Energetics of the OH radical H-abstraction reactions from simple aldehydes and their geminal diol forms

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Supplementary Inofrmation

Table SI1. Energies at different levels of calculation for the radical and closed-shell species related to formaldehyde (**F**)

Table SI2. Energies at different levels of calculation for the radical and closed-shell species related to acetaldehyde (**A**)

Table SI3. Energies at different levels of calculation for the radical and closed-shell species related to glycolaldehyde (**G**)

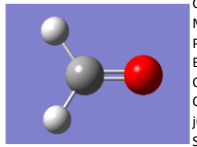
Table SI4. Energies at different levels of calculation for the radical and closed-shell species related to glyoxal (**Gl**)

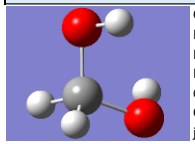
Table SI5. Energies at different levels of calculation for the radical and closed-shell species related to methylglyoxal (**MG**)

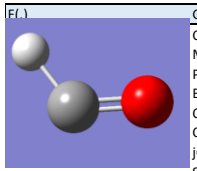
Table SI6. Energies at different levels of calculation for the radical and closed-shell species related to acrolein (**AC**)

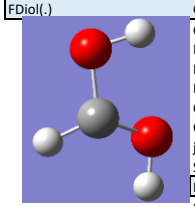
Table SI7. Cartesian coordinates for the optimized geometries of the molecules considered in this study.

Table SI1. Energies at different levels of calculation for the radical and closed-shell species related to formaldehyde (**F**)

F	Gas phase				
	CBS-QB3	-114.370381	-114.344163	-114.340350	-114.365818
	M06-2X-D3	-114.498971	-114.471958	-114.468148	-114.493603
	PW6B95-D3	-114.678858	-114.652036	-114.648225	-114.673022
	B2PLYP	-114.468075	-114.441399	-114.437587	-114.463056
	CCSD(T)-freq//B2PLYP	-114.342880	-114.316177	-114.312364	-114.337180
	CCSD(T)//B2PLYP+B2PLYP freq	-114.342880	-114.316204	-114.312392	-114.337861
	jChS	-114.495408	-114.468586	-114.464775	-114.489572
	SVECV-f12	-114.487381	-114.460368	-114.456558	-114.482013
	Bulk				
	CBS-QB3	-114.375678	-114.349342	-114.345529	-114.371001
	M06-2X-D3	-114.504636	-114.477498	-114.473688	-114.499148
	PW6B95-D3	-114.684178	-114.657210	-114.653400	-114.678201
	B2PLYP	-114.473469	-114.446623	-114.442812	-114.468283
	CCSD(T)-freq//B2PLYP	-114.347986	-114.321106	-114.317293	-114.342112
	CCSD(T)//B2PLYP+B2PLYP freq	-114.347986	-114.321140	-114.317329	-114.342800
	jChS	-114.500498	-114.473530	-114.469720	-114.494521
	SVECV-f12				

FDiol	Gas phase				
	CBS-QB3	-190.751507	-190.694733	-190.690014	-190.719608
	M06-2X-D3	-190.957530	-190.899602	-190.894838	-190.924512
	PW6B95-D3	-191.245493	-191.187769	-191.183006	-191.212668
	B2PLYP	-190.903108	-190.845690	-190.840916	-190.870611
	CCSD(T)-freq//B2PLYP	-190.707717	-190.650309	-190.645473	-190.675285
	CCSD(T)//B2PLYP+B2PLYP freq	-190.707717	-190.650299	-190.645525	-190.675220
	jChS	-190.951225	-190.893501	-190.888738	-190.918400
	SVECV-f12	-190.937266	-190.879338	-190.874574	-190.904248
	Bulk				
	CBS-QB3	-190.759173	-190.702662	-190.697872	-190.727596
	M06-2X-D3	-190.965063	-190.907401	-190.902568	-190.932373
	PW6B95-D3	-191.252811	-191.195313	-191.190480	-191.220274
	B2PLYP	-190.910583	-190.853397	-190.848549	-190.878384
	CCSD(T)-freq//B2PLYP	-190.715108	-190.657915	-190.653005	-190.682965
	CCSD(T)//B2PLYP+B2PLYP freq	-190.715108	-190.657922	-190.653074	-190.682909
	jChS	-190.958562	-190.901064	-190.896231	-190.926025
	SVECV-f12				

