

SUPPORTING INFORMATION FILE

Donor's Position-Specific Channel Interference in Substituted Biphenyl molecules

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A) Optimized Coordinates (in Å) of all the systems in different solvent phases

Table : ST – 1

1) PDPA

In Vacuum				In CH3CN			In CH3OH		
At.No.	X	Y	Z	X	Y	Z	X	Y	Z
6	-1.301	0.001	0.011	-1.301	-0.000	-0.000	-1.301	-0.000	-0.000
6	-2.038	1.130	0.428	-2.035	-1.150	-0.370	-2.035	-1.150	-0.371
6	-3.428	1.135	0.417	-3.425	-1.158	-0.370	-3.425	-1.157	-0.370
6	-4.137	-0.003	-0.011	-4.137	0.000	0.000	-4.137	0.000	0.000
6	-3.419	-1.139	-0.427	-3.425	1.158	0.370	-3.425	1.157	0.370
6	-2.028	-1.130	-0.417	-2.035	1.150	0.370	-2.035	1.150	0.371
6	0.178	0.004	0.021	0.177	-0.000	-0.000	0.177	-0.000	-0.001
6	0.918	1.174	-0.235	0.919	-1.177	0.230	0.919	-1.177	0.229
6	2.308	1.185	-0.233	2.309	-1.187	0.236	2.309	-1.187	0.236
6	3.050	0.010	0.046	3.054	-0.000	-0.001	3.054	-0.000	-0.001
6	2.309	-1.172	0.297	2.309	1.187	-0.237	2.309	1.187	-0.238
6	0.919	-1.165	0.283	0.919	1.177	-0.230	0.919	1.177	-0.231
6	-5.572	-0.004	-0.021	-5.571	0.000	0.000	-5.571	0.000	0.001
6	5.158	-1.237	0.186	5.160	1.238	-0.217	5.160	1.238	-0.217
6	5.158	1.212	-0.316	5.160	-1.237	0.219	5.160	-1.237	0.221
1	-1.509	2.012	0.792	-1.508	-2.050	-0.689	-1.508	-2.050	-0.689
1	-3.978	2.017	0.751	-3.968	-2.057	-0.666	-3.968	-2.056	-0.667
1	-3.961	-2.022	-0.770	-3.968	2.057	0.667	-3.968	2.056	0.668
1	-1.492	-2.011	-0.774	-1.507	2.050	0.688	-1.507	2.050	0.689
1	0.394	2.100	-0.480	0.400	-2.114	0.441	0.399	-2.114	0.441
1	2.819	2.119	-0.462	2.821	-2.127	0.439	2.821	-2.127	0.438
1	2.821	-2.107	0.517	2.821	2.127	-0.440	2.821	2.126	-0.440
1	0.396	-2.096	0.511	0.400	2.114	-0.442	0.400	2.114	-0.442
1	4.951	-1.926	-0.656	4.909	2.001	0.540	4.911	2.000	0.543
1	6.235	-1.029	0.201	6.235	1.035	-0.151	6.235	1.035	-0.153
1	4.909	-1.766	1.122	4.956	1.671	-1.213	4.954	1.673	-1.212
1	4.882	2.074	0.315	4.909	-2.003	-0.537	4.909	-2.004	-0.534
1	6.234	1.039	-0.188	6.235	-1.035	0.151	6.235	-1.035	0.152
1	4.978	1.497	-1.372	4.956	-1.668	1.216	4.956	-1.666	1.218
7	-6.737	-0.006	-0.030	-6.737	0.000	0.000	-6.736	0.000	0.001
7	4.433	0.017	0.076	4.428	-0.000	-0.001	4.428	-0.000	-0.002
In C2H5OH				In CH2Cl2			In CHCl3		
6	-1.301	-0.000	-0.000	-1.301	-0.000	-0.000	-1.301	-0.001	-0.007
6	-2.035	-1.149	-0.372	-2.035	-1.147	-0.378	-2.037	-1.144	-0.391
6	-3.425	-1.157	-0.371	-3.425	-1.155	-0.378	-3.428	-1.150	-0.384
6	-4.137	0.000	0.000	-4.137	0.000	0.000	-4.137	0.001	0.006
6	-3.425	1.157	0.371	-3.425	1.155	0.378	-3.422	1.152	0.390
6	-2.035	1.149	0.372	-2.035	1.147	0.378	-2.032	1.144	0.384
6	0.177	-0.000	-0.000	0.177	-0.000	-0.001	0.177	-0.002	-0.014
6	0.919	-1.177	0.230	0.919	-1.176	0.233	0.919	-1.177	0.224
6	2.309	-1.187	0.237	2.309	-1.186	0.240	2.309	-1.189	0.225
6	3.054	-0.000	-0.001	3.053	-0.000	-0.001	3.053	-0.006	-0.030
6	2.309	1.187	-0.238	2.309	1.186	-0.242	2.309	1.180	-0.265
6	0.919	1.177	-0.231	0.919	1.176	-0.235	0.919	1.172	-0.254
6	-5.571	0.000	0.000	-5.571	0.000	0.001	-5.571	0.003	0.013
6	5.160	1.237	-0.218	5.160	1.237	-0.222	5.159	1.240	-0.190
6	5.160	-1.237	0.221	5.160	-1.236	0.226	5.160	-1.225	0.274
1	-1.507	-2.049	-0.691	-1.507	-2.044	-0.703	-1.510	-2.038	-0.726
1	-3.968	-2.056	-0.669	-3.968	-2.051	-0.681	-3.973	-2.044	-0.692
1	-3.968	2.056	0.669	-3.968	2.051	0.681	-3.964	2.046	0.703
1	-1.507	2.049	0.691	-1.506	2.044	0.703	-1.500	2.037	0.714
1	0.399	-2.113	0.442	0.399	-2.112	0.449	0.397	-2.110	0.448
1	2.821	-2.126	0.440	2.821	-2.125	0.446	2.820	-2.126	0.437
1	2.821	2.126	-0.441	2.821	2.125	-0.447	2.821	2.119	-0.471
1	0.399	2.113	-0.443	0.399	2.111	-0.450	0.399	2.108	-0.467
1	4.911	2.000	0.541	4.912	2.002	0.536	4.942	1.947	0.633
1	6.235	1.035	-0.153	6.235	1.034	-0.158	6.235	1.030	-0.184
1	4.954	1.672	-1.213	4.953	1.669	-1.218	4.920	1.746	-1.141
1	4.909	-2.004	-0.533	4.909	-2.006	-0.525	4.890	-2.051	-0.406
1	6.235	-1.035	0.152	6.235	-1.034	0.157	6.235	-1.038	0.163
1	4.956	-1.666	1.219	4.956	-1.661	1.226	4.975	-1.566	1.310
7	-6.736	0.000	0.001	-6.736	0.000	0.001	-6.736	0.003	0.019
7	4.428	-0.000	-0.002	4.428	-0.000	-0.002	4.430	-0.010	-0.050

