

Theoretical Study of the Anisotropy Spectra of the Valine Zwitterion and Glyceraldehyde

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Table S1: Cartesian coordinates (in Å) of the M06-2X/cc-pVTZ optimized geometries of the L-valine zwitterions: *Trans/Gauche+* and *Gauche+/Gauche-*

Atom	X	Y	Z	Atom	X	Y	Z
	<i>Trans/Gauche+</i>				<i>Gauche-/Trans</i>		
C	1.032781	0.766627	-0.001253	C	-1.448974	-0.274271	-0.213884
O	0.628846	1.914743	-0.068634	O	-2.127976	0.492478	0.522420
C	0.168539	-0.330470	-0.732658	C	-0.057639	0.355211	-0.594021
H	0.098101	-0.113458	-1.796049	H	-0.024319	0.553924	-1.663470
C	1.219851	-0.510991	-0.116166	C	1.109589	-0.524623	-0.171248
H	1.627655	-1.453367	-0.503163	H	0.939505	-1.453253	-0.717609
C	1.142480	-0.592106	1.407823	C	2.454509	0.066747	-0.580503
H	0.451722	-1.361920	1.760602	H	2.493469	0.267639	-1.651606
H	0.801832	0.362056	1.811059	H	2.659200	1.004562	-0.053887
H	2.124457	-0.813466	1.823818	H	3.267341	-0.615696	-0.334143
C	2.146605	0.618521	-0.554423	C	1.064359	-0.847184	1.320488
H	2.247089	0.646494	-1.640020	H	1.854323	-1.552613	1.574673
H	3.137288	0.474464	-0.123704	H	1.228870	0.038979	1.942452
H	1.744768	1.574837	-0.225664	H	0.107234	-1.287196	1.597118
H	1.720789	-1.147763	0.065582	H	0.631647	1.742747	0.849152
H	0.489736	-2.324532	-0.087930	H	0.001175	2.483224	-0.487803
H	1.401913	-1.922761	-1.407895	H	-1.020825	1.584585	0.530173
O	2.030578	0.260588	0.583908	O	-1.662037	-1.391313	-0.651963
N	0.999225	-1.576102	-0.545537	N	-0.078368	1.681214	0.126614

Table S2: Cartesian coordinates (in Å) of the M06-2X/cc-pVTZ optimized geometries of the L-valine zwitterions: *Gauche-/Trans*

Atom	X	Y	Z
C	-1.436258	0.349377	0.045590
O	-1.577601	1.513129	0.379270
C	-0.072030	-0.337225	0.452124
H	0.107192	-0.218162	1.519644
C	1.135036	0.140450	-0.353781
H	0.905603	-0.034565	-1.411493
C	1.367514	1.635571	-0.151856
H	2.239100	1.949311	-0.726200
H	0.501664	2.218054	-0.449294
H	1.561180	1.845846	0.901932
C	2.401299	-0.631150	0.022155
H	2.640305	-0.466759	1.074889
H	2.330158	-1.70980	-0.138642
H	3.246176	-0.280776	-0.569529
H	-1.230375	-1.660680	-0.331063
H	0.363286	-2.227646	-0.420000
H	-0.481240	-2.353645	0.9953260
O	-2.187461	-0.443762	-0.583538
N	-0.347988	-1.794035	0.157597

Table S3: Cartesian coordinates (in Å) of the M06-2X/cc-pVTZ/PCM optimized geometries of the L-valine zwitterions: *Trans/Gauche+* and *Gauche+/Gauche-*

Atom	X	Y	Z	Atom	X	Y	Z
	<i>Trans/Gauche+</i>				<i>Gauche+/Gauche-</i>		
C	1.056899	0.721400	0.018022	C	-1.443689	-0.242103	-0.206327
O	0.766116	1.912516	-0.128346	O	-2.121746	0.456361	0.589025
C	0.175198	-0.311523	-0.740915	C	-0.061779	0.361750	-0.582969
H	0.103524	-0.044905	-1.791789	H	-0.026888	0.532573	-1.656315
C	-1.224620	-0.455436	-0.129732	C	1.092339	-0.544735	-0.160381
H	-1.665417	-1.352283	-0.575684	H	0.912522	-1.472684	-0.703790
C	-1.164641	-0.637781	1.385340	C	2.441889	0.021439	-0.589730
H	-0.522946	-1.467890	1.685531	H	2.464316	0.220243	-1.661102
H	-0.783451	0.268513	1.858974	H	2.674885	0.953146	-0.068385
H	-2.162186	-0.832023	1.776711	H	3.238005	-0.683730	-0.354134
C	-2.109564	0.728919	-0.501699	C	1.060263	-0.854967	1.334289
H	-2.169685	0.852134	-1.583323	H	1.853254	-1.558589	1.583372
H	-3.117118	0.568020	-0.119174	H	1.225875	0.037248	1.943370
H	-1.713449	1.647778	-0.073867	H	0.108159	-1.295769	1.629503
H	1.623991	-1.381053	0.115805	H	0.758407	1.800450	0.748797
H	0.331529	-2.396686	-0.362496	H	0.010249	2.478900	-0.553227
H	1.410951	-1.855531	-1.485131	H	-0.935957	1.683391	0.614844
O	1.962261	0.210865	0.724823	O	-1.715650	-1.335190	-0.710412
N	0.919658	-1.609513	-0.629066	N	-0.016828	1.698165	0.096981

Table S4: Cartesian coordinates (in Å) of the M06-2X/cc-pVTZ/PCM optimized geometries of the L-valine zwitterions: *Gauche-/Trans*