Abstraction of H-C	rad	E	E+ZPE	H	G
F(.)	Gas phase				
	CBS-QB3	-113.717546	-113.704757	-113.700954	-113.726423
	M06-2X-D3	-113.849422	-113.836155	-113.832353	-113.857801
	PW6B95-D3	-114.028415	-114.015260	-114.011459	-114.036903
	B2PLYP	-113.821440	-113.808442	-113.804641	-113.830100
	CCSD(T)-freq//B2PLYP	-113.692483	-113.679415	-113.675613	-113.701073
	CCSD(T)//B2PLYP+B2PLYP freq	-113.692483	-113.679485	-113.675684	-113.701143
	jChS	-113.842515	-113.829360	-113.825559	-113.851003
	SVECV-f12	-113.835363	-113.822096	-113.818294	-113.843742
	Bulk				
	CBS-QB3	-113.720279	-113.707376	-113.703573	-113.729035
	M06-2X-D3	-113.852705	-113.839340	-113.835538	-113.860979
	PW6B95-D3	-114.031446	-114.018184	-114.014382	-114.039819
	B2PLYP	-113.824366	-113.811243	-113.807442	-113.832894
	CCSD(T)-freq//B2PLYP	-113.695044	-113.681851	-113.678049	-113.703501
	CCSD(T)//B2PLYP+B2PLYP freq	-113.695044	-113.681921	-113.678120	-113.703572
	jChS	-113.845091	-113.831829	-113.828027	-113.853464
	SVECV-f12				

Abstraction of H-C	rad1	E	E+ZPE	H	G
FDiol(.)	Gas phase				
	CBS-QB3	-190.085127	-190.042197	-190.037310	-190.067670
	M06-2X-D3	-190.295834	-190.252051	-190.247096	-190.277599
	PW6B95-D3	-190.583278	-190.539577	-190.534675	-190.565047
	B2PLYP	-190.242999	-190.199580	-190.194671	-190.225072
	CCSD(T)-freq//B2PLYP	-190.043189	-189.999754	-189.994767	-190.025336
	CCSD(T)//B2PLYP+B2PLYP freq	-190.043189	-189.999770	-189.994861	-190.025262
	jChS	-190.284528	-190.240827	-190.235925	-190.266297
	SVECV-f12	-190.271760	-190.227977	-190.223022	-190.253525
	Bulk				
	CBS-QB3	-190.092537	-190.049866	-190.044923	-190.075394
	M06-2X-D3	-190.303311	-190.259767	-190.254791	-190.285327
	PW6B95-D3	-190.590442	-190.546981	-190.542035	-190.572495
	B2PLYP	-190.250249	-190.207062	-190.202111	-190.232596
	CCSD(T)-freq//B2PLYP	-190.050328	-190.007118	-190.002088	-190.032749
	CCSD(T)//B2PLYP+B2PLYP freq	-190.050328	-190.007141	-190.002190	-190.032675
	jChS	-190.291506	-190.248045	-190.243099	-190.273559
	SVECV-f12				