2) PDOA

In Vaccum				In CH3CN			In CH3OH		
At.No.	X	Y	Z	X	Y	Z	X	Y	Z
6	1.788	-0.395	0.097	-1.785	-0.399	-0.093	-1.785	-0.399	-0.093
6	2.399	-1.635	0.367	-2.385	-1.644	-0.366	-2.385	-1.644	-0.366
6	3.785	-1.786	0.392	-3.771	-1.799	-0.419	-3.770	-1.799	-0.419
6	4.619	-0.689	0.151	-4.616	-0.704	-0.203	-4.616	-0.704	-0.203
6	4.049	0.551	-0.123	-4.059	0.540	0.079	-4.059	0.540	0.079
6	2.649	0.706	-0.158	-2.659	0.697	0.144	-2.659	0.697	0.144
6	0.309	-0.291	0.085	-0.308	-0.280	-0.058	-0.308	-0.280	-0.058
6	-0.474	-1.283	-0.533	0.479	-1.258	0.581	0.479	-1.258	0.581
6	-1.864	-1.226	-0.545	1.867	-1.186	0.610	1.867	-1.186	0.610
6	-2.556	-0.166	0.091	2.559	-0.114	-0.016	2.559	-0.114	-0.016
6	-1.768	0.836	0.710	1.767	0.860	-0.680	1.767	0.860	-0.680
6	-0.379	0.768	0.703	0.379	0.776	-0.688	0.379	0.776	-0.688
6	-4.605	1.086	0.592	4.613	1.033	-0.709	4.613	1.033	-0.709
6	-4.706	-1.062	-0.676	4.717	-1.100	0.606	4.717	-1.100	0.606
6	2.142	2.006	-0.504	-2.163	1.994	0.515	-2.163	1.994	0.515
1	1.761	-2.493	0.587	-1.742	-2.502	-0.566	-1.742	-2.502	-0.566
1	4.217	-2.765	0.614	-4.194	-2.781	-0.643	-4.194	-2.781	-0.643
1	0.017	-2.110	-1.052	-0.008	-2.092	1.091	-0.008	-2.093	1.091
1	-2.411	-2.012	-1.063	2.417	-1.967	1.132	2.417	-1.967	1.132
1	-2.241	1.679	1.210	2.239	1.689	-1.204	2.239	1.689	-1.204
1	0.178	1.557	1.209	-0.180	1.540	-1.231	-0.180	1.540	-1.231
1	-4.347	1.988	0.002	4.283	2.031	-0.373	4.282	2.031	-0.374
1	-5.691	0.940	0.538	5.691	0.959	-0.527	5.691	0.959	-0.526
1	-4.349	1.290	1.645	4.442	0.972	-1.801	4.443	0.971	-1.801
1	-4.488	-2.100	-0.373	4.572	-2.063	0.081	4.573	-2.063	0.079
1	-5.777	-0.888	-0.506	5.781	-0.838	0.551	5.781	-0.838	0.552
1	-4.512	-0.981	-1.764	4.463	-1.255	1.669	4.462	-1.256	1.668
1	5.704	-0.799	0.175	-5.700	-0.820	-0.252	-5.700	-0.820	-0.252
1	4.678	1.419	-0.327	-4.699	1.403	0.268	-4.699	1.403	0.268
7	-3.940	-0.111	0.108	3.932	-0.025	0.020	3.932	-0.025	0.020
7	1.787	3.078	-0.792	-1.814	3.059	0.836	-1.814	3.059	0.835

In C2H5OH				In CH2Cl2			In CHCl3		
At.No.	X	Y	Z	X	Y	Z	X	Y	Z
6	-1.785	-0.399	-0.093	-1.787	-0.398	-0.095	-1.787	-0.397	-0.095
6	-2.385	-1.644	-0.366	-2.394	-1.640	-0.364	-2.397	-1.639	-0.363
6	-3.770	-1.800	-0.419	-3.779	-1.791	-0.406	-3.783	-1.788	-0.400
6	-4.616	-0.704	-0.203	-4.619	-0.693	-0.183	-4.620	-0.689	-0.173
6	-4.059	0.539	0.079	-4.055	0.548	0.095	-4.053	0.552	0.103
6	-2.659	0.697	0.144	-2.654	0.701	0.149	-2.652	0.703	0.151
6	-0.308	-0.280	-0.058	-0.309	-0.286	-0.070	-0.309	-0.289	-0.076
6	0.479	-1.259	0.580	0.477	-1.271	0.559	0.476	-1.275	0.551
6	1.867	-1.186	0.609	1.866	-1.206	0.579	1.866	-1.214	0.567
6	2.559	-0.114	-0.016	2.559	-0.140	-0.054	2.559	-0.152	-0.072
6	1.767	0.860	-0.679	1.768	0.848	-0.698	1.768	0.841	-0.706
6	0.379	0.776	-0.688	0.379	0.771	-0.697	0.379	0.768	-0.702
6	4.613	1.034	-0.708	4.610	1.063	-0.658	4.608	1.073	-0.632
6	4.717	-1.101	0.605	4.714	-1.081	0.647	4.711	-1.070	0.663
6	-2.163	1.994	0.514	-2.152	1.997	0.514	-2.147	2.000	0.512
1	-1.742	-2.502	-0.566	-1.754	-2.500	-0.570	-1.759	-2.499	-0.572
1	-4.194	-2.781	-0.642	-4.208	-2.771	-0.627	-4.213	-2.767	-0.620
1	-0.008	-2.093	1.090	-0.011	-2.102	1.073	-0.013	-2.104	1.069
1	2.417	-1.968	1.131	2.416	-1.989	1.099	2.415	-1.996	1.089
1	2.239	1.690	-1.203	2.240	1.683	-1.212	2.240	1.679	-1.217
1	-0.180	1.541	-1.230	-0.180	1.545	-1.226	-0.179	1.546	-1.224
1	4.282	2.032	-0.371	4.324	2.021	-0.186	4.341	2.007	-0.101
1	5.691	0.960	-0.525	5.694	0.938	-0.544	5.693	0.934	-0.551
1	4.443	0.973	-1.800	4.390	1.141	-1.737	4.366	1.213	-1.700
1	4.572	-2.063	0.079	4.532	-2.091	0.239	4.507	-2.097	0.313
1	5.781	-0.839	0.550	5.780	-0.857	0.527	5.779	-0.873	0.511
1	4.463	-1.257	1.668	4.490	-1.110	1.729	4.506	-1.038	1.750
1	-5.700	-0.820	-0.251	-5.704	-0.805	-0.222	-5.705	-0.799	-0.208
1	-4.699	1.403	0.268	-4.690	1.414	0.289	-4.686	1.419	0.300
7	3.932	-0.025	0.020	3.934	-0.070	-0.048	3.936	-0.091	-0.079
7	-1.815	3.059	0.834	-1.800	3.063	0.828	-1.794	3.067	0.821