Atom	X	Y	Z
C	1.414544	-0.282434	0.075569
O	1.671543	-1.365521	0.608657
C	0.060961	0.385005	0.454390
H	-0.128372	0.275996	1.519853
C	-1.121727	-0.151308	-0.360308
H	-0.943107	0.127023	-1.404252
C	-1.217331	-1.671469	-0.276518
H	-2.099417	-2.008153	-0.820291
H	-0.339657	-2.158325	-0.692892
H	-1.316499	-1.988531	0.763210
C	-2.435480	0.472104	0.110976
H	-2.637653	0.176502	1.141991
H	-2.444054	1.562102	0.069223
H	-3.258513	0.121160	-0.510046
H	1.064384	1.796412	-0.528687
H	-0.550301	2.283919	-0.288987
H	0.531258	2.387318	0.951331
O	2.091556	0.370569	-0.758120
N	0.258763	1.838972	0.138657

Table S5: Cartesian coordinates (in Å) of the M06-2X/cc-pVTZ optimized geometries of D-glyceraldehyde: 1-4.

Atom	X	Y	Z	Atom	X	Y	Z
Geometry 1				Geometry 2			
C	-1.066008	-0.644329	0.402191	C	-1.362796	-0.635545	0.216768
C	-0.033219	0.433134	0.636874	C	-0.037180	0.029632	0.466987
C	1.367312	-0.152476	0.522942	C	1.079992	-0.718678	-0.259210
O	1.568554	-0.691472	-0.759805	O	2.308357	-0.075887	-0.044306
O	-0.180145	1.455897	-0.309155	O	-0.052040	1.361637	0.032452
O	-1.933209	-0.520051	-0.418222	O	-2.262936	-0.064778	-0.338198
H	-0.985737	-1.548767	1.028930	H	-1.464369	-1.682107	0.551276
H	-1.016863	1.293907	-0.767567	H	-0.915043	1.517265	-0.375916
H	1.344583	0.001508	-1.390530	H	2.178682	0.853872	-0.261444
H	-0.182882	0.810212	1.658961	H	0.169025	-0.007979	1.544172
H	1.497004	-0.961746	1.242705	H	0.833097	-0.764867	-1.326615
H	2.093783	0.631931	0.752920	H	1.171460	-1.736425	0.121674
Geometry 3				Geometry 4			
C	-1.315293	0.360873	-0.011606	C	-0.804612	-0.894057	0.166107
C	0.078212	0.683241	0.504187	C	-0.071297	0.403695	0.407797
C	0.899585	-0.579526	0.687124	C	1.237254	0.416684	-0.376132
O	1.110535	-1.194590	-0.570572	O	2.034645	-0.635568	0.129561
O	0.683324	1.567663	-0.414009	O	-0.856173	1.495901	0.038827
O	-1.754215	-0.754337	-0.105667	O	-1.926649	-0.904273	-0.267657
H	-1.895810	1.238034	-0.348829	H	-0.257919	-1.820882	0.394014
H	1.049376	1.016166	-1.117158	H	-1.704983	1.139506	-0.258528
H	0.290781	-1.638509	-0.811335	H	2.876993	-0.646644	-0.328167
H	-0.022727	1.217302	1.453685	H	0.182606	0.437873	1.475775
H	0.405865	-1.254819	1.388340	H	1.704433	1.393905	-0.234789
H	1.880337	-0.315595	1.079047	H	1.016213	0.289833	-1.440788

Table S6: Cartesian coordinates (in Å) of the M06-2X/cc-pVTZ optimized geometries of D-glyceraldehyde: 5-8.

Atom	X	Y	Z	Atom	X	Y	Z
Geometry 5				Geometry 6			
C	-0.822147	-0.889654	0.158102	C	-0.986872	-0.631367	0.483134
C	-0.063806	0.393217	0.395215	C	-0.056663	0.560269	0.546314
C	1.237110	0.383347	-0.413832	C	1.379471	0.067471	0.463179
O	2.098535	-0.654270	0.003849	O	1.464836	-0.792740	-0.652954
O	-0.835434	1.501184	0.048927	O	-0.352808	1.475295	-0.462169
O	-1.959109	-0.879842	-0.234111	O	-1.865809	-0.706706	-0.329112
H	-0.276460	-1.827035	0.344395	H	-0.811529	-1.430174	1.224362
H	-1.704133	1.165639	-0.213766	H	-1.028525	1.067752	-1.020805
H	2.535263	-0.392535	0.817417	H	2.383867	-0.931177	-0.887393
H	0.201530	0.416618	1.463341	H	-0.196205	1.025980	1.531865
H	1.697713	1.369902	-0.332569	H	1.638204	-0.456633	1.390890
H	1.007211	0.209373	-1.465050	H	2.028824	0.939229	0.359203
Geometry 7				Geometry 8			
C	-1.540860	0.211656	-0.042123	C	-1.296473	0.237452	-0.297932
C	-0.083266	0.353792	0.332024	C	-0.032813	0.577965	0.484817
C	0.735595	-0.789711	-0.233273	C	0.816074	-0.665658	0.663331
O	2.075189	-0.523818	0.148692	O	1.325208	-0.954884	-0.630806
O	0.359809	1.596198	-0.155030	O	0.683815	1.611492	-0.140301
O	-2.136464	-0.826932	0.020687	O	-2.002000	-0.692848	-0.030873
H	-2.020563	1.147317	-0.382254	H	-1.523280	0.931733	-1.128906
H	1.319028	1.604431	-0.069430	H	1.220526	1.202063	-0.828988
H	2.661470	-1.149599	-0.280327	H	1.863702	-1.747218	-0.599729
H	-0.017822	0.314863	1.428268	H	-0.353930	0.940040	1.464838
H	0.369173	-1.734490	0.171602	H	0.188700	-1.474812	1.041744
H	0.631625	-0.800522	-1.322427	H	1.627372	-0.460439	1.365589

Table S7: Cartesian coordinates (in Å) of the M06-2X/cc-pVTZ optimized geometries of D-glyceraldehyde: 13-16.