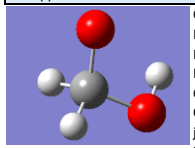
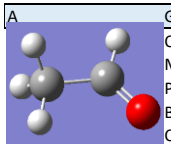
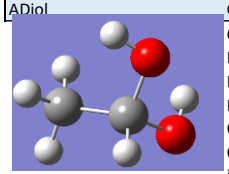
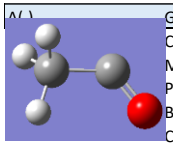
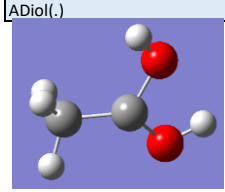
Abstraction from O (identical to addition of OH to CH2O) rad2		E	E+ZPE	H	G
FDiol(.)	Gas phase				
	CBS-QB3	-190.069856	-190.028969	-190.024188	-190.054545
	M06-2X-D3	-190.280830	-190.238250	-190.233577	-190.263704
	PW6B95-D3	-190.571684	-190.529950	-190.525157	-190.555569
	B2PLYP	-190.228283	-190.186193	-190.181503	-190.211658
	CCSD(T)-freq//B2PLYP	-190.029064	-189.986877	-189.982117	-190.012470
	CCSD(T)//B2PLYP+B2PLYP freq	-190.029064	-189.986974	-189.982284	-190.012439
	jChS	-190.268024	-190.226290	-190.221497	-190.251909
	SVECV-f12	-190.256249	-190.213669	-190.208996	-190.239123
	Bulk				
	CBS-QB3	-190.076905	-190.035858	-190.031121	-190.061369
	M06-2X-D3	-190.288008	-190.245344	-190.240727	-190.270728
	PW6B95-D3	-190.578454	-190.536478	-190.531774	-190.561950
	B2PLYP	-190.235397	-190.193217	-190.188568	-190.218632
	CCSD(T)-freq//B2PLYP	-190.028716	-189.986207	-189.981558	-190.011633
	CCSD(T)//B2PLYP+B2PLYP freq	-190.028716	-189.986536	-189.981887	-190.011951
	jChS	-190.275038	-190.233062	-190.228358	-190.258534
	SVECV-f12				

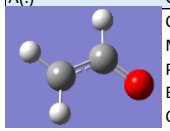
Table SI2. Energies at different levels of calculation for the radical and closed-shell species related to acetaldehyde (**A**)

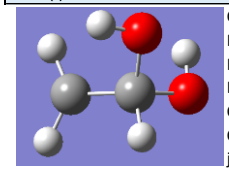
A		E	E+ZPE	H	G
	Gas phase				
	CBS-QB3	-153.637112	-153.582459	-153.577608	-153.607403
	M06-2X-D3	-153.820805	-153.764850	-153.760020	-153.789775
	PW6B95-D3	-154.072141	-154.016362	-154.011531	-154.041272
	B2PLYP	-153.771970	-153.716347	-153.711517	-153.741278
	CCSD(T)-freq//B2PLYP	-153.598393	-153.542929	-153.537901	-153.568558
	CCSD(T)//B2PLYP+B2PLYP freq	-153.598394	-153.542771	-153.537941	-153.567702
	jChS	-153.817045	-153.761266	-153.756435	-153.786176
	SVECV-f12	-153.805219	-153.749264	-153.744434	-153.774189
	Bulk				
	CBS-QB3	-153.643145	-153.588484	-153.583646	-153.613402
	M06-2X-D3	-153.827336	-153.771383	-153.766565	-153.796288
	PW6B95-D3	-154.078442	-154.022648	-154.017829	-154.047538
	B2PLYP	-153.778242	-153.722570	-153.717752	-153.747478
	CCSD(T)-freq//B2PLYP	-153.604234	-153.548671	-153.543685	-153.574090
	CCSD(T)//B2PLYP+B2PLYP freq	-153.604234	-153.548562	-153.543744	-153.573470
	jChS	-153.820457	-153.764663	-153.759844	-153.789553
	SVECV-f12				

ADiol		E	E+ZPE	H	G
	Gas phase				
	CBS-QB3	-230.008207	-229.924780	-229.918582	-229.952046
	M06-2X-D3	-230.267951	-230.183045	-230.176663	-230.210850
	PW6B95-D3	-230.625880	-230.541261	-230.534839	-230.569024
	B2PLYP	-230.194483	-230.110081	-230.103725	-230.137682
	CCSD(T)-freq//B2PLYP	-229.953083			
	CCSD(T)//B2PLYP+B2PLYP freq	-229.953083	-229.868681	-229.862325	-229.896282
	jChS	-230.262372	-230.177753	-230.171331	-230.205516
	SVECV-f12	-230.244632	-230.159726	-230.153344	-230.187531
	Bulk				
	CBS-QB3	-230.017642	-229.934420	-229.928170	-229.961798
	M06-2X-D3	-230.277198	-230.192343	-230.186068	-230.219824
	PW6B95-D3	-230.636586	-230.551496	-230.545394	-230.578664
	B2PLYP	-230.203608	-230.119359	-230.113008	-230.146973
	CCSD(T)-freq//B2PLYP	-229.962110			
	CCSD(T)//B2PLYP+B2PLYP freq	-229.962110	-229.877861	-229.871510	-229.905475
	jChS	-230.272991	-230.187901	-230.181799	-230.215069
	SVECV-f12				