3) PDMA

In Vacuum				In CH ₃ CN			In CH ₃ OH		
At.No.	X	Y	Z	X	Y	Z	X	Y	Z
6	1.424	-0.513	0.116	-1.424	-0.511	-0.106	-1.424	-0.511	-0.106
6	1.982	-1.777	0.396	-1.981	-1.781	-0.369	-1.981	-1.781	-0.369
6	3.364	-1.973	0.421	-3.363	-1.982	-0.397	-3.363	-1.982	-0.397
6	4.236	-0.912	0.177	-4.240	-0.921	-0.171	-4.240	-0.921	-0.171
6	3.700	0.358	-0.101	-3.703	0.353	0.090	-3.703	0.353	0.090
6	2.309	0.550	-0.135	-2.313	0.554	0.127	-2.313	0.554	0.127
6	-0.044	-0.308	0.087	0.043	-0.303	-0.074	0.043	-0.303	-0.074
6	-0.918	-1.302	-0.387	0.924	-1.314	0.360	0.924	-1.314	0.359
6	-2.296	-1.119	-0.422	2.302	-1.129	0.396	2.302	-1.130	0.395
6	-2.887	0.084	0.037	2.891	0.095	-0.019	2.891	0.094	-0.020
6	-2.008	1.092	0.505	2.005	1.118	-0.449	2.005	1.117	-0.450
6	-0.631	0.892	0.527	0.629	0.915	-0.472	0.629	0.915	-0.472
6	-4.813	1.573	0.335	4.815	1.585	-0.324	4.815	1.585	-0.323
6	-5.114	-0.723	-0.599	5.127	-0.753	0.528	5.127	-0.753	0.529
6	4.578	1.465	-0.366	-4.584	1.462	0.336	-4.584	1.462	0.336
1	1.319	-2.615	0.620	-1.319	-2.623	-0.577	-1.320	-2.624	-0.577
1	3.767	-2.963	0.647	-3.760	-2.976	-0.610	-3.761	-2.976	-0.609
1	1.920	1.539	-0.382	-1.929	1.548	0.360	-1.929	1.548	0.359
1	-0.510	-2.239	-0.774	0.523	-2.268	0.710	0.523	-2.268	0.709
1	-2.916	-1.921	-0.822	2.925	-1.945	0.761	2.925	-1.945	0.760
1	-2.399	2.041	0.868	2.393	2.079	-0.781	2.393	2.079	-0.781
1	0.001	1.690	0.924	-0.004	1.728	-0.837	-0.004	1.727	-0.837
1	-4.485	2.354	-0.379	4.476	2.370	0.378	4.476	2.369	0.381
1	-5.909	1.517	0.301	5.908	1.528	-0.271	5.908	1.529	-0.270
1	-4.530	1.905	1.349	4.543	1.906	-1.344	4.543	1.908	-1.342
1	-4.988	-1.716	-0.136	5.003	-1.707	-0.014	5.002	-1.707	-0.011
1	-6.163	-0.429	-0.468	6.170	-0.437	0.413	6.170	-0.437	0.413
1	-4.919	-0.830	-1.685	4.942	-0.948	1.601	4.942	-0.946	1.603
1	5.317	-1.054	0.198	-5.320	-1.068	-0.196	-5.320	-1.068	-0.195
7	-4.260	0.265	0.033	4.255	0.280	-0.007	4.256	0.280	-0.009
7	5.290	2.362	-0.577	-5.300	2.360	0.533	-5.299	2.360	0.533
In C ₂ H ₅ OH				In CH ₂ Cl ₂			In CHCl ₃		
6	-1.424	-0.511	-0.106	-1.424	-0.511	-0.107	-1.424	-0.511	-0.109
6	-1.981	-1.781	-0.369	-1.981	-1.780	-0.374	-1.981	-1.779	-0.378
6	-3.363	-1.981	-0.397	-3.363	-1.980	-0.401	-3.363	-1.979	-0.405
6	-4.240	-0.921	-0.171	-4.239	-0.920	-0.172	-4.239	-0.918	-0.173
6	-3.703	0.353	0.091	-3.703	0.354	0.092	-3.702	0.354	0.094
6	-2.313	0.554	0.127	-2.312	0.554	0.128	-2.312	0.553	0.130
6	0.043	-0.303	-0.074	0.043	-0.303	-0.076	0.043	-0.304	-0.078
6	0.924	-1.314	0.360	0.923	-1.312	0.364	0.922	-1.310	0.369
6	2.302	-1.130	0.396	2.301	-1.128	0.400	2.300	-1.126	0.405
6	2.891	0.094	-0.020	2.890	0.093	-0.022	2.890	0.091	-0.025
6	2.005	1.117	-0.451	2.005	1.114	-0.458	2.006	1.110	-0.467
6	0.629	0.915	-0.474	0.629	0.912	-0.481	0.630	0.908	-0.490
6	4.814	1.585	-0.323	4.814	1.583	-0.325	4.814	1.581	-0.327
6	5.126	-0.752	0.530	5.125	-0.748	0.539	5.123	-0.744	0.550
6	-4.584	1.462	0.336	-4.583	1.462	0.340	-4.582	1.463	0.345
1	-1.320	-2.623	-0.578	-1.319	-2.622	-0.584	-1.319	-2.620	-0.591
1	-3.761	-2.976	-0.609	-3.761	-2.974	-0.616	-3.762	-2.972	-0.622
1	-1.929	1.548	0.360	-1.928	1.546	0.364	-1.927	1.545	0.368
1	0.522	-2.267	0.711	0.520	-2.263	0.720	0.518	-2.258	0.731
1	2.925	-1.944	0.762	2.923	-1.941	0.771	2.922	-1.937	0.782
1	2.393	2.078	-0.783	2.394	2.073	-0.795	2.395	2.067	-0.809
1	-0.004	1.727	-0.839	-0.003	1.722	-0.851	-0.003	1.716	-0.865
1	4.476	2.369	0.381	4.478	2.367	0.381	4.480	2.364	0.381
1	5.908	1.528	-0.270	5.908	1.526	-0.276	5.908	1.524	-0.281
1	4.543	1.909	-1.342	4.540	1.908	-1.343	4.538	1.908	-1.344
1	5.002	-1.708	-0.008	4.999	-1.710	0.013	4.995	-1.712	0.037
1	6.170	-0.437	0.414	6.170	-0.437	0.419	6.169	-0.437	0.425
1	4.942	-0.943	1.604	4.940	-0.927	1.616	4.939	-0.907	1.629
1	-5.320	-1.067	-0.195	-5.319	-1.066	-0.196	-5.319	-1.064	-0.197
7	4.256	0.280	-0.010	4.256	0.278	-0.013	4.257	0.275	-0.017
7	-5.299	2.360	0.534	-5.298	2.360	0.540	-5.297	2.360	0.547