Atom	X	Y	Z	Atom	X	Y	Z
Geometry 13				Geometry 14			
C	-1.305728	-0.691566	0.211483	C	-1.223195	0.061763	-0.392604
C	-0.033343	0.100931	0.382603	C	-0.057762	0.510521	0.473111
C	1.113851	-0.581457	-0.345496	C	0.904010	-0.654422	0.655696
O	2.314787	-0.029344	0.142765	O	1.426722	-1.063935	-0.586366
O	-0.201937	1.416089	-0.048846	O	0.684936	1.539334	-0.153013
O	-2.306866	-0.198751	-0.232446	O	-2.134466	-0.585786	0.035746
H	-1.275528	-1.750496	0.521654	H	-1.166376	0.367787	-1.454918
H	-1.125635	1.505379	-0.320128	H	0.156950	2.338065	-0.218522
H	3.028905	-0.237115	-0.462376	H	1.840838	-0.294579	-0.989931
H	0.211902	0.074008	1.455342	H	-0.450444	0.814199	1.448011
H	1.075875	-1.662349	-0.160956	H	0.366949	-1.500210	1.081571
H	0.987929	-0.400832	-1.416860	H	1.696231	-0.349347	1.345631
Geometry 15				Geometry 16			
C	-1.318243	-0.676922	0.218182	C	-1.252481	0.229099	-0.338633
C	-0.032707	0.092947	0.401133	C	-0.009196	0.542465	0.474830
C	1.106897	-0.625458	-0.319215	C	0.829098	-0.716303	0.645392
O	2.357418	-0.032042	-0.080353	O	1.289854	-1.169452	-0.604681
O	-0.169034	1.408211	-0.034180	O	0.711022	1.531928	-0.241945
O	-2.299352	-0.167995	-0.251010	O	-2.075008	-0.558217	0.028731
H	-1.314763	-1.734165	0.535057	H	-1.343813	0.785320	-1.288955
H	-1.083034	1.513264	-0.331973	H	1.333266	1.964010	0.347644
H	2.525022	-0.014584	0.865254	H	1.668020	-0.411034	-1.061791
H	0.185943	0.068678	1.482382	H	-0.341872	0.908754	1.451287
H	1.103717	-1.685038	-0.033619	H	0.211048	-1.502506	1.076825
H	0.935174	-0.556952	-1.393354	H	1.661875	-0.510181	1.328611

Table S8: Cartesian coordinates (in Å) of the M06-2X/cc-pVTZ optimized geometries of D-glyceraldehyde: 17-20.

Atom	X	Y	Z	Atom	X	Y	Z
Geometry 17				Geometry 18			
C	1.542536	0.207631	-0.063924	C	-1.405062	-0.574824	0.232336
C	0.059917	0.346600	-0.346352	C	-0.067386	0.093742	0.434924
C	-0.750955	-0.796144	0.237319	C	1.017408	-0.728375	-0.246918
O	-2.104724	-0.685616	-0.125463	O	2.235694	-0.062262	0.032257
O	-0.425442	1.603898	0.092235	O	-0.093025	1.397269	-0.057842
O	2.100663	-0.845446	0.058025	O	-2.333488	-0.087737	-0.340058
H	2.084335	1.169696	0.025760	H	-1.464969	-1.594171	0.665757
H	-0.320845	1.663952	1.047431	H	0.818827	1.707731	-0.062566
H	-2.368821	0.229760	0.010907	H	2.927763	-0.404807	-0.536480
H	-0.068392	0.350422	-1.432813	H	0.135612	0.071207	1.517459
H	-0.374103	-1.743839	-0.140909	H	1.023296	-1.751497	0.140941
H	-0.625136	-0.801199	1.328982	H	0.816261	-0.749881	-1.322017
Geometry 19				Geometry 20			
C	-1.150647	0.632343	-0.082855	C	-1.119313	-0.550279	0.428254
C	0.270650	0.623077	0.451751	C	-0.028494	0.487356	0.595706
C	0.788691	-0.800422	0.594963	C	1.327686	-0.207581	0.532370
O	0.668085	-1.547055	-0.589853	O	1.492429	-0.845954	-0.708193
O	1.109443	1.352524	-0.418093	O	-0.148810	1.435082	-0.437206
O	-1.911585	-0.289788	0.020127	O	-1.960918	-0.520340	-0.417211
H	-1.447689	1.564583	-0.602513	H	-1.068277	-1.370230	1.171640
H	0.974751	2.293928	-0.288975	H	0.408781	2.190063	-0.232831
H	-0.261499	-1.764611	-0.704442	H	1.162868	-0.246239	-1.387432
H	0.243201	1.077661	1.452233	H	-0.162549	0.936846	1.588957
H	0.262702	-1.278001	1.426073	H	1.402052	-0.970534	1.308800
H	1.848825	-0.749003	0.837020	H	2.116249	0.532805	0.713773

Table S9: Cartesian coordinates (in Å) of the M06-2X/cc-pVTZ optimized geometries of D-glyceraldehyde: 21-24.

