Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Electronic Supplementary Information

Solvent effects on the electrical and magnetic spectroscopic properties of azo-enaminone derivatives in methanol and in water

Leonardo Bruno Assis Oliveira[1*]; Luizmar Adriano Júnior[2]; Guilherme Colherinhas[1]

[1] Departamento de Física – CEPAE, Universidade Federal de Goiás, Campus Samambaia, 74.690-900, Goiânia–GO - Brazil.

[2] Pró-Reitoria de Pesquisa e Inovação, Universidade Federal de Goiás, Campus Samambaia, 74.690-900, Goiânia–GO - Brazil.

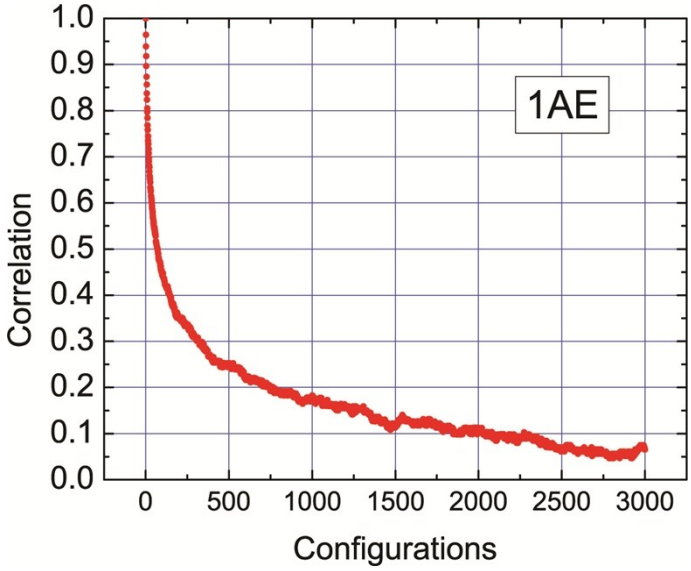

Figure S1: Example of the correlation between the 3,000 configurations saved during the Monte Carlo simulation process. In the example, for the 1AE molecule in water, the 100 uncorrelated configurations are obtained by selecting one in 25 configurations. For this case, the correlation found for the selected settings will be approximately 0.08 (8%). In all simulations, similar analyzes were performed, guaranteeing a selection of configurations with correlation less than 10%.

Table S1: Geometry and OPLS parameters for Lennard-Jones potential used in the S-MC/QM calculations. σ in Å and ε in Kcal.mol^{-1}.

1AE (x,y,z,σ,ε)					
N1	4.817176	1.310647	-0.002797	0.170	3.300
N2	1.474681	-0.183584	-0.000165	0.170	3.300
N3	0.673755	0.807116	-0.007523	0.170	3.300
N4	-4.886878	-0.072811	0.000103	0.120	3.250
O1	4.834191	-1.281871	-0.016459	0.210	2.960
O2	-0.452500	-1.910905	0.015077	0.170	3.070
O3	-5.319727	-1.221531	0.010325	0.170	2.960
O4	-5.612371	0.917637	-0.008447	0.170	2.960
C1	2.854965	-2.574627	-0.001753	0.066	3.500
C2	3.595454	-1.254739	-0.007308	0.105	3.750
C3	2.835032	-0.004147	-0.001501	0.066	3.500
C4	3.502040	1.261730	0.005633	0.070	3.550
C5	2.801169	2.582423	0.026147	0.066	3.500
C6	-0.688765	0.491838	-0.005135	0.070	3.550
C7	-1.238160	-0.818615	0.006100	0.070	3.550
C8	-2.616484	-0.990052	0.007905	0.070	3.550
C9	-3.439774	0.126784	-0.001888	0.070	3.550
C10	-2.935159	1.424866	-0.013415	0.070	3.550
C11	-1.564787	1.587348	-0.014813	0.070	3.550
H1	3.591867	-3.373680	-0.004335	0.030	2.500
H2	2.214808	-2.675441	-0.879071	0.030	2.500
H3	2.223428	-2.672961	0.882082	0.030	2.500
H4	3.533106	3.389374	0.044284	0.030	2.500
H5	2.146419	2.656623	0.892155	0.030	2.500
H6	2.155894	2.687824	-0.843818	0.030	2.500
H7	-3.028692	-1.990117	0.016658	0.030	2.420
H8	5.305623	2.201343	0.008197	0.000	0.000
H9	5.333464	0.431205	-0.014386	0.000	0.000
H10	-1.133583	2.581335	-0.023717	0.030	2.420
H11	0.478471	-1.563690	0.011873	0.000	0.000
H12	-3.601886	2.275117	-0.021048	0.030	2.420