H-Abstraction from CHO or CH(OH)2 A(.)		E	E+ZPE	H	G
	Gas phase				
	CBS-QB3	-152.984570	-152.942041	-152.937125	-152.967671
	M06-2X-D3	-153.171242	-153.127757	-153.122848	-153.153404
	PW6B95-D3	-153.421884	-153.378452	-153.373557	-153.404047
	B2PLYP	-153.125052	-153.081738	-153.076848	-153.107343
	CCSD(T)-freq//B2PLYP	-152.947746	-152.904591	-152.900404	-152.929372
	CCSD(T)//B2PLYP+B2PLYP freq	-152.947746	-152.904432	-152.899542	-152.930037
	jChS	-153.163945	-153.120513	-153.115618	-153.146108
	SVECV-f12	-153.153179	-153.109694	-153.104785	-153.135341
	Bulk				
	CBS-QB3	-152.988363	-152.945896	-152.940982	-152.971526
	M06-2X-D3	-153.175732	-153.132330	-153.127427	-153.157964
	PW6B95-D3	-153.426261	-153.382905	-153.378014	-153.408495
	B2PLYP	-153.129219	-153.085953	-153.081068	-153.111549
	CCSD(T)-freq//B2PLYP	-152.951399	-152.908278	-152.904097	-152.933051
	CCSD(T)//B2PLYP+B2PLYP freq	-152.951399	-152.908133	-152.903248	-152.933729
	jChS	-153.167608	-153.124252	-153.119361	-153.149842
	SVECV-f12				

H-Abstraction from CHO or CH(OH)2 ADiol(.)		E	E+ZPE	H	G
	Gas phase				
	CBS-QB3	-229.349311	-229.278714	-229.272559	-229.306531
	M06-2X-D3	-229.613200	-229.541080	-229.534948	-229.568883
	PW6B95-D3	-229.971282	-229.899391	-229.893235	-229.927213
	B2PLYP	-229.541835	-229.470174	-229.464039	-229.497984
	CCSD(T)-freq//B2PLYP	-229.295317			
	CCSD(T)//B2PLYP+B2PLYP freq	-229.295317	-229.223656	-229.217521	-229.251466
	jChS	-229.602588	-229.530697	-229.524541	-229.558519
	SVECV-f12	-229.585848	-229.513728	-229.507596	-229.541531
	Bulk				
	CBS-QB3	-229.356530	-229.286236	-229.280055	-229.314072
	M06-2X-D3	-229.620524	-229.548684	-229.542544	-229.576492
	PW6B95-D3	-229.978265	-229.906615	-229.900460	-229.934427
	B2PLYP	-229.548893	-229.477470	-229.471335	-229.505273
	CCSD(T)-freq//B2PLYP	-229.302289			
	CCSD(T)//B2PLYP+B2PLYP freq	-229.302289	-229.230866	-229.224731	-229.258669
	jChS	-229.609567	-229.537917	-229.531762	-229.565729
	SVECV-f12				

H-Abstraction from CH3		E	E+ZPE	H	G
A(.)	Gas phase				
	CBS-QB3	-152.974689	-152.932833	-152.928349	-152.957753
	M06-2X-D3	-153.161756	-153.118813	-153.114353	-153.143715
	PW6B95-D3	-153.411205	-153.368416	-153.363958	-153.393308
	B2PLYP	-153.112833	-153.070073	-153.065586	-153.094998
	CCSD(T)-freq//B2PLYP	-152.936210	-152.893701	-152.889148	-152.918665
	CCSD(T)//B2PLYP+B2PLYP freq	-152.936210	-152.893450	-152.888963	-152.918375
	jChS	-153.151698	-153.108909	-153.104451	-153.133801
	SVECV-f12	-153.142208	-153.099265	-153.094805	-153.124167
	Bulk				
	CBS-QB3	-152.980832	-152.938784	-152.934312	-152.963701
	M06-2X-D3	-153.168884	-153.125729	-153.121285	-153.150627
	PW6B95-D3	-153.417731	-153.374719	-153.370275	-153.399609
	B2PLYP	-153.119720	-153.076748	-153.072276	-153.101669
	CCSD(T)-freq//B2PLYP	-152.942499	-152.899738	-152.895203	-152.924697
	CCSD(T)//B2PLYP+B2PLYP freq	-152.942499	-152.899527	-152.895055	-152.924448
	jChS	-153.157983	-153.114971	-153.110527	-153.139861
	SVECV-f12				