Atom	X	Y	Z	Atom	X	Y	Z
Geometry 21				Geometry 22			
C	0.974517	-0.563776	0.385304	C	-1.409173	-0.566657	0.247142
C	0.110196	0.468028	-0.319355	C	-0.064441	0.091775	0.443611
C	-1.326695	0.347830	0.135888	C	1.009473	-0.726180	-0.273289
O	-1.725394	-0.977111	-0.146614	O	2.268823	-0.094718	-0.140033
O	0.549083	1.757614	0.068767	O	-0.082236	1.403465	-0.023889
O	1.792139	-1.239566	-0.169935	O	-2.327541	-0.083633	-0.344300
H	0.838121	-0.602115	1.484404	H	-1.482042	-1.576940	0.699864
H	1.412686	1.921619	-0.318685	H	0.834652	1.662172	-0.170025
H	-2.612963	-1.122404	0.185267	H	2.600134	-0.236666	0.750658
H	0.188107	0.306593	-1.397147	H	0.142775	0.050246	1.527267
H	-1.367416	0.568010	1.208353	H	1.029362	-1.755898	0.093547
H	-1.933266	1.088309	-0.390958	H	0.787602	-0.737454	-1.340328
Geometry 23				Geometry 24			
C	1.517190	0.092584	0.128018	C	-1.191103	-0.021470	-0.373931
C	0.076963	0.359574	-0.276723	C	-0.047134	0.579896	0.430458
C	-0.833675	-0.665955	0.392417	C	0.994143	-0.497827	0.656403
O	-2.152849	-0.614205	-0.093225	O	1.322493	-1.042671	-0.605369
O	-0.326959	1.648874	0.117841	O	0.560172	1.652302	-0.252473
O	2.101731	-0.915310	-0.152240	O	-2.037669	-0.710841	0.119021
H	1.988049	0.901718	0.719890	H	-1.178730	0.222873	-1.452204
H	-0.088580	2.289601	-0.554518	H	-0.048325	2.393812	-0.289701
H	-2.175333	-0.997428	-0.973065	H	1.952131	-1.756134	-0.488902
H	0.010078	0.221885	-1.362634	H	-0.443643	0.881802	1.405240
H	-0.386422	-1.655788	0.272982	H	0.559916	-1.252356	1.318455
H	-0.886038	-0.432071	1.456066	H	1.863247	-0.043909	1.140060

Table S10: Cartesian coordinates (in Å) of the M06-2X/cc-pVTZ optimized geometries of D-glyceraldehyde: 25-28.

Atom	X	Y	Z	Atom	X	Y	Z
Geometry 25				Geometry 26			
C	0.449986	-1.225123	-0.138470	C	1.126764	-0.479204	0.323380
C	0.577469	0.270236	-0.364595	C	0.177646	0.507294	-0.323075
C	-0.541197	1.045219	0.320889	C	-1.217071	0.329229	0.267843
O	-1.796364	0.743192	-0.229643	O	-1.723768	-0.9042512	-0.178126
O	1.864839	0.695219	0.029382	O	0.682698	1.788076	-0.007328
O	-0.552545	-1.769177	0.242232	O	1.435520	-1.531626	-0.151321
H	1.377270	-1.797255	-0.325923	H	1.508471	-0.141744	1.307705
H	1.914108	0.695988	0.990129	H	0.151041	2.454718	-0.448612
H	-1.973158	-0.184613	-0.039879	H	-2.503175	-1.135016	0.330153
H	0.509629	0.441538	-1.442878	H	0.148009	0.309668	-1.397389
H	-0.510522	0.838839	1.399426	H	-1.146015	0.381023	1.360159
H	-0.362308	2.109646	0.176426	H	-1.837966	1.169857	-0.066705
Geometry 27				Geometry 28			
C	1.072924	-0.457276	0.361941	C	-1.010946	-0.775821	0.412083
C	0.132900	0.503244	-0.342797	C	-0.234356	0.535776	0.388817
C	-1.289420	0.303250	0.154957	C	1.032806	0.444200	-0.441926
O	-1.644768	-1.035690	-0.095742	O	1.983274	-0.401205	0.168611
O	0.554247	1.832995	-0.116970	O	-1.126236	1.530693	-0.086437
O	1.642450	-1.369320	-0.157071	O	-0.880386	-1.632854	-0.414684
H	1.215788	-0.227980	1.442545	H	-1.783643	-0.851950	1.198883
H	0.484261	2.032730	0.821932	H	-1.377144	1.308227	-0.989000
H	-2.545110	-1.190634	0.195523	H	2.394350	0.067652	0.898187
H	0.189127	0.317660	-1.413552	H	0.013387	0.823462	1.413368
H	-1.320950	0.533291	1.230064	H	0.798236	0.000018	-1.409851
H	-1.936969	1.015745	-0.362852	H	1.416575	1.454584	-0.605357

Table S11: Cartesian coordinates (in Å) of the M06-2X/cc-pVTZ optimized geometries of D-glyceraldehyde: 29-32.