1BE (x,y,z,σ,ε)					
N1	4.584807	-0.811027	-0.000555	0.170	3.250
N2	1.132480	0.398211	-0.000048	0.170	3.300
N3	0.401605	-0.647814	-0.002684	0.170	3.300
N4	-5.206742	-0.161799	-0.000296	0.120	3.250
O1	4.388892	1.760209	-0.005513	0.210	2.960
O2	-0.912999	1.984641	0.009503	0.170	3.070
O3	-5.720443	0.953541	0.003963	0.170	2.960
O4	-5.860723	-1.201216	-0.004518	0.170	2.960
C1	2.313436	2.887576	-0.005450	0.066	3.500
C2	3.153459	1.629434	-0.003862	0.105	3.750
C3	2.500125	0.322373	-0.000716	0.066	3.500
C4	3.269958	-0.894787	0.001981	0.070	3.550
C5	2.648753	-2.253399	0.008538	0.066	3.500
C6	-0.979030	-0.428513	-0.001673	0.070	3.550
C7	-1.620294	0.839700	0.004455	0.070	3.550
C8	-3.006971	0.913537	0.005418	0.070	3.550
C9	-3.750110	-0.258532	-0.000219	0.070	3.550
C10	-3.154739	-1.517730	-0.006370	0.070	3.550
C11	-1.776434	-1.582884	-0.006868	0.070	3.550
C12	5.544210	-1.908211	0.002309	0.066	3.500
H1	2.987275	3.740484	-0.010303	0.030	2.500
H2	1.675320	2.941581	0.877388	0.030	2.500
H3	1.669128	2.935904	-0.884019	0.030	2.500
H4	3.400154	-3.035812	0.015671	0.030	2.500
H5	2.002505	-2.374867	-0.858953	0.030	2.500
H6	1.996976	-2.364101	0.873259	0.030	2.500
H7	-3.488264	1.882175	0.010137	0.030	2.420
H8	4.937863	0.152687	-0.004579	0.000	0.000
H9	-1.276062	-2.543992	-0.011608	0.030	2.420
H10	-3.759430	-2.413171	-0.010745	0.030	2.420
H11	5.437251	-2.535716	-0.882488	0.030	2.500
H12	6.539248	-1.471362	-0.001862	0.030	2.500
H13	5.441242	-2.527681	0.893236	0.030	2.500
H14	0.039748	1.702081	0.007224	0.000	0.000

1CE (x,y,z,σ,ε)					
N1	3.750259	-0.092555	0.000190	0.170	3.250
N2	0.178982	0.697722	-0.001920	0.170	3.300
N3	-0.438206	-0.419553	-0.002554	0.170	3.300
N4	-6.066651	-0.530528	0.002352	0.120	3.250
O1	3.246694	2.436472	0.001960	0.210	2.960
O2	-2.024393	2.059204	-0.003585	0.170	3.070
O3	-6.695921	0.524013	-0.000314	0.170	2.960
O4	-6.607016	-1.633432	0.007084	0.170	2.960
C1	1.051624	3.302344	0.002735	0.066	3.500
C2	2.036176	2.153556	0.001088	0.105	3.750
C3	1.546448	0.776125	-0.001145	0.066	3.500
C4	2.457550	-0.347975	-0.001693	0.070	3.550
C5	1.962268	-1.757871	-0.004403	0.066	3.500
C6	-1.834186	-0.346877	-0.002438	0.070	3.550
C7	-2.606870	0.845836	-0.002565	0.070	3.550
C8	-3.993489	0.772587	-0.001352	0.070	3.550
C9	-4.608339	-0.471896	0.000011	0.070	3.550
C10	-3.882290	-1.660612	-0.000420	0.070	3.550
C11	-2.504820	-1.579377	-0.001730	0.070	3.550
C12	4.967401	-0.959307	0.001197	0.066	3.500
C13	6.141475	0.032455	0.004917	0.066	3.500
C1	5.049832	-1.810370	-1.274841	0.066	3.500
C5	5.044948	-1.814161	1.275005	0.066	3.500
H1	1.620039	4.228865	0.005227	0.030	2.500
H2	0.408185	3.276113	0.882853	0.030	2.500
H3	0.409872	3.279972	-0.878735	0.030	2.500
H4	2.771970	-2.472886	-0.005638	0.030	2.500
H5	1.324663	-1.925560	-0.870455	0.030	2.500
H6	1.324367	-1.928879	0.860786	0.030	2.500
H7	-4.574947	1.684719	-0.001094	0.030	2.420
H8	3.938917	0.919055	0.001497	0.000	0.000
H9	-1.905315	-2.481915	-0.001967	0.030	2.420
H10	-1.047161	1.878882	-0.003268	0.000	0.000
H11	-4.388254	-2.615189	0.000460	0.030	2.420
H12	7.084014	-0.512477	0.005913	0.030	2.500
H13	6.117560	0.669963	-0.880173	0.030	2.500
H14	6.114197	0.667339	0.891799	0.030	2.500
H15	4.274719	-2.570730	-1.331888	0.030	2.500
H16	4.975592	-1.178258	-2.160006	0.030	2.500
H17	6.013836	-2.319108	-1.300184	0.030	2.500
H18	4.967658	-1.184634	2.161751	0.030	2.500
H19	4.269411	-2.574417	1.326924	0.030	2.500
H20	6.008707	-2.323259	1.302354	0.030	2.500