H-Abstraction from CH3		E	E+ZPE	H	G
ADiol(.)	Gas phase				
	CBS-QB3	-229.331373	-229.262182	-229.255846	-229.290097
	M06-2X-D3	-229.595337	-229.524880	-229.518454	-229.552946
	PW6B95-D3	-229.950304	-229.880126	-229.873645	-229.908258
	B2PLYP	-229.523016	-229.453099	-229.446618	-229.481254
	CCSD(T)-freq//B2PLYP	-229.278446	-229.208268	-229.201787	-229.236400
	CCSD(T)//B2PLYP+B2PLYP freq	-229.278446	-229.208529	-229.202048	-229.236684
	jChS	-229.585007	-229.514829	-229.508348	-229.542961
	SVECV-f12	-229.568421	-229.497964	-229.491538	-229.526030
	Bulk				
	CBS-QB3	-229.340318	-229.271448	-229.265008	-229.299513
	M06-2X-D3	-229.604251	-229.534067	-229.527566	-229.562283
	PW6B95-D3	-229.958805	-229.888921	-229.882335	-229.917267
	B2PLYP	-229.531758	-229.462127	-229.455543	-229.490482
	CCSD(T)-freq//B2PLYP	-229.287076	-229.217192	-229.210606	-229.245538
	CCSD(T)//B2PLYP+B2PLYP freq	-229.287076	-229.217445	-229.210861	-229.245800
	jChS	-229.593609	-229.523725	-229.517139	-229.552071
	SVECV-f12				

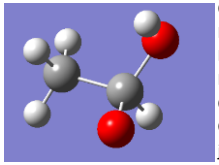
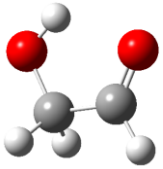
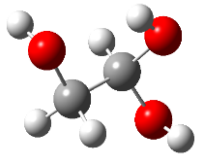
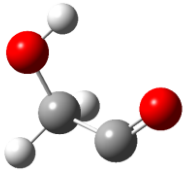
Abstraction from oxygen (identical to addition of OH to CH3Cl		E	E+ZPE	H	G
ADiol(.)	Gas phase				
	CBS-QB3	-229.331684	-229.262448	-229.256531	-229.290113
	M06-2X-D3	-229.594686	-229.523444	-229.517464	-229.551297
	PW6B95-D3	-229.956536	-229.886020	-229.880095	-229.913696
	B2PLYP	-229.523355	-229.452885	-229.446703	-229.481268
	CCSD(T)-freq//B2PLYP	-229.278200			
	CCSD(T)//B2PLYP+B2PLYP freq	-229.278200	-229.207730	-229.201548	-229.236113
	jChS	-229.583990	-229.513474	-229.507549	-229.541150
	SVECV-f12	-229.567254	-229.496012	-229.490032	-229.523865
	Bulk				
	CBS-QB3	-229.337474	-229.268159	-229.262112	-229.296016
	M06-2X-D3	-229.601665	-229.530324	-229.524509	-229.557895
	PW6B95-D3	-229.962798	-229.892407	-229.886462	-229.920104
	B2PLYP	-229.530183	-229.459414	-229.453494	-229.487111
	CCSD(T)-freq//B2PLYP	-229.284913			
	CCSD(T)//B2PLYP+B2PLYP freq	-229.284913	-229.214144	-229.208224	-229.241841
	jChS	-229.590190	-229.519799	-229.513854	-229.547496
	SVECV-f12				