Atom	X	Y	Z	Atom	X	Y	Z
Geometry 29				Geometry 30			
C	0.857511	-0.878906	-0.154158	C	-0.868757	-0.872965	0.151215
C	0.085206	0.404470	-0.375023	C	-0.079080	0.399097	0.374309
C	-1.229936	0.346186	0.401826	C	1.232789	0.330131	-0.418309
O	-2.020817	-0.668086	-0.182076	O	2.065720	-0.720110	0.019342
O	0.870010	1.490271	0.029078	O	-0.858485	1.494919	-0.009199
O	1.984560	-0.925120	0.243482	O	-2.004058	-0.902078	-0.222675
H	0.278727	-1.791823	-0.380645	H	-0.294290	-1.795189	0.351078
H	0.465891	2.301506	-0.286794	H	-0.387942	2.304505	0.203073
H	-2.793967	-0.826003	0.362750	H	2.431564	-0.497230	0.878603
H	-0.166598	0.437807	-1.444211	H	0.172118	0.422422	1.447206
H	-1.014257	0.146255	1.455846	H	1.008649	0.144173	-1.468339
H	-1.716509	1.325244	0.333317	H	1.734774	1.301896	-0.354656
Geometry 31				Geometry 32			
C	-1.071615	-0.825716	0.226242	C	1.044086	0.830059	0.248455
C	-0.319193	0.491379	0.326185	C	0.308831	-0.499172	0.335453
C	0.988500	0.482065	-0.455618	C	-0.992825	-0.495826	-0.449043
O	1.995279	-0.245011	0.208733	O	-1.995006	0.233333	0.223357
O	-1.235060	1.459898	-0.143971	O	1.145985	-1.507627	-0.200906
O	-0.623449	-1.821549	-0.259717	O	0.626913	1.812397	-0.288220
H	-2.100782	-0.782619	0.628059	H	2.058989	0.814983	0.701186
H	-0.895722	2.337930	0.043362	H	1.942149	-1.589772	0.330486
H	2.289398	0.252474	0.975068	H	-2.350793	-0.307508	0.931576
H	-0.095414	0.645117	1.393076	H	0.084018	-0.693548	1.393766
H	0.831260	-0.004718	-1.416496	H	-0.834932	-0.006259	-1.408301
H	1.290944	1.518740	-0.644284	H	-1.283126	-1.533081	-0.631761

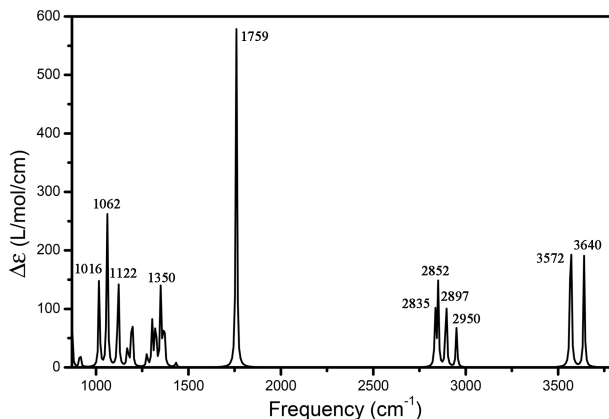


Figure S1: IR spectra of glyceraldehyde of the lowest energy geometry.

Harmonic vibrational analysis using DFT/M06-2X is performed to the lowest-energy structure and the spectra are drawn in Figure S1. The calculated frequencies have been scaled by a factor of 0.949.¹ In Figure S1, the strong IR peak at 1759 cm⁻¹ is readily assigned to the carbonyl group, which is in agreement with the typical C=O vibrational frequency in between 1760 and 1668 cm⁻¹ found in organic compounds,²⁻⁴ and reasonably close to the experimental result⁵ of 1735 cm⁻¹ obtained from melting dimeric forms as well as from an other *ab initio* work.⁶ The latter agrees remarkably well with the slightly lower dimer frequencies.⁷ Two C-O bonds stretching locate at 1081 and 1090 cm⁻¹. The C1-H7 and C2-H10 stretching modes have the vibrational frequency of 2841 and 2857 cm⁻¹. The IR bands at 1435, 2990 and 2958 cm⁻¹ are assigned to the bending of H11-C3-H12 angle, the symmetric and asymmetric stretches of the two C-H bonds, respectively.

Table S12: Comparing the excitation wavelengths(λ) and oscillator strength(f) of 30 excited states of the lowest energy geometry of D-glyceraldehyde calculated by TDDFT/B3LYP with different basis sets.

State	cc-pVTZ		aug-cc-pVTZ		cc-pVQZ		aug-cc-pVQZ	
	$\lambda(nm)$	f	$\lambda(nm)$	f	$\lambda(nm)$	f	$\lambda(nm)$	f
1	274.94	0.0001	277.11	0.0001	275.95	0.0001	277.24	0.0001
2	229.56	0.0151	229.72	0.0161	229.08	0.0156	229.75	0.0161
3	204.38	0.0061	204.89	0.0068	204.26	0.0064	204.92	0.0068
4	169.47	0.0062	187.08	0.0040	170.83	0.0003	187.10	0.0040
5	165.20	0.0023	182.41	0.0112	169.14	0.0100	182.41	0.0112
6	163.33	0.0044	180.65	0.0076	165.81	0.0095	180.70	0.0076
7	160.01	0.0118	175.18	0.0603	164.54	0.0109	175.24	0.0591
8	158.99	0.0087	169.94	0.0054	163.40	0.0038	170.03	0.0044
9	154.14	0.0880	169.44	0.0122	159.45	0.0853	169.62	0.0143
10	148.64	0.0208	169.03	0.0142	153.33	0.0161	169.25	0.0124
11	144.14	0.0107	165.37	0.0170	149.29	0.0219	165.59	0.0158
12	143.20	0.0381	163.89	0.0049	147.87	0.0308	164.05	0.0054
13	140.54	0.0455	163.45	0.0048	145.46	0.0482	163.65	0.0030
14	139.79	0.0244	162.20	0.0211	145.02	0.0232	162.38	0.0217
15	139.25	0.0144	160.89	0.0111	143.09	0.0041	160.98	0.0109
16	137.77	0.0051	155.51	0.0043	139.80	0.0044	155.88	0.0042
17	135.39	0.0436	153.38	0.0063	138.82	0.0208	154.00	0.0047
18	133.51	0.0458	152.45	0.0094	136.46	0.0265	152.82	0.0087
19	131.56	0.0357	150.70	0.0105	134.69	0.0264	151.20	0.0142
20	130.53	0.0033	149.98	0.0037	134.41	0.0465	150.35	0.0033
21	130.33	0.0246	148.64	0.0012	133.56	0.0253	149.23	0.0010
22	128.88	0.0333	147.32	0.0092	132.77	0.0148	148.82	0.0123
23	127.54	0.0344	146.36	0.0220	131.09	0.0159	148.18	0.0112
24	126.81	0.0153	144.29	0.0070	130.18	0.0261	145.86	0.0068
25	126.70	0.0316	143.54	0.0078	129.40	0.0241	145.02	0.0019
26	124.18	0.0229	143.15	0.0087	127.85	0.0260	144.93	0.0097
27	123.21	0.0100	142.47	0.0126	126.95	0.0163	143.52	0.0156
28	122.29	0.0973	141.24	0.0196	125.66	0.0414	141.66	0.0143
29	120.80	0.0061	140.10	0.0053	125.38	0.0622	141.24	0.0032
30	119.19	0.0091	139.72	0.0011	122.25	0.0008	140.64	0.0004