4) ODPA

In Vacuum				In CH ₃ CN			In CH ₃ OH		
At.No.	X	Y	Z	X	Y	Z	X	Y	Z
6	0.436	-0.486	-0.037	0.439	-0.483	-0.029	0.439	-0.483	-0.029
6	1.026	0.428	-0.934	1.024	0.434	-0.927	1.024	0.434	-0.927
6	2.405	0.608	-0.971	2.403	0.616	-0.970	2.403	0.616	-0.970
6	3.239	-0.120	-0.100	3.237	-0.116	-0.102	3.237	-0.116	-0.102
6	2.664	-1.032	0.801	2.669	-1.032	0.801	2.669	-1.032	0.801
6	1.282	-1.209	0.825	1.288	-1.209	0.829	1.288	-1.209	0.829
6	-1.033	-0.740	-0.041	-1.030	-0.739	-0.032	-1.030	-0.739	-0.032
6	-2.003	0.303	-0.023	-2.003	0.303	-0.025	-2.003	0.303	-0.025
6	-3.362	-0.043	-0.127	-3.361	-0.048	-0.144	-3.361	-0.048	-0.144
6	-3.772	-1.374	-0.227	-3.765	-1.382	-0.244	-3.766	-1.382	-0.243
6	-2.827	-2.399	-0.210	-2.818	-2.406	-0.209	-2.818	-2.406	-0.209
6	-1.473	-2.072	-0.115	-1.465	-2.074	-0.102	-1.466	-2.074	-0.102
6	-0.968	2.036	1.352	-0.968	2.037	1.350	-0.968	2.037	1.350
6	-2.524	2.673	-0.377	-2.542	2.672	-0.366	-2.541	2.672	-0.366
6	4.662	0.070	-0.132	4.659	0.074	-0.139	4.659	0.074	-0.139
1	-3.135	-3.444	-0.287	-3.122	-3.452	-0.281	-3.122	-3.452	-0.281
1	-0.725	-2.867	-0.146	-0.716	-2.868	-0.119	-0.716	-2.868	-0.119
1	-4.837	-1.604	-0.308	-4.829	-1.615	-0.335	-4.829	-1.615	-0.334
1	2.849	1.311	-1.677	2.842	1.321	-1.677	2.842	1.321	-1.677
1	0.389	1.001	-1.606	0.386	1.008	-1.597	0.386	1.008	-1.597
1	3.305	-1.595	1.482	3.310	-1.598	1.479	3.310	-1.598	1.479
1	-4.119	0.741	-0.111	-4.121	0.733	-0.141	-4.121	0.733	-0.141
1	0.846	-1.911	1.538	0.857	-1.914	1.542	0.856	-1.914	1.542
1	-0.443	2.997	1.233	-0.444	2.998	1.227	-0.445	2.998	1.227
1	-1.720	2.150	2.162	-1.717	2.154	2.162	-1.717	2.153	2.162
1	-0.233	1.286	1.667	-0.233	1.287	1.666	-0.233	1.287	1.665
1	-3.383	2.835	0.310	-3.397	2.819	0.327	-3.397	2.819	0.327
1	-1.989	3.632	-0.462	-2.012	3.634	-0.443	-2.012	3.634	-0.443
1	-2.917	2.410	-1.369	-2.936	2.415	-1.359	-2.936	2.415	-1.359
7	-1.588	1.659	0.081	-1.596	1.658	0.082	-1.595	1.658	0.082
7	5.816	0.226	-0.157	5.814	0.229	-0.170	5.814	0.229	-0.169
In C ₂ H ₅ OH				In CH ₂ Cl ₂			In CHCl ₃		
At.No.	X	Y	Z	X	Y	Z	X	Y	Z
6	0.439	-0.483	-0.030	0.439	-0.484	-0.031	0.438	-0.484	-0.032
6	1.024	0.434	-0.927	1.025	0.433	-0.928	1.025	0.432	-0.929
6	2.403	0.615	-0.970	2.403	0.614	-0.970	2.403	0.613	-0.970
6	3.237	-0.116	-0.102	3.237	-0.117	-0.102	3.237	-0.118	-0.101
6	2.669	-1.032	0.801	2.669	-1.032	0.801	2.668	-1.032	0.801
6	1.287	-1.209	0.829	1.287	-1.209	0.829	1.286	-1.209	0.828
6	-1.030	-0.739	-0.032	-1.031	-0.739	-0.033	-1.031	-0.740	-0.035
6	-2.003	0.303	-0.025	-2.002	0.303	-0.025	-2.002	0.303	-0.024
6	-3.361	-0.048	-0.144	-3.361	-0.047	-0.141	-3.361	-0.046	-0.138
6	-3.766	-1.382	-0.243	-3.767	-1.381	-0.241	-3.768	-1.379	-0.238
6	-2.819	-2.406	-0.209	-2.820	-2.405	-0.209	-2.821	-2.404	-0.209
6	-1.466	-2.074	-0.102	-1.467	-2.073	-0.104	-1.468	-2.073	-0.106
6	-0.968	2.037	1.350	-0.968	2.037	1.351	-0.969	2.037	1.352
6	-2.541	2.672	-0.366	-2.538	2.672	-0.368	-2.535	2.672	-0.370
6	4.659	0.074	-0.139	4.659	0.073	-0.138	4.660	0.073	-0.136
1	-3.122	-3.452	-0.282	-3.124	-3.451	-0.283	-3.126	-3.449	-0.284
1	-0.716	-2.868	-0.119	-0.718	-2.868	-0.123	-0.719	-2.868	-0.128
1	-4.829	-1.615	-0.334	-4.830	-1.613	-0.330	-4.832	-1.611	-0.326
1	2.842	1.321	-1.677	2.843	1.319	-1.677	2.844	1.318	-1.677
1	0.386	1.008	-1.597	0.386	1.007	-1.598	0.387	1.005	-1.600
1	3.310	-1.598	1.479	3.309	-1.598	1.479	3.309	-1.597	1.480
1	-4.121	0.733	-0.140	-4.120	0.734	-0.136	-4.119	0.736	-0.131
1	0.856	-1.914	1.542	0.855	-1.914	1.541	0.853	-1.914	1.540
1	-0.445	2.998	1.227	-0.445	2.998	1.228	-0.446	2.999	1.231
1	-1.717	2.153	2.162	-1.718	2.153	2.162	-1.719	2.151	2.162
1	-0.233	1.287	1.666	-0.233	1.287	1.666	-0.233	1.287	1.667
1	-3.397	2.819	0.326	-3.395	2.821	0.323	-3.392	2.824	0.320
1	-2.011	3.634	-0.444	-2.008	3.633	-0.447	-2.003	3.633	-0.450
1	-2.935	2.414	-1.359	-2.932	2.414	-1.361	-2.929	2.413	-1.363
7	-1.595	1.658	0.082	-1.594	1.658	0.082	-1.592	1.658	0.082
7	5.814	0.229	-0.169	5.814	0.228	-0.167	5.814	0.228	-0.165