2AE (x,y,z,σ,ε)					
N1	4.828124	-1.131609	-0.006627	0.170	3.300
N2	1.437452	0.251533	0.002664	0.170	3.300
N3	0.665671	-0.756402	0.003044	0.170	3.300
N4	-4.881142	0.222037	-0.001672	0.120	3.250
O1	4.742811	1.468513	0.004881	0.210	2.960
O2	-5.293599	1.379904	-0.011792	0.170	2.960
O3	-5.628575	-0.753685	0.007183	0.170	2.960
C1	2.702090	2.669512	0.009404	0.066	3.500
C2	3.506234	1.388246	0.005020	0.105	3.750
C3	2.795476	0.106365	0.001205	0.066	3.500
C4	3.512219	-1.132531	-0.004900	0.070	3.550
C5	2.858349	-2.476319	-0.010468	0.066	3.500
C6	-0.703063	-0.426245	0.002109	0.070	3.550
C7	-1.219600	0.881491	-0.010108	0.070	3.550
C8	-2.582359	1.094026	-0.011131	0.070	3.550
C9	-3.444206	-0.003214	-0.000078	0.070	3.550
C10	-2.959065	-1.307880	0.011943	0.070	3.550
C11	-1.592039	-1.510865	0.012765	0.070	3.550
H1	3.396886	3.506004	0.012361	0.030	2.500
H2	2.054295	2.722597	0.883878	0.030	2.500
H3	2.054602	2.728670	-0.864928	0.030	2.500
H4	3.615502	-3.259913	-0.017162	0.030	2.500
H5	2.207015	-2.580686	-0.876156	0.030	2.500
H6	2.212488	-2.590328	0.858106	0.030	2.500
H7	-2.985710	2.097843	-0.020727	0.030	2.420
H8	5.350165	-2.003016	-0.013735	0.000	0.000
H9	5.310285	-0.232925	-0.003366	0.000	0.000
H10	-1.189232	-2.516716	0.021912	0.030	2.420
H11	-3.645440	-2.143765	0.020370	0.030	2.420
H12	-0.540906	1.719965	-0.019162	0.030	2.420

2BE (x,y,z,σ,ε)					
N1	4.544967	-0.678541	0.005038	0.170	3.250
N2	1.071461	0.454562	-0.035082	0.170	3.300
N3	0.364954	-0.602321	-0.091995	0.170	3.300
N4	-5.229984	0.016814	0.034207	0.120	3.250
O1	4.277839	1.888274	-0.201034	0.210	2.960
O2	-5.711702	1.108849	0.327335	0.170	2.960
O3	-5.913120	-0.968304	-0.236524	0.170	2.960
C1	2.162533	2.949707	-0.160056	0.066	3.500
C2	3.049173	1.724819	-0.130665	0.105	3.750
C3	2.431981	0.400847	-0.029271	0.066	3.500
C4	3.235641	-0.789800	0.084485	0.070	3.550
C5	2.651364	-2.143263	0.325027	0.066	3.500
C6	-1.018316	-0.363855	-0.050925	0.070	3.550
C7	-1.614740	0.867375	0.275751	0.070	3.550
C8	-2.988030	0.992302	0.301555	0.070	3.550
C9	-3.781438	-0.115760	0.004612	0.070	3.550
C10	-3.216253	-1.347812	-0.312887	0.070	3.550
C11	-1.840506	-1.465086	-0.333914	0.070	3.550
C12	5.534479	-1.741528	0.125716	0.066	3.500
H1	2.800882	3.829458	-0.184284	0.030	2.500
H2	1.509560	2.987010	0.710330	0.030	2.500
H3	1.517126	2.941282	-1.037755	0.030	2.500
H4	3.413704	-2.856990	0.619797	0.030	2.500
H5	2.154925	-2.500295	-0.577034	0.030	2.500
H6	1.877966	-2.090790	1.086066	0.030	2.500
H7	-3.455688	1.931417	0.552319	0.030	2.420
H8	4.869673	0.285383	-0.129793	0.000	0.000
H9	-1.375438	-2.410304	-0.574996	0.030	2.420
H10	-3.851828	-2.189885	-0.535756	0.030	2.420
H11	5.361776	-2.529439	-0.605256	0.030	2.500
H12	6.510589	-1.303774	-0.059742	0.030	2.500
H13	5.534065	-2.176786	1.124804	0.030	2.500
H14	-0.986564	1.711885	0.511347	0.030	2.420