Table S13: Comparing the excitation wavelengths(λ) and oscillator strength(f) of 30 excited states of the lowest energy geometry of D-glyceraldehyde calculated by TDDFT/M06-2X with different basis sets.

State	cc-pVTZ		aug-cc-pVTZ		cc-pVQZ		aug-cc-pVQZ	
	$\lambda(nm)$	f	$\lambda(nm)$	f	$\lambda(nm)$	f	$\lambda(nm)$	f
1	289.76	0.0000	287.73	0.0001	287.44	0.0001	288.18	0.0001
2	183.85	0.0338	185.01	0.0270	183.31	0.0296	185.08	0.0270
3	164.63	0.0039	169.86	0.0133	163.86	0.0064	169.73	0.0136
4	153.50	0.0077	166.57	0.0099	156.30	0.0070	166.55	0.0109
5	145.79	0.0059	164.65	0.0006	150.46	0.0044	164.64	0.0005
6	145.28	0.0076	162.78	0.0085	147.52	0.0296	162.83	0.0091
7	141.61	0.0310	156.87	0.0713	145.20	0.0182	157.06	0.0751
8	140.00	0.0101	155.42	0.0121	141.99	0.0576	155.41	0.0115
9	138.14	0.0235	154.25	0.0089	141.00	0.0601	154.42	0.0093
10	135.78	0.0973	149.43	0.0247	139.77	0.0077	149.57	0.0251
11	134.94	0.0109	148.10	0.0112	135.52	0.0240	148.17	0.0111
12	129.39	0.0201	146.62	0.0149	134.20	0.0024	146.74	0.0155
13	127.74	0.1313	145.84	0.0112	132.49	0.0365	145.86	0.0116
14	127.22	0.0678	141.87	0.0052	130.51	0.1054	141.91	0.0056
15	125.45	0.0029	141.07	0.0034	129.31	0.0153	141.15	0.0024
16	125.00	0.0566	140.36	0.0061	128.01	0.0835	140.55	0.0057
17	121.75	0.0209	139.08	0.0054	127.01	0.0058	139.58	0.0054
18	120.69	0.0502	138.92	0.0070	124.30	0.0552	139.13	0.0062
19	118.30	0.0110	137.40	0.0302	122.25	0.0183	138.17	0.0362
20	117.77	0.0048	137.03	0.0106	121.07	0.0144	137.31	0.0103
21	116.96	0.0170	135.60	0.0214	120.42	0.0033	136.54	0.0147
22	116.57	0.0072	134.88	0.0262	119.96	0.0121	135.37	0.0160
23	115.60	0.0714	134.39	0.0024	119.13	0.0508	134.57	0.0036
24	115.17	0.0283	133.99	0.0044	117.30	0.0738	134.37	0.0054
25	113.18	0.0808	133.55	0.0127	116.39	0.0081	134.27	0.0065
26	112.60	0.0136	133.05	0.0116	116.01	0.0124	133.40	0.0169
27	111.73	0.0178	132.06	0.0070	115.41	0.0516	133.16	0.0092
28	110.68	0.0062	130.51	0.0088	114.46	0.0049	130.59	0.0117
29	109.76	0.0292	129.59	0.0037	114.10	0.0067	130.47	0.0020
30	108.79	0.0200	128.64	0.0698	112.67	0.0124	129.11	0.0253

Table S14: Comparing excitation wavelength ($\lambda(nm)$) and oscillator strength(f) of 30 excited states of the lowest energy geometry of D-glyceraldehyde calculated by TDDFT/cc-pVTZ with different functions.