5) MDPA

In Vaccum				In CH3CN			In CH3OH		
At.No.	X	Y	Z	X	Y	Z	X	Y	Z
6	-1.054	0.374	-0.069	-1.056	0.372	-0.064	-1.056	0.372	-0.064
6	-1.554	-0.782	-0.700	-1.545	-0.811	-0.654	-1.546	-0.811	-0.655
6	-2.908	-1.103	-0.656	-2.899	-1.133	-0.614	-2.899	-1.133	-0.614
6	-3.808	-0.265	0.026	-3.807	-0.268	0.024	-3.807	-0.268	0.024
6	-3.325	0.894	0.659	-3.337	0.919	0.618	-3.337	0.918	0.618
6	-1.969	1.203	0.608	-1.981	1.227	0.570	-1.980	1.227	0.570
6	0.393	0.714	-0.116	0.391	0.714	-0.109	0.391	0.714	-0.109
6	1.356	-0.300	-0.008	1.356	-0.300	-0.001	1.356	-0.300	-0.001
6	2.742	-0.020	-0.049	2.744	-0.019	-0.041	2.744	-0.019	-0.041
6	3.131	1.335	-0.185	3.131	1.340	-0.176	3.131	1.340	-0.176
6	2.171	2.339	-0.294	2.169	2.343	-0.285	2.169	2.343	-0.285
6	0.807	2.050	-0.261	0.803	2.052	-0.253	0.803	2.052	-0.253
6	3.257	-2.383	0.370	3.259	-2.385	0.355	3.259	-2.385	0.355
6	5.086	-0.695	0.216	5.091	-0.692	0.197	5.091	-0.692	0.197
6	-5.206	-0.591	0.076	-5.204	-0.593	0.070	-5.204	-0.593	0.070
1	-0.871	-1.428	-1.256	-0.858	-1.480	-1.173	-0.858	-1.480	-1.174
1	-3.279	-1.998	-1.158	-3.259	-2.050	-1.083	-3.259	-2.049	-1.084
1	1.014	-1.322	0.145	1.018	-1.324	0.148	1.018	-1.324	0.148
1	2.501	3.375	-0.411	2.497	3.379	-0.400	2.497	3.379	-0.401
1	0.072	2.847	-0.376	0.069	2.851	-0.365	0.069	2.851	-0.365
1	-4.019	1.543	1.197	-4.035	1.589	1.120	-4.035	1.588	1.121
1	-1.606	2.093	1.124	-1.629	2.139	1.054	-1.628	2.139	1.055
1	4.185	1.610	-0.207	4.184	1.616	-0.197	4.184	1.616	-0.197
1	4.131	-3.047	0.368	4.136	-3.044	0.353	4.136	-3.044	0.353
1	2.771	-2.455	1.364	2.768	-2.467	1.344	2.768	-2.467	1.345
1	2.546	-2.769	-0.380	2.554	-2.765	-0.403	2.554	-2.765	-0.403
1	5.280	-0.118	1.142	5.298	-0.115	1.119	5.298	-0.115	1.119
1	5.677	-1.619	0.258	5.679	-1.618	0.233	5.679	-1.618	0.233
1	5.462	-0.101	-0.634	5.455	-0.100	-0.659	5.455	-0.100	-0.659
7	3.685	-1.035	0.044	3.684	-1.029	0.049	3.684	-1.029	0.049
7	-6.339	-0.856	0.117	-6.338	-0.857	0.107	-6.338	-0.857	0.107
In C2H5OH				In CH2Cl2			In CHCl3		
6	-1.056	0.372	-0.064	-1.056	0.373	-0.065	-1.055	0.373	-0.066
6	-1.546	-0.810	-0.656	-1.547	-0.805	-0.663	-1.548	-0.801	-0.671
6	-2.899	-1.132	-0.616	-2.901	-1.127	-0.623	-2.902	-1.122	-0.630
6	-3.807	-0.268	0.024	-3.807	-0.267	0.024	-3.807	-0.267	0.025
6	-3.336	0.918	0.619	-3.335	0.914	0.626	-3.333	0.910	0.633
6	-1.980	1.226	0.571	-1.978	1.223	0.578	-1.977	1.219	0.584
6	0.391	0.714	-0.109	0.391	0.714	-0.110	0.391	0.714	-0.111
6	1.356	-0.300	-0.001	1.356	-0.301	-0.002	1.356	-0.301	-0.003
6	2.744	-0.019	-0.041	2.744	-0.019	-0.042	2.744	-0.019	-0.043
6	3.131	1.340	-0.176	3.131	1.339	-0.178	3.131	1.338	-0.179
6	2.169	2.343	-0.286	2.169	2.342	-0.287	2.170	2.342	-0.289
6	0.803	2.052	-0.253	0.804	2.052	-0.255	0.804	2.051	-0.256
6	3.259	-2.385	0.356	3.259	-2.385	0.358	3.259	-2.385	0.361
6	5.091	-0.692	0.197	5.090	-0.692	0.200	5.089	-0.693	0.203
6	-5.204	-0.593	0.070	-5.204	-0.593	0.071	-5.204	-0.592	0.072
1	-0.859	-1.479	-1.176	-0.861	-1.470	-1.190	-0.863	-1.461	-1.204
1	-3.260	-2.048	-1.086	-3.263	-2.040	-1.098	-3.266	-2.031	-1.111
1	1.017	-1.324	0.148	1.017	-1.324	0.148	1.016	-1.323	0.148
1	2.497	3.379	-0.401	2.498	3.378	-0.403	2.499	3.377	-0.405
1	0.069	2.850	-0.366	0.069	2.850	-0.367	0.070	2.849	-0.369
1	-4.035	1.587	1.123	-4.032	1.580	1.136	-4.029	1.573	1.148
1	-1.628	2.138	1.057	-1.624	2.131	1.068	-1.621	2.123	1.080
1	4.184	1.616	-0.197	4.184	1.615	-0.200	4.184	1.614	-0.201
1	4.136	-3.045	0.353	4.135	-3.045	0.357	4.134	-3.045	0.359
1	2.768	-2.467	1.345	2.768	-2.466	1.348	2.768	-2.464	1.351
1	2.554	-2.766	-0.402	2.554	-2.766	-0.399	2.553	-2.767	-0.396
1	5.298	-0.115	1.120	5.295	-0.113	1.122	5.293	-0.114	1.125
1	5.679	-1.618	0.234	5.678	-1.618	0.240	5.678	-1.618	0.243
1	5.455	-0.100	-0.659	5.457	-0.102	-0.656	5.458	-0.102	-0.652
7	3.684	-1.029	0.049	3.684	-1.030	0.049	3.684	-1.031	0.049
7	-6.338	-0.857	0.107	-6.338	-0.857	0.109	-6.338	-0.857	0.111

