rotational Con. (GHz)	1.53497	1.45	1.51077
Rotational Con. (GHz)	0.42401	0.42576	0.48408
Rotational Con. (GHz)	0.41401	0.41349	0.47216

* "solvent=average": ϵ = average of ϵ of CCl4 and ϵ of ethanol