2CE (x,y,z,σ,ε)					
N1	3.663910	-0.015519	-0.000340	0.170	3.250
N2	0.080538	0.717600	-0.001745	0.170	3.300
N3	-0.526557	-0.400422	-0.002943	0.170	3.300
N4	-6.156708	-0.298928	0.001601	0.120	3.250
O1	3.100415	2.511180	-0.003286	0.210	2.960
O2	-6.746421	0.780144	0.003644	0.170	2.960
O3	-6.742770	-1.379911	0.000551	0.170	2.960
C1	0.875012	3.310885	-0.002531	0.066	3.500
C2	1.897882	2.196697	-0.002527	0.105	3.750
C3	1.440225	0.805817	-0.001695	0.066	3.500
C4	2.376661	-0.297395	-0.000326	0.070	3.550
C5	1.903629	-1.714202	0.001483	0.066	3.500
C6	-1.928074	-0.285766	-0.001694	0.070	3.550
C7	-2.643927	0.925238	0.004605	0.070	3.550
C8	-4.023031	0.921934	0.005562	0.070	3.550
C9	-4.703723	-0.296394	0.000410	0.070	3.550
C10	-4.019755	-1.509320	-0.005715	0.070	3.550
C11	-2.638366	-1.495956	-0.006716	0.070	3.550
C12	4.897139	-0.858601	0.001770	0.066	3.500
C13	6.053094	0.153951	0.000370	0.066	3.500
C14	4.992813	-1.712754	-1.271252	0.066	3.500
C15	4.991643	-1.707907	1.278136	0.066	3.500
H1	1.408927	4.258320	-0.002740	0.030	2.500
H2	0.228351	3.251123	0.872069	0.030	2.500
H3	0.228151	3.250916	-0.876977	0.030	2.500
H4	2.721737	-2.419884	0.003693	0.030	2.500
H5	1.266948	-1.891393	-0.863532	0.030	2.500
H6	1.264752	-1.888522	0.865466	0.030	2.500
H7	-4.578211	1.850419	0.010461	0.030	2.420
H8	3.830948	0.999795	-0.001842	0.000	0.000
H9	-2.083064	-2.426386	-0.011599	0.030	2.420
H10	-4.566588	-2.442419	-0.009696	0.030	2.420
H11	7.005391	-0.373838	0.001963	0.030	2.500
H12	6.016654	0.787845	-0.886901	0.030	2.500
H13	6.015680	0.791443	0.885021	0.030	2.500
H14	4.229875	-2.485653	-1.324762	0.030	2.500
H15	4.907331	-1.085086	-2.158592	0.030	2.500
H16	5.964971	-2.205791	-1.295939	0.030	2.500
H17	4.905748	-1.076814	2.163003	0.030	2.500
H18	4.228423	-2.480367	1.334083	0.030	2.500
H19	5.963633	-2.201144	1.305399	0.030	2.500
H20	-2.105049	1.859660	0.008862	0.030	2.420