Table SI3. Energies at different levels of calculation for the radical and closed-shell species related to glycolaldehyde (**G**)

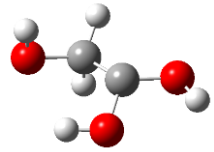
		E	E+ZPE	H	G
G	Gas phase				
	CBS-QB3	-228.782623	-228.722414	-228.716943	-228.749092
	M06-2X-D3	-229.045738	-228.983897	-228.978499	-229.010474
	PW6B95-D3	-229.401685	-229.340049	-229.334704	-229.366556
	B2PLYP	-228.976065	-228.914796	-228.909402	-228.941378
	CCSD(T)-freq//B2PLYP	-228.728400			
	CCSD(T)//B2PLYP+B2PLYP freq	-228.728400	-228.667131	-228.661737	-228.693713
	jChS	-229.034530	-228.972894	-228.967549	-228.999401
	SVECV-f12	-229.018431	-228.956590	-228.951192	-228.983167
	Bulk				
	CBS-QB3	-228.790452	-228.730351	-228.724804	-228.757117
	M06-2X-D3	-229.053692	-228.992070	-228.986549	-229.018793
	PW6B95-D3	-229.409337	-229.347850	-229.342418	-229.374440
	B2PLYP	-228.983862	-228.922727	-228.917239	-228.949407
	CCSD(T)-freq//B2PLYP	-228.735896			
	CCSD(T)//B2PLYP+B2PLYP freq	-228.735896	-228.674761	-228.669273	-228.701441
	jChS	-229.041991	-228.980504	-228.975072	-229.007094
	SVECV-f12				

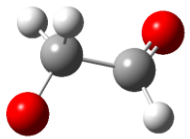
		E	E+ZPE	H	G
GDiol	Gas phase				
	CBS-QB3	-305.155165	-305.065835	-305.058955	-305.094626
	M06-2X-D3	-305.493842	-305.402874	-305.395885	-305.431787
	PW6B95-D3	-305.955905	-305.865285	-305.858288	-305.894203
	B2PLYP	-305.399594	-305.309452	-305.302432	-305.338408
	CCSD(T)-freq//B2PLYP	-305.084561			
	CCSD(T)//B2PLYP+B2PLYP freq	-305.084561	-304.994419	-304.987399	-305.023375
	jChS	-305.481079	-305.390459	-305.383462	-305.419377
	SVECV-f12	-305.458985	-305.368017	-305.361028	-305.396930
	Bulk				
	CBS-QB3	-305.166606	-305.077408	-305.070532	-305.106207
	M06-2X-D3	-305.504960	-305.414225	-305.407226	-305.443139
	PW6B95-D3	-305.966761	-305.876332	-305.869324	-305.905273
	B2PLYP	-305.410628	-305.320684	-305.313644	-305.349673
	CCSD(T)-freq//B2PLYP	-305.095472			
	CCSD(T)//B2PLYP+B2PLYP freq	-305.095472	-305.005528	-304.998488	-305.034517
	jChS	-305.491946	-305.401517	-305.394509	-305.430458
	SVECV-f12				

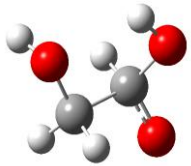
H-Abstraction from CHO or CH(OH)2 Conformation 2 / OH toward oxygen

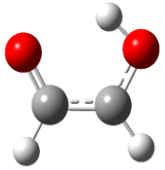
		E	E+ZPE	H	G
G(.)	Gas phase				
	CBS-QB3	-228.126291	-228.078170	-228.072543	-228.105646
	M06-2X-D3	-228.392341	-228.343161	-228.337491	-228.370717
	PW6B95-D3	-228.747324	-228.698331	-228.692655	-228.725900
	B2PLYP	-228.325581	-228.276822	-228.271164	-228.304369
	CCSD(T)-freq//B2PLYP	-228.074099			
	CCSD(T)//B2PLYP+B2PLYP freq	-228.074099	-228.025340	-228.019682	-228.052887
	jChS	-228.377640	-228.328647	-228.322971	-228.356216
	SVECV-f12	-228.362597	-228.313417	-228.307747	-228.340973
	Bulk				
	CBS-QB3	-228.133039	-228.084907	-228.079280	-228.112423
	M06-2X-D3	-228.399375	-228.350101	-228.344509	-228.377566
	PW6B95-D3	-228.754287	-228.705167	-228.699570	-228.732637
	B2PLYP	-228.332606	-228.283735	-228.278137	-228.311220
	CCSD(T)-freq//B2PLYP	-228.080548			
	CCSD(T)//B2PLYP+B2PLYP freq	-228.080548	-228.031677	-228.026079	-228.059162
	jChS	-228.384054	-228.334934	-228.329337	-228.362404
	SVECV-f12				