B) List of all the TP tensor elements (in a.u.) of all the five molecules in different solvent phases

Table : ST – 2

System	Solvent	Sxx	Syy	Szz	Sxy	Sxz	Syz
PDPA	CH3CN	-1.3	-8.7	360.5	-0.1	-0.0	0.0
	CH3OH	1.3	8.6	-357.1	0.1	0.0	-0.0
	C2H5OH	-1.4	-8.8	361.4	-0.1	-0.0	0.0
	CH2Cl2	-1.4	-9.1	362.7	-0.1	-0.0	0.0
	CHCl3	-1.7	-9.0	353.0	-0.1	-0.5	0.1
	Vacuum	-1.8	-6.5	225.4	0.1	1.3	-0.3
PDOA	CH3CN	1.8	-2.3	-197.8	3.0	3.9	-21.6
	CH3OH	1.8	-2.3	-196.1	2.9	3.8	-21.4
	C2H5OH	-1.8	2.2	199.0	-3.0	-3.8	21.6
	CH2Cl2	1.8	-1.9	-204.9	3.1	4.3	-22.0
	CHCl3	-1.9	1.5	203.5	-3.0	-4.4	21.6
	Vacuum	1.7	-0.0	-143.4	-1.7	3.7	15.8
PDMA	CH3CN	0.8	2.3	-159.7	0.6	-6.6	42.6
	CH3OH	-0.8	-2.3	157.8	-0.6	6.5	-42.1
	C2H5OH	0.8	2.3	-161.5	0.6	-6.6	42.9
	CH2Cl2	0.9	2.4	-168.4	0.7	-6.7	43.8
	CHCl3	-1.0	-2.4	171.0	-0.8	6.6	-43.6
	Vacuum	1.2	2.1	-115.3	-0.2	-3.6	-28.8
ODPA	CH3CN	2.3	-12.6	-89.9	2.5	5.2	-17.6
	CH3OH	-2.3	12.5	89.0	-2.5	-5.2	17.5
	C2H5OH	-2.3	12.7	90.1	-2.5	-5.2	17.7
	CH2Cl2	2.4	-13.0	-90.3	2.5	5.2	-17.7
	CHCl3	-2.5	13.0	88.3	-2.5	-5.1	17.5
	Vacuum	2.1	-9.8	-55.5	1.7	3.5	-13.1
MDPA	CH3CN	-0.6	-7.4	69.0	-0.7	-4.0	-39.0
	CH3OH	0.6	7.4	-68.3	0.7	3.9	38.6
	C2H5OH	0.6	7.5	-69.3	0.7	4.0	39.2
	CH2Cl2	-0.6	-7.6	70.4	-0.7	-4.0	-39.8
	CHCl3	-0.7	-7.8	72.2	-0.7	-3.7	-38.1
	Vacuum	0.4	5.8	-46.6	0.5	2.5	25.9

C) List of oscillator strengths, excitation energies (in eV) and all the different transition moment vectors (in a.u.)- all the three components and the total value, of the first and second excited states of all the five molecules

Table : ST – 3a)

		Oscillator strengths						
	Solvents Systems	→ ↓	Vacuum	CH3CN	CH3OH	C2H5OH	CH2Cl2	CHCl3
1st Ex. State	PDPA		0.873	1.037	1.031	1.041	1.055	1.057
	PDOA		0.364	0.422	0.419	0.426	0.441	0.452
	PDMA		0.263	0.274	0.270	0.282	0.314	0.339
	ODPA		0.152	0.180	0.178	0.182	0.189	0.194
	MDPA		0.071	0.079	0.078	0.080	0.085	0.088

		Oscillator strengths						
	Solvents Systems	↕	Vacuum	CH3CN	CH3OH	C2H5OH	CH2Cl2	CHCl3
2nd Ex. State	PDPA		0.021	0.025	0.025	0.025	0.027	0.028
	PDOA		0.168	0.033	0.033	0.033	0.035	0.035
	PDMA		0.302	0.494	0.493	0.490	0.471	0.446
	ODPA		0.049	0.081	0.080	0.082	0.084	0.083
	MDPA		0.317	0.542	0.535	0.547	0.563	0.586

Table : ST – 3b)

		ω^{01}					
	Solvent System $\rightarrow$ $\downarrow$	Vacuum	CH3CN	CH3OH	C2H5OH	CH2Cl2	CHCl3
	PDPA	4.098	3.764	3.768	3.766	3.781	3.815
	PDOA	4.114	3.888	3.891	3.890	3.891	3.917
	PDMA	4.268	4.003	4.005	4.006	4.024	4.051
	ODPA	4.134	3.933	3.935	3.936	3.952	3.974
	MDPA	4.074	3.841	3.843	3.845	3.863	3.890

		ω^{02}					
	Solvent System $\rightarrow$ $\downarrow$	Vacuum	CH3CN	CH3OH	C2H5OH	CH2Cl2	CHCl3
	PDPA	4.455	4.335	4.336	4.336	4.344	4.363
	PDOA	4.627	4.426	4.428	4.428	4.428	4.447
	PDMA	4.445	4.253	4.256	4.255	4.265	4.284
	ODPA	4.844	4.778	4.779	4.779	4.783	4.790
	MDPA	4.793	4.648	4.651	4.649	4.653	4.649