3AE (x,y,z,σ,ε)					
N1	4.292490	-2.286521	-0.001954	0.170	3.300
N2	1.111979	-0.461036	0.001139	0.170	3.300
N3	0.193615	-1.342621	0.001259	0.170	3.300
N4	-5.173941	0.357136	-0.001256	0.120	3.250
O1	4.557058	0.334400	-0.000568	0.210	2.960
O2	-0.523270	1.525503	-0.000763	0.170	3.070
O3	2.680142	1.561293	0.000952	0.170	3.000
O4	-5.430965	1.557906	-0.006045	0.170	2.960
O5	-6.040256	-0.513320	0.002768	0.170	2.960
C1	3.330938	0.388264	0.000610	0.105	3.750
C2	2.439215	-0.782979	0.000775	0.066	3.500
C3	2.986939	-2.094871	-0.000146	0.070	3.550
C4	2.148430	-3.333220	0.000876	0.066	3.500
C5	-1.107985	-0.827163	0.000868	0.070	3.550
C6	-1.452083	0.553853	-0.000313	0.070	3.550
C7	-2.792031	0.924078	-0.001129	0.070	3.550
C8	-3.773822	-0.056669	-0.000407	0.070	3.550
C9	-3.469218	-1.415758	0.000947	0.070	3.550
C10	-2.137886	-1.778810	0.001429	0.070	3.550
C11	3.492551	2.763424	0.000564	0.105	3.750
C12	2.552167	3.946320	0.001328	0.066	3.500
H1	2.787083	-4.215627	0.000403	0.030	2.500
H2	1.491239	-3.351810	-0.866532	0.030	2.500
H3	1.492930	-3.351527	0.869569	0.030	2.500
H4	-3.051287	1.974156	-0.002177	0.030	2.420
H5	4.678148	-3.225592	-0.003850	0.000	0.000
H6	4.912985	-1.481832	-0.002997	0.000	0.000
H7	-1.858023	-2.825690	0.002226	0.030	2.420
H8	0.361066	1.067451	-0.000370	0.000	0.000
H9	-4.254572	-2.157663	0.001394	0.030	2.420
H10	4.132174	2.751358	0.883385	0.030	2.500
H11	4.131018	2.751608	-0.883097	0.030	2.500
H12	1.915996	3.940621	0.886379	0.030	2.500
H13	3.132343	4.869861	0.001135	0.030	2.500
H14	1.914920	3.940907	-0.882949	0.030	2.500

3BE (x,y,z,σ,ε)					
N1	4.261112	-1.631689	0.000057	0.170	3.250
n2	0.888459	-0.201162	-0.000295	0.170	3.300
N3	0.065299	-1.175188	0.000937	0.170	3.300
N4	-5.449279	-0.040579	-0.000469	0.120	3.250
O1	4.212394	0.987882	-0.003330	0.210	2.960
O2	-0.946362	1.605456	-0.003923	0.170	3.070
O3	2.206421	1.985981	0.000027	0.170	3.000
O4	-5.830426	1.127159	-0.002500	0.170	2.960
O5	-6.221121	-0.996434	0.001355	0.170	2.960
C1	2.985816	0.895818	-0.001325	0.105	3.750
C2	2.240308	-0.372479	-0.000273	0.066	3.500
C3	2.939841	-1.620316	0.000455	0.070	3.550
C4	2.222027	-2.930727	0.001692	0.066	3.500
C5	-1.281625	-0.796525	0.000490	0.070	3.550
C6	-1.768486	0.541444	-0.001915	0.070	3.550
C7	-3.139251	0.770793	-0.002293	0.070	3.550
C8	-4.014934	-0.306207	-0.000186	0.070	3.550
C9	-3.570246	-1.626041	0.002232	0.070	3.550
C11	-2.208552	-1.849444	0.002491	0.070	3.550
C12	2.877183	3.273290	-0.001295	0.105	3.750
C13	1.809769	4.342634	0.005866	0.066	3.500
C15	5.135131	-2.798320	0.000993	0.066	3.500
H1	2.913155	-3.766629	0.001754	0.030	2.500
H2	1.565399	-2.999279	-0.863971	0.030	2.500
H3	1.566434	-2.998275	0.868213	0.030	2.500
H4	-3.505863	1.788427	-0.004150	0.030	2.420
H5	4.693338	-0.706978	-0.001083	0.000	0.000
H6	-1.822225	-2.861891	0.004337	0.030	2.420
H7	-0.018996	1.243252	-0.003010	0.000	0.000
H8	-4.274618	-2.445365	0.003864	0.030	2.420
H9	3.517930	3.331981	0.878772	0.030	2.500
H10	3.508905	3.334729	-0.887713	0.030	2.500
H11	1.182388	4.265079	0.893798	0.030	2.500
H12	2.283323	5.325143	0.004942	0.030	2.500
H13	1.173119	4.267882	-0.875689	0.030	2.500
H14	4.984696	-3.412797	-0.886608	0.030	2.500
H15	6.160180	-2.437432	0.000796	0.030	2.500
H16	4.984558	-3.411403	0.889530	0.030	2.500