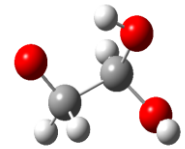
H-Abstraction from CHO or CH(OH)2

		E	E+ZPE	H	G
GDiol(.)	Gas phase				
	CBS-QB3	-304.495940	-304.419484	-304.412608	-304.448949
	M06-2X-D3	-304.839177	-304.761110	-304.754229	-304.790571
	PW6B95-D3	-305.301412	-305.223701	-305.216792	-305.253195
	B2PLYP	-304.746767	-304.669491	-304.662561	-304.699030
	CCSD(T)-freq//B2PLYP	-304.426415			
	CCSD(T)//B2PLYP+B2PLYP freq	-304.426415	-304.349139	-304.342209	-304.378678
	jChS	-304.821036	-304.743325	-304.736416	-304.772819
	SVECV-f12	-304.800179	-304.722112	-304.715231	-304.751573
	Bulk				
	CBS-QB3	-304.504545	-304.428566	-304.421587	-304.458174
	M06-2X-D3	-304.847717	-304.770288	-304.763226	-304.799985
	PW6B95-D3	-305.309570	-305.232327	-305.225315	-305.261970
	B2PLYP	-304.755129	-304.678347	-304.671297	-304.708059
	CCSD(T)-freq//B2PLYP	-304.434668			
	CCSD(T)//B2PLYP+B2PLYP freq	-304.434668	-304.357886	-304.350836	-304.387598
	jChS	-304.829237	-304.751994	-304.744982	-304.781637
	SVECV-f12				

Abstraction of H from the OH		E	E+ZPE	H	G
G(.)	Gas phase				
	CBS-QB3	-228.095756	-228.050057	-228.044648	-228.077412
	M06-2X-D3	-228.363415	-228.316191	-228.310830	-228.343592
	PW6B95-D3	-228.721811	-228.675174	-228.669770	-228.702543
	B2PLYP	-228.296190	-228.249522	-228.244145	-228.276934
	CCSD(T)-freq//B2PLYP	-228.045145			
	CCSD(T)//B2PLYP+B2PLYP freq	-228.045145	-227.998477	-227.993100	-228.025889
	jChS	-228.346128	-228.299491	-228.294087	-228.326860
	SVECV-f12	-228.332305	-228.285081	-228.279720	-228.312482
	Bulk				
	CBS-QB3	-228.102650	-228.057033	-228.051612	-228.084395
	M06-2X-D3	-228.370915	-228.323675	-228.318312	-228.351075
	PW6B95-D3	-228.729059	-228.682531	-228.677121	-228.709901
	B2PLYP	-228.303538	-228.256790	-228.251417	-228.284196
	CCSD(T)-freq//B2PLYP	-228.051923			
	CCSD(T)//B2PLYP+B2PLYP freq	-228.051923	-228.005175	-227.999802	-228.032581
	jChS	-228.352765	-228.306237	-228.300827	-228.333607
	SVECV-f12				