Table : ST – 3c)

		μ^{01}				μ^{02}			
System	Solvent	X	Y	Z	Total	X	Y	Z	Total
PDPA	Vacuum	-0.037	0.007	2.950	2.950	-0.139	-0.440	-0.005	0.462
	CH3CN	0.000	-0.000	3.353	3.353	0.146	0.483	0.000	0.505
	CH3OH	-0.001	0.000	-3.341	3.341	0.145	0.480	0.000	0.501
	C2H5OH	0.001	-0.000	3.358	3.358	0.147	0.487	0.000	0.509
	CH2Cl2	0.001	-0.000	3.375	3.375	-0.153	-0.505	0.000	0.528
	CHCl3	0.021	-0.004	3.362	3.362	-0.156	-0.512	0.001	0.535
PDOA	Vacuum	-0.031	-0.265	1.900	1.919	-0.158	-0.339	-1.216	1.273
	CH3CN	0.074	-0.318	-2.105	2.130	-0.344	-0.531	0.006	0.632
	CH3OH	0.074	-0.317	-2.096	2.121	-0.342	-0.526	0.005	0.628
	C2H5OH	-0.074	0.319	2.115	2.140	-0.346	-0.533	0.002	0.635
	CH2Cl2	0.054	-0.307	-2.152	2.174	0.353	0.549	0.018	0.653
	CHCl3	-0.042	0.300	2.169	2.190	0.352	0.543	0.030	0.648
PDMA	Vacuum	0.193	0.358	1.584	1.636	0.081	-0.431	-1.662	1.719
	CH3CN	-0.177	0.442	-1.668	1.735	0.071	0.324	-2.177	2.202
	CH3OH	0.176	-0.439	1.656	1.722	0.069	0.324	-2.173	2.199
	C2H5OH	-0.178	0.445	-1.691	1.758	0.072	0.322	-2.169	2.194

	CH ₂ Cl ₂	-0.183	0.458	-1.782	1.848	0.079	0.317	-2.123	2.148
	CHCl ₃	0.186	-0.464	1.847	1.913	0.085	0.317	-2.060	2.086
ODPA	Vaccum	-0.126	0.302	1.224	1.268	-0.116	0.130	0.642	0.665
	CH ₃ CN	-0.129	0.332	1.365	1.411	0.103	-0.048	-0.832	0.840
	CH ₃ OH	0.129	-0.331	-1.358	1.404	0.103	-0.050	-0.825	0.833
	C ₂ H ₅ OH	0.129	-0.333	-1.372	1.417	-0.104	0.047	0.835	0.843
	CH ₂ Cl ₂	-0.131	0.336	1.397	1.443	-0.106	0.046	0.844	0.852
	CHCl ₃	0.132	-0.337	-1.409	1.455	0.107	-0.053	-0.839	0.847
MDPA	Vaccum	0.086	0.602	-0.784	0.993	-0.153	-0.333	1.644	1.684
	CH ₃ CN	-0.094	-0.697	0.827	1.086	-0.052	-0.325	2.181	2.206
	CH ₃ OH	0.094	0.693	-0.822	1.079	-0.052	-0.325	2.166	2.191
	C ₂ H ₅ OH	0.095	0.701	-0.833	1.093	0.051	0.324	-2.190	2.215
	CH ₂ Cl ₂	-0.096	-0.716	0.859	1.122	-0.051	-0.320	2.222	2.245
	CHCl ₃	0.095	0.707	-0.884	1.136	-0.044	-0.299	2.267	2.287

		μ^{11}				μ^{12}			
System	Solvent	X	Y	Z	Total	X	Y	Z	Total
PDPA	Vaccum	-0.010	0.005	-3.580	3.580	0.031	0.191	-0.013	0.194
	CH ₃ CN	0.000	-0.000	-4.478	4.478	-0.036	-0.231	-0.000	0.234
	CH ₃ OH	0.000	-0.000	-4.458	4.458	0.035	0.230	0.000	0.232
	C ₂ H ₅ OH	0.000	-0.000	-4.488	4.488	-0.036	-0.233	-0.000	0.235
	CH ₂ Cl ₂	0.000	-0.000	-4.516	4.516	0.036	0.239	0.000	0.241
	CHCl ₃	0.005	-0.002	-4.473	4.473	0.036	0.236	0.009	0.239
PDOA	Vaccum	-0.090	-0.355	3.833	3.851	0.025	0.193	-0.579	0.611
	CH ₃ CN	0.113	-0.485	-4.485	4.512	-0.081	-0.108	-0.042	0.141
	CH ₃ OH	0.113	-0.483	-4.469	4.496	-0.081	-0.107	-0.042	0.141
	C ₂ H ₅ OH	0.112	-0.483	-4.492	4.519	0.082	0.109	0.044	0.143
	CH ₂ Cl ₂	0.115	-0.480	-4.537	4.564	0.085	0.121	0.032	0.151
	CHCl ₃	0.112	-0.466	-4.504	4.529	-0.083	-0.123	-0.036	0.153
PDMA	Vaccum	0.037	0.413	3.950	3.972	0.032	0.107	0.133	0.174
	CH ₃ CN	-0.037	0.417	-5.130	5.147	0.048	-0.210	-0.352	0.413
	CH ₃ OH	-0.036	0.413	-5.110	5.127	-0.048	0.210	0.343	0.405
	C ₂ H ₅ OH	-0.037	0.425	-5.121	5.139	0.048	-0.207	-0.362	0.420
	CH ₂ Cl ₂	-0.042	0.455	-5.087	5.108	0.047	-0.192	-0.395	0.442
	CHCl ₃	-0.045	0.477	-5.004	5.027	-0.046	0.173	0.401	0.439
ODPA	Vaccum	-0.205	1.074	2.686	2.901	-0.055	0.304	-0.357	0.472
	CH ₃ CN	-0.228	1.182	3.420	3.625	0.061	-0.405	0.380	0.558
	CH ₃ OH	-0.228	1.178	3.406	3.611	-0.060	0.401	-0.380	0.556
	C ₂ H ₅ OH	-0.228	1.184	3.420	3.627	0.061	-0.407	0.378	0.559
	CH ₂ Cl ₂	-0.227	1.194	3.410	3.620	-0.062	0.415	-0.371	0.560
	CHCl ₃	-0.225	1.196	3.364	3.578	-0.063	0.415	-0.364	0.556
MDPA	Vaccum	-0.086	-0.283	-3.710	3.722	0.077	0.275	-0.370	0.468
	CH ₃ CN	-0.083	-0.266	-4.677	4.685	-0.055	-0.356	0.289	0.462
	CH ₃ OH	-0.083	-0.266	-4.661	4.669	0.055	0.354	-0.297	0.465
	C ₂ H ₅ OH	-0.083	-0.266	-4.678	4.686	-0.055	-0.358	0.283	0.460
	CH ₂ Cl ₂	-0.084	-0.266	-4.664	4.673	-0.056	-0.365	0.259	0.451
	CHCl ₃	-0.083	-0.254	-4.594	4.602	0.054	0.362	-0.223	0.428