3CE (x,y,z,σ,ε)					
N1	-3.691364	-0.572024	0.000094	0.170	3.250
N2	-0.110221	0.192751	0.000647	0.170	3.300
N3	0.529919	-0.910821	0.001572	0.170	3.300
N4	6.157882	-0.764084	-0.001109	0.120	3.250
O1	-3.144945	1.989289	-0.000293	0.210	2.960
O2	2.015033	1.649013	-0.003005	0.170	3.070
O3	-0.986044	2.582609	0.000329	0.170	3.000
O4	6.739088	0.318245	0.000037	0.170	2.960
O5	6.749372	-1.841035	-0.002935	0.170	2.960
C1	-1.958728	1.660839	0.000153	0.105	3.750
C2	-1.470125	0.272004	0.000641	0.066	3.500
C3	-2.394980	-0.827940	0.000694	0.070	3.550
C4	-1.897716	-2.237216	0.001232	0.066	3.500
C5	1.922319	-0.773960	0.000983	0.070	3.550
C6	2.637429	0.457160	-0.001374	0.070	3.550
C7	4.027062	0.441563	-0.002115	0.070	3.550
C8	4.699671	-0.772859	-0.000412	0.070	3.550
C9	4.029213	-1.993710	0.002021	0.070	3.550
C10	2.649550	-1.973549	0.002692	0.070	3.550
C11	-1.398136	3.974389	0.000014	0.105	3.750
C12	-0.143991	4.817459	0.001218	0.066	3.500
C13	-4.906716	-1.441225	-0.000087	0.066	3.500
C14	-6.082509	-0.451654	-0.000804	0.066	3.500
C15	-4.986045	-2.294298	1.274827	0.066	3.500
C16	-4.985111	-2.295049	-1.274558	0.066	3.500
H1	-2.704355	-2.955401	0.001164	0.030	2.500
H2	-1.259144	-2.404299	0.866937	0.030	2.500
H3	-1.258642	-2.404754	-0.864030	0.030	2.500
H4	4.567099	1.378655	-0.003990	0.030	2.500
H5	-3.889009	0.431738	-0.000247	0.030	2.500
H6	2.090484	-2.901806	0.004638	0.030	2.500
H7	1.038383	1.455533	-0.001781	0.030	2.500
H8	4.577970	-2.924357	0.003405	0.030	2.500
H9	-2.009839	4.155690	-0.883910	0.030	2.500
H10	-2.011460	4.155582	0.882826	0.030	2.500
H11	0.461841	4.619261	-0.882834	0.030	2.500
H12	-0.418181	5.873066	0.000912	0.030	2.500
H13	0.460128	4.619312	0.886454	0.030	2.420
H14	-6.057829	0.184258	-0.887114	0.000	0.000
H15	-7.024166	-0.998052	-0.001086	0.030	2.420
H16	-6.058577	0.184640	0.885252	0.000	0.000
H17	-4.207989	-3.051778	1.330529	0.030	2.420
H18	-4.913477	-1.663075	2.160755	0.030	2.500
H19	-5.947966	-2.806989	1.300222	0.030	2.500
H20	-4.912309	-1.664302	-2.160806	0.030	2.500
H21	-4.206776	-3.052297	-1.329404	0.030	2.500
H22	-5.946856	-2.808063	-1.300145	0.030	2.500

4AE (x,y,z,σ,ε)					
N1	4.236799	-2.229299	-0.002310	0.170	3.300
N2	1.066283	-0.382090	0.000993	0.170	3.300
N3	0.162564	-1.275253	0.001241	0.170	3.300
N4	4.523291	0.374194	-0.000531	0.210	2.960
N5	-5.185845	0.486837	-0.001113	0.120	3.250
O1	2.673450	1.635116	0.000768	0.170	3.000
O2	-5.428535	1.692083	-0.005287	0.170	2.960
O3	-6.065815	-0.371598	0.002629	0.170	2.960
C1	3.296360	0.450264	0.000165	0.105	3.750
C2	2.387702	-0.712555	0.000512	0.066	3.500
C3	2.933012	-2.030439	-0.000334	0.070	3.550
C4	2.092692	-3.267499	0.000971	0.066	3.500
C5	-1.144889	-0.754204	0.000662	0.070	3.550
C6	-1.467762	0.614597	-0.001547	0.070	3.550
C7	-2.785784	1.020412	-0.002235	0.070	3.550
C8	-3.796619	0.058055	-0.000554	0.070	3.550
C9	-3.503706	-1.303160	0.001591	0.070	3.550
C10	-2.180222	-1.700217	0.002081	0.070	3.550
C11	3.519049	2.812495	0.000898	0.105	3.750
C12	2.614840	4.023791	0.001817	0.066	3.500
H1	2.730392	-4.150928	0.000493	0.030	2.500
H2	1.434203	-3.284079	-0.865249	0.030	2.500
H3	1.436205	-3.283594	0.868723	0.030	2.500
H4	-3.041016	2.071710	-0.003954	0.030	2.420
H5	4.859029	-1.425300	-0.003422	0.030	2.500
H6	-1.925954	-2.753497	0.003578	0.030	2.420
H7	-4.302839	-2.031947	0.002762	0.030	2.420
H8	4.159140	2.784412	0.883265	0.030	2.500
H9	4.158371	2.785199	-0.882049	0.030	2.500
H10	1.979122	4.038381	0.887258	0.030	2.500
H11	3.222699	4.929472	0.002086	0.030	2.500
H12	1.978513	4.039297	-0.883168	0.030	2.500
H13	-0.671223	1.342325	-0.002755	0.030	2.420
H14	4.617604	-3.170396	-0.004045	0.030	2.500