State	B3LYP		PBE0		CAM-B3LYP		ω B97XD		M062X	
	$\lambda(nm)$	f	$\lambda(nm)$	f	$\lambda(nm)$	f	$\lambda(nm)$	f	$\lambda(nm)$	f
1	274.94	0.0001	270.99	0.0001	269.64	0.0001	269.93	0.0001	289.76	0.0000
2	229.56	0.0151	218.71	0.0191	195.39	0.0228	198.66	0.0245	183.85	0.0338
3	204.38	0.0061	194.91	0.0067	175.56	0.0037	177.33	0.0029	164.63	0.0039
4	169.47	0.0062	162.35	0.0070	156.11	0.0043	151.96	0.0037	153.50	0.0077
5	165.20	0.0023	158.56	0.0024	150.28	0.0122	150.62	0.0110	145.79	0.0059
6	163.33	0.0044	157.54	0.0044	148.86	0.0037	148.13	0.0057	145.28	0.0076
7	160.01	0.0118	153.57	0.0211	147.40	0.0070	144.99	0.0043	141.61	0.0310
8	158.99	0.0087	152.12	0.0040	146.94	0.0243	142.58	0.0452	140.00	0.0101
9	154.14	0.0880	147.71	0.0970	142.67	0.0716	138.90	0.0517	138.14	0.0235
10	148.64	0.0208	142.82	0.0224	140.65	0.0672	137.46	0.0950	135.78	0.0973
11	144.14	0.0107	138.66	0.0132	134.86	0.0235	133.01	0.0011	134.94	0.0109
12	143.20	0.0381	137.61	0.0363	132.60	0.0022	131.16	0.0308	129.39	0.0201
13	140.54	0.0445	136.43	0.0066	132.19	0.0303	128.10	0.0220	127.74	0.1313
14	139.79	0.0244	134.69	0.0683	128.34	0.1040	127.58	0.1835	127.22	0.0678
15	139.25	0.0144	133.61	0.0318	128.36	0.0075	125.76	0.0527	125.45	0.0029
16	137.77	0.0051	131.92	0.0280	127.65	0.1073	124.87	0.0051	125.00	0.0566
17	135.39	0.0436	130.68	0.0734	125.14	0.0270	121.16	0.0425	121.75	0.0209
18	133.51	0.0458	128.67	0.0141	123.92	0.0269	120.26	0.0190	120.69	0.0502
19	131.56	0.0357	126.40	0.0300	122.31	0.0049	119.40	0.0194	118.30	0.0110
20	130.53	0.0033	125.58	0.0248	121.41	0.0154	119.07	0.0065	117.77	0.0048
21	130.33	0.0246	125.03	0.0220	119.88	0.0266	117.80	0.0178	116.96	0.0170
22	128.88	0.0333	124.26	0.0405	119.39	0.0020	116.38	0.0247	116.57	0.0072
23	127.54	0.0344	122.85	0.0113	118.82	0.0328	116.00	0.0267	115.60	0.0714
24	126.81	0.0153	121.84	0.0322	117.62	0.0734	114.62	0.0490	115.17	0.0283
25	126.70	0.0316	121.64	0.0184	116.54	0.0281	113.69	0.0595	113.18	0.0808
26	124.18	0.0229	119.19	0.0261	115.99	0.0275	113.00	0.0232	112.60	0.0136
27	123.21	0.0100	118.09	0.0189	115.55	0.0199	112.37	0.0218	111.73	0.0178
28	122.29	0.0973	117.67	0.0531	113.56	0.0078	110.72	0.0081	110.68	0.0062
29	120.80	0.0061	117.27	0.0402	111.37	0.0392	110.14	0.0160	109.76	0.0292
30	119.19	0.0091	115.24	0.0212	110.75	0.0053	108.83	0.0119	108.79	0.0200