H-Abstraction from the exposed OH of C(OH)2		E	E+ZPE	H	G
GDiol(.) rad 2 from C(OH)2	Gas phase				
	CBS-QB3	-304.473294	-304.398185	-304.391612	-304.427312
	M06-2X-D3	-304.816318	-304.739683	-304.733021	-304.768964
	PW6B95-D3	-305.282609	-305.206301	-305.199680	-305.235482
	B2PLYP	-304.724567	-304.648630	-304.641954	-304.677924
	CCSD(T)-freq//B2PLYP	-304.405482			
	CCSD(T)//B2PLYP+B2PLYP freq	-304.405482	-304.329545	-304.322869	-304.358839
	jChS	-304.797623	-304.721315	-304.714694	-304.750496
	SVECV-f12	-304.777578	-304.700943	-304.694281	-304.730224
	Bulk				
	CBS-QB3	-304.485147	-304.410233	-304.403590	-304.439400
	M06-2X-D3	-304.828536	-304.752542	-304.745802	-304.781810
	PW6B95-D3	-305.295591	-305.219492	-305.212812	-305.248689
	B2PLYP	-304.736707	-304.661437	-304.654606	-304.690825
	CCSD(T)-freq//B2PLYP	-304.416471			
	CCSD(T)//B2PLYP+B2PLYP freq	-304.416471	-304.341201	-304.334370	-304.370589
	jChS	-304.808435	-304.732336	-304.725656	-304.761533
	SVECV-f12				

Abstraction of H from the CH2		E	E+ZPE	H	G
G(.)	Gas phase				
	CBS-QB3	-228.146457	-228.097376	-228.092446	-228.124077
	M06-2X-D3	-228.414332	-228.364021	-228.359118	-228.390699
	PW6B95-D3	-228.771022	-228.720866	-228.715974	-228.747529
	B2PLYP	-228.345514	-228.295666	-228.290739	-228.322374
	CCSD(T)-freq//B2PLYP	-228.091697			
	CCSD(T)//B2PLYP+B2PLYP freq	-228.091697	-228.041849	-228.036922	-228.068557
	jChS	-228.395959	-228.345803	-228.340911	-228.372466
	SVECV-f12	-228.381798	-228.331487	-228.326584	-228.358165
	Bulk				
	CBS-QB3	-228.153004	-228.104012	-228.099031	-228.130771
	M06-2X-D3	-228.421579	-228.371361	-228.366414	-228.398086
	PW6B95-D3	-228.777744	-228.727708	-228.722752	-228.754443
	B2PLYP	-228.352542	-228.302816	-228.297830	-228.329592
	CCSD(T)-freq//B2PLYP	-228.098180			
	CCSD(T)//B2PLYP+B2PLYP freq	-228.098180	-228.048454	-228.043468	-228.075230
	jChS	-228.402431	-228.352395	-228.347439	-228.379130
	SVECV-f12				

H-Abstraction from the OH in the CH2OH substituent		E	E+ZPE	H	G
GDiol(.) rad 3 from C(OH)2	Gas phase				
	CBS-QB3	-304.472450	-304.397274	-304.390687	-304.426348
	M06-2X-D3	-304.817094	-304.740703	-304.734039	-304.770000
	PW6B95-D3	-305.282194	-305.205748	-305.199160	-305.234801
	B2PLYP	-304.724570	-304.648793	-304.642114	-304.678149
	CCSD(T)-freq//B2PLYP	-304.405892			
	CCSD(T)//B2PLYP+B2PLYP freq	-304.405892	-304.330115	-304.323436	-304.359471
	jChS	-304.796577	-304.720131	-304.713543	-304.749184
	SVECV-f12	-304.777968	-304.701577	-304.694913	-304.730874
	Bulk				
	CBS-QB3	-304.482610	-304.408415	-304.401681	-304.437785
	M06-2X-D3	-304.826182	-304.749903	-304.743220	-304.779236
	PW6B95-D3	-305.290350	-305.214826	-305.208091	-305.244271
	B2PLYP	-304.733690	-304.658110	-304.651363	-304.687564
	CCSD(T)-freq//B2PLYP	-304.414759			
	CCSD(T)//B2PLYP+B2PLYP freq	-304.414759	-304.339179	-304.332432	-304.368633
	jChS	-304.806741	-304.731217	-304.724482	-304.760662
	SVECV-f12				

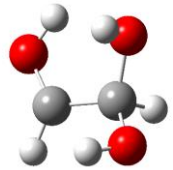
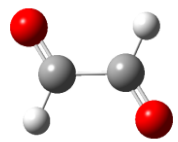
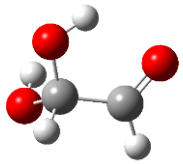