4BE (x,y,z,σ,ε)					
N1	4.193170	-1.577226	0.000639	0.170	3.300
N2	0.824807	-0.133048	-0.000832	0.170	3.300
N3	0.016618	-1.116960	-0.000620	0.170	3.300
N4	-5.478892	0.108135	0.000878	0.120	3.250
O1	4.160116	1.029477	-0.001488	0.210	2.960
O2	2.172969	2.057070	-0.001572	0.170	3.000
O3	-5.840219	1.283748	0.002531	0.170	2.960
O4	-6.270585	-0.833043	-0.000157	0.170	2.960
C1	2.930337	0.955101	-0.001309	0.105	3.750
C2	2.171397	-0.310089	-0.000727	0.066	3.500
C3	2.872772	-1.562411	-0.000006	0.070	3.550
C4	2.155523	-2.872899	0.000109	0.066	3.500
C5	-1.334919	-0.729190	-0.000617	0.070	3.550
C6	-1.792256	0.601402	-0.000838	0.070	3.550
C7	-3.143491	0.875882	-0.000407	0.070	3.550
C8	-4.055496	-0.181006	0.000139	0.070	3.550
C9	-3.629236	-1.506838	0.000085	0.070	3.550
C10	-2.273456	-1.772290	-0.000224	0.070	3.550
C11	2.873148	3.326916	-0.001898	0.105	3.750
C12	1.831724	4.422181	0.002920	0.066	3.500
C13	5.066462	-2.744375	0.001840	0.066	3.500
H1	2.846809	-3.708858	0.000105	0.030	2.500
H2	1.497974	-2.939701	-0.864775	0.030	2.500
H3	1.498065	-2.939638	0.865084	0.030	2.500
H4	-3.500901	1.897061	-0.000471	0.030	2.420
H5	4.624773	-0.651236	0.000280	0.030	2.500
H6	-1.917023	-2.795649	-0.000073	0.030	2.420
H7	-4.352997	-2.310624	0.000436	0.030	2.420
H8	3.514298	3.373659	0.878867	0.030	2.500
H9	3.508783	3.376072	-0.886553	0.030	2.500
H10	1.201246	4.360757	0.890122	0.030	2.500
H11	2.328100	5.393440	0.002710	0.030	2.500
H12	1.195507	4.363294	-0.880349	0.030	2.500
H13	4.916576	-3.358401	-0.886161	0.030	2.500
H14	6.091826	-2.384269	0.002982	0.030	2.500
H15	4.914490	-3.358086	0.889691	0.030	2.500
H16	-1.070766	1.403552	-0.001271	0.030	2.420