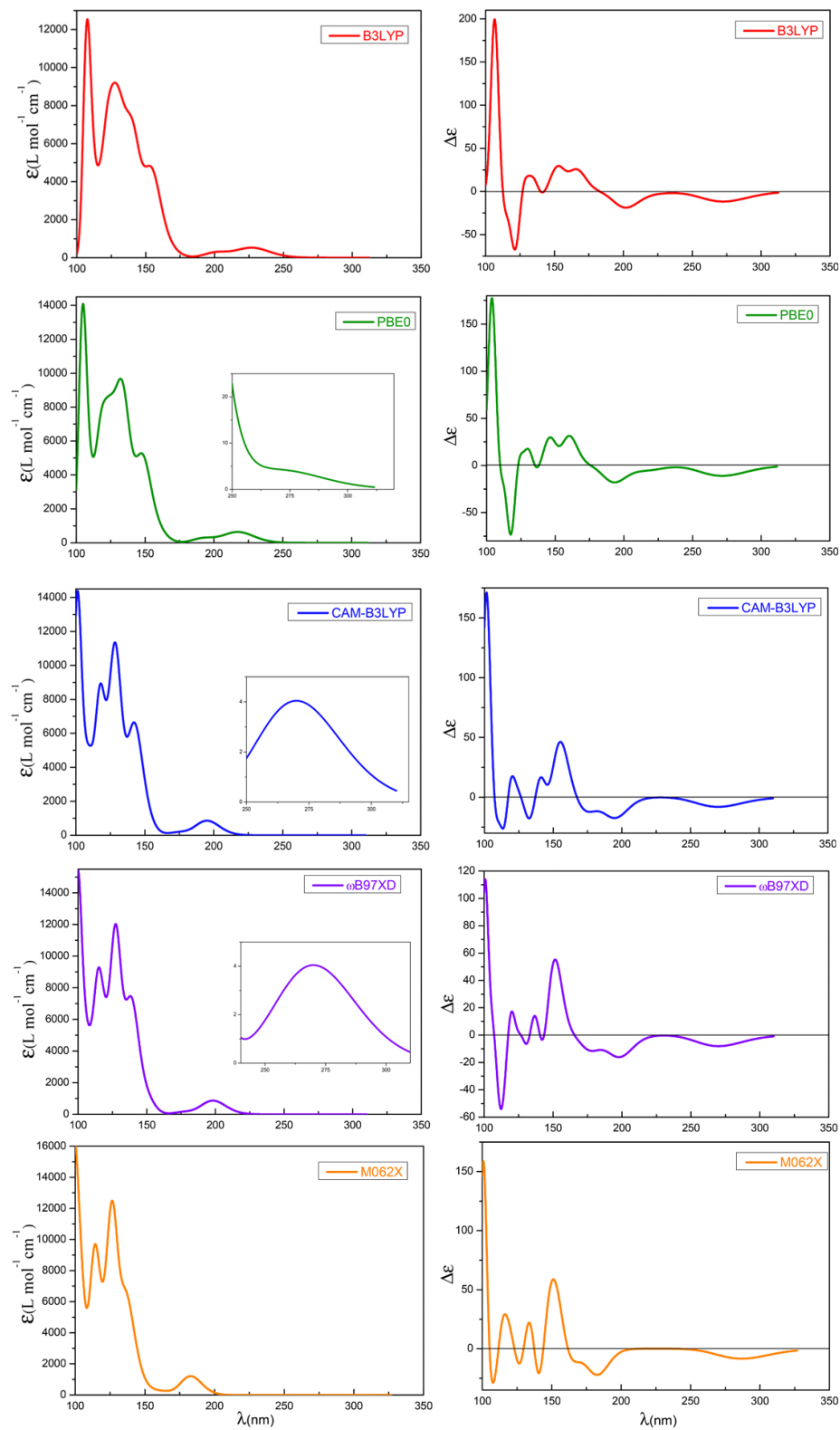


Figure S2: Comparing the absorption and ECD spectra of glyceraldehyde on its lowest energy geometry (optimized with B3LPY) calculated by TDDFT/cc-pVTZ with the different functionals

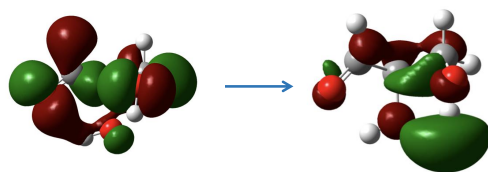
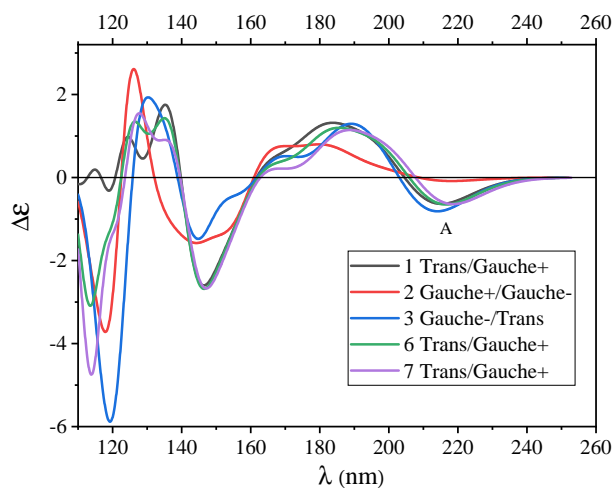
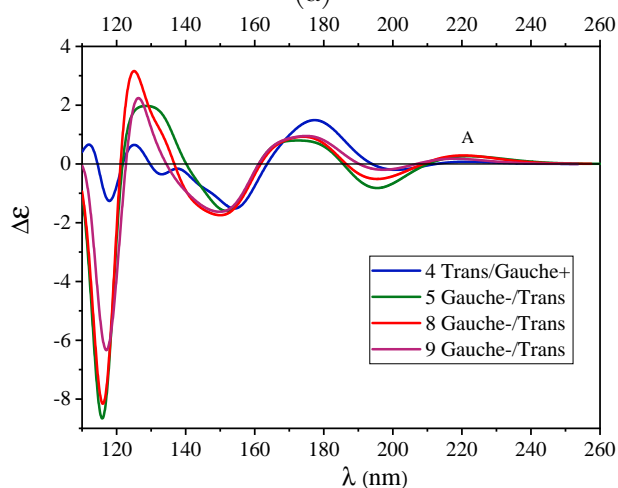


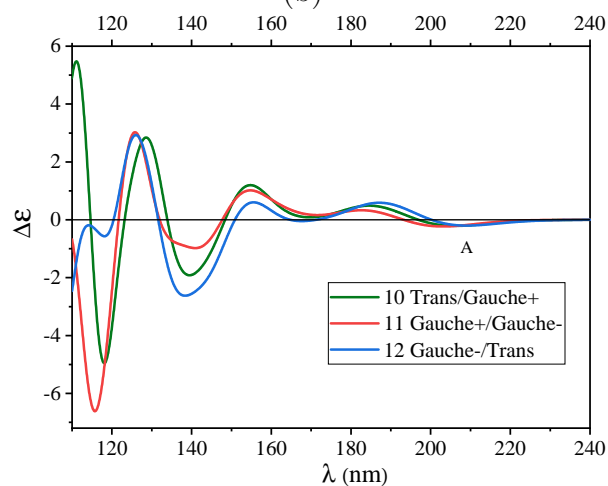
Figure S3: Natural transition orbitals (NTOs) of the S3 state of glyceraldehyde from TDDFT/M06-2X. Left is the hole NTO, right the particle NTO.



(a)



(b)



(c)

Figure S4: M06-2X theoretical ECD spectra of individual structures of the L-valine zwitterion. The longest wavelength feature is labelled as “A” on all subfigures. (a) Structures optimized without PCM and with negative “A” peak (b) Structures optimized without PCM and with positive “A” bump (c) Structures optimized with PCM

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