μ^{22}						
System	Solvent	x	y	z	Total	
PDPA	Vacuum	0.035	-0.004	-0.824	0.825	
	CH3CN	-0.000	0.000	-1.294	1.294	
	CH3OH	-0.001	0.000	-1.290	1.290	
	C2H5OH	-0.001	0.000	-1.289	1.289	
	CH2Cl2	-0.001	0.000	-1.252	1.252	
	CHCl3	-0.025	0.002	-1.193	1.193	
PDOA	Vacuum	0.147	0.304	2.693	2.714	
	CH3CN	0.014	0.007	-0.960	0.960	
	CH3OH	0.014	0.008	-0.956	0.956	
	C2H5OH	0.014	0.010	-0.959	0.959	
	CH2Cl2	-0.015	0.046	-0.953	0.954	
	CHCl3	-0.028	0.066	-0.936	0.939	
PDMA	Vacuum	0.098	0.010	1.972	1.975	
	CH3CN	-0.070	0.021	-3.200	3.201	
	CH3OH	-0.071	0.022	-3.179	3.179	
	C2H5OH	-0.070	0.018	-3.207	3.208	
	CH2Cl2	-0.071	0.005	-3.231	3.232	
	CHCl3	-0.073	-0.003	-3.196	3.196	
ODPA	Vacuum	-0.079	0.423	0.243	0.494	
	CH3CN	-0.095	0.444	0.610	0.760	
	CH3OH	-0.094	0.444	0.603	0.755	
	C2H5OH	-0.094	0.444	0.608	0.759	
	CH2Cl2	-0.093	0.446	0.591	0.747	
	CHCl3	-0.092	0.448	0.556	0.720	
MDPA	Vacuum	-0.054	0.202	-1.259	1.276	
	CH3CN	0.001	0.193	-2.046	2.055	
	CH3OH	0.000	0.191	-2.038	2.047	
	C2H5OH	0.001	0.193	-2.045	2.054	
	CH2Cl2	0.002	0.192	-2.033	2.042	
	CHCl3	0.006	0.192	-1.983	1.992	

D) List of different angles (in degree) between different transition dipole moment vectors, different δ -terms (in a.u.) appeared in 3SM calculations, of all the five molecules in different solvent phases.

Table : ST – 4

System	Solvent	θ_{01}^{02}	θ_{11}^{21}	θ_{01}^{11}	θ_{02}^{21}	θ_{01}^{21}	θ_{02}^{11}	δ_{TP}^{11}	δ_{TP}^{22}	$2\delta_{TP}^{12}$
PDPA	Vacuum	90.545	86.289	179.180	170.790	93.737	89.480	471807.459	24.214	2240.483
	CH3CN	90.031	90.005	180.084	172.026	90.086	90.060	1130978.892	40.652	4505.353
	CH3OH	90.068	90.155	0.017	8.070	90.154	90.067	1110330.134	39.633	4407.757
	C2H5OH	90.015	89.967	180.076	172.023	90.123	90.075	1138351.426	41.851	4586.201
	CH2Cl2	90.028	90.161	180.072	171.895	89.932	90.065	1155383.419	47.266	4909.669
	CHCl3	89.977	92.217	179.660	171.509	87.899	90.151	1104342.424	47.552	4812.253
PDOA	Vacuum	155.253	166.932	2.688	35.250	169.527	157.584	228948.408	1265.350	33571.972
	CH3CN	84.511	68.747	2.493	18.330	67.218	86.236	433751.231	21.511	2127.626
	CH3OH	84.360	68.635	2.512	18.270	67.098	86.092	426294.378	20.973	2087.536
	C2H5OH	95.956	111.983	177.588	161.603	66.569	85.862	438866.148	22.331	2194.462
	CH2Cl2	97.633	106.340	2.077	10.923	108.026	95.879	461766.182	27.377	2519.347
	CHCl3	81.408	72.518	178.102	169.202	109.351	96.874	455562.000	27.411	2542.411
PDMA	Vacuum	170.420	34.168	9.200	152.504	26.053	170.914	161896.386	255.090	-12031.726
	CH3CN	10.004	36.191	11.537	39.538	47.356	4.423	344383.799	2113.499	47506.150
	CH3OH	170.119	143.351	168.508	139.931	47.943	4.454	336027.704	2006.337	45537.267
	C2H5OH	9.942	35.156	11.359	38.403	46.144	4.357	352138.441	2213.982	49562.546
	CH2Cl2	9.766	31.669	10.650	34.558	41.961	4.259	382222.984	2474.524	55928.397
	CHCl3	170.530	150.668	170.057	147.922	39.106	4.364	392624.918	2370.793	56277.621
ODPA	Vacuum	4.904	117.047	8.090	125.756	124.511	11.850	55454.958	127.228	-3770.881
	CH3CN	169.583	66.570	5.612	128.318	61.531	163.992	119472.544	290.792	-7531.515
	CH3OH	10.360	113.813	174.478	51.651	61.241	164.137	117235.966	284.686	-7428.764
	C2H5OH	169.553	66.903	174.417	52.010	118.293	16.192	120416.333	292.433	-7534.266
	CH2Cl2	10.505	111.905	5.972	127.055	117.320	16.465	123287.765	295.699	-7479.943
	CHCl3	10.010	111.102	173.781	54.047	63.219	163.773	120899.590	282.442	-7141.784
MDPA	Vacuum	154.093	42.158	42.335	154.820	4.545	163.011	40793.249	1273.944	-14044.278
	CH3CN	31.834	125.408	136.304	42.718	10.916	168.116	84873.863	1718.735	-23233.475
	CH3OH	148.342	53.764	43.781	138.373	10.007	168.035	83242.554	1743.251	-23241.958
	C2H5OH	31.830	124.641	43.724	136.547	168.347	11.916	85975.485	1693.717	-23145.484
	CH2Cl2	31.746	121.645	136.656	46.744	15.024	168.377	89728.651	1592.136	-22616.501
	CHCl3	148.783	61.934	42.188	129.045	19.749	169.191	89825.225	1393.272	-20689.465