4CE (x,y,z,σ,ε)					
N1	-3.564739	-0.574874	-0.023026	0.170	3.300
N2	-0.008002	0.293280	-0.035513	0.170	3.300
N3	0.619824	-0.806355	-0.171155	0.170	3.300
N4	6.236826	-0.585150	0.078110	0.120	3.250
O1	-3.100829	1.991156	-0.169941	0.210	2.960
O2	-0.972577	2.673805	-0.083758	0.170	3.000
O3	6.784678	0.415907	0.537071	0.170	2.960
O4	6.864216	-1.560177	-0.332241	0.170	2.960
C1	-1.902063	1.712619	-0.097865	0.105	3.750
C2	-1.366670	0.340053	-0.030252	0.066	3.500
C3	-2.263019	-0.782842	0.065208	0.070	3.550
C4	-1.735288	-2.161434	0.306382	0.066	3.500
C5	2.014749	-0.672290	-0.094969	0.070	3.550
C6	2.682237	0.453797	0.419689	0.070	3.550
C7	4.060136	0.484253	0.473678	0.070	3.550
C8	4.786037	-0.616498	0.016837	0.070	3.550
C9	4.148534	-1.748185	-0.487586	0.070	3.550
C10	2.768510	-1.771892	-0.533889	0.070	3.550
C11	-1.450528	4.041031	-0.154455	0.105	3.750
C12	-0.241609	4.948116	-0.126140	0.066	3.500
C14	-4.753799	-1.474199	0.069552	0.066	3.500
C15	-5.947796	-0.562076	-0.253113	0.066	3.500
C16	-4.925421	-2.022443	1.494788	0.066	3.500
C17	-4.699508	-2.595719	-0.977641	0.066	3.500
H1	-2.512405	-2.837475	0.635120	0.030	2.500
H2	-0.937872	-2.131473	1.043912	0.030	2.500
H3	-1.278046	-2.551763	-0.602397	0.030	2.500
H4	4.579598	1.345996	0.871114	0.030	2.420
H5	-3.789432	0.415156	-0.153257	0.030	2.500
H6	2.248230	-2.641348	-0.918722	0.030	2.420
H7	4.730935	-2.591123	-0.834073	0.030	2.420
H8	-2.027020	4.163378	-1.071834	0.030	2.500
H9	-2.114760	4.225228	0.690406	0.030	2.500
H10	0.417274	4.749442	-0.971496	0.030	2.500
H11	-0.567452	5.987525	-0.182518	0.030	2.500
H12	0.325930	4.816873	0.795217	0.030	2.500
H13	-5.860951	-0.147066	-1.258299	0.030	2.500
H14	-6.873245	-1.132987	-0.198830	0.030	2.500
H15	-6.015463	0.262119	0.458970	0.030	2.500
H16	-4.130511	-2.705604	1.786183	0.030	2.500
H17	-4.955668	-1.205871	2.216475	0.030	2.500
H18	-5.867833	-2.567509	1.557500	0.030	2.500
H19	-4.536813	-2.181102	-1.972786	0.030	2.500
H20	-3.921560	-3.328419	-0.779206	0.030	2.500
H21	-5.654264	-3.122226	-0.981560	0.030	2.500
H22	2.103071	1.290675	0.780766	0.030	2.420

Table S2: DFT/CAM-B3LYP/6-311+G(d) results for $\langle\beta_{vec}\rangle$ and $\langle\beta_{tot}\rangle$ of E azo-enaminones isomers type in gas phase and in CH_3OH solution using PCM and ASEC approaches. The $\langle\beta_{vec}\rangle$ and $\langle\beta_{tot}\rangle$ expressions are available in Reference [3].

	Gas-phase			CH_3OH					
				PCM			ASEC		
	$\lvert\langle\beta_{vec}\rangle\rvert$	$\langle\beta_{tot}\rangle$	$\lvert\langle\beta_{vec}\rangle\rvert/\langle\beta_{tot}\rangle$	$\lvert\langle\beta_{vec}\rangle\rvert$	$\langle\beta_{tot}\rangle$	$\lvert\langle\beta_{vec}\rangle\rvert/\langle\beta_{tot}\rangle$	$\lvert\langle\beta_{vec}\rangle\rvert$	$\langle\beta_{tot}\rangle$	$\lvert\langle\beta_{vec}\rangle\rvert/\langle\beta_{tot}\rangle$
1AE	24,56	29,04	0,85	136,30	159,46	0,85	41,22	49,26	0,84
1BE	30,88	35,82	0,86	157,56	181,23	0,87	49,50	58,15	0,85
1CE	33,63	39,01	0,86	163,36	186,87	0,87	52,36	62,01	0,84
2AE	34,13	37,87	0,90	157,87	175,75	0,90	49,22	56,31	0,87
2BE	42,02	46,05	0,91	181,84	199,72	0,91	59,40	66,37	0,89
2CE	46,14	50,41	0,92	184,23	203,09	0,91	54,65	62,50	0,87
3AE	24,89	27,03	0,92	147,07	157,92	0,93	48,69	52,85	0,92
3BE	31,14	33,61	0,93	170,83	181,62	0,94	52,07	56,50	0,92
3CE	33,47	36,41	0,92	176,26	187,34	0,94	57,52	61,42	0,94
4AE	35,42	36,57	0,97	171,41	177,89	0,96	53,10	55,53	0,96
4BE	43,28	44,65	0,97	196,65	202,81	0,97	63,80	66,16	0,96
4CE	47,12	48,79	0,97	203,12	209,85	0,97	62,06	65,51	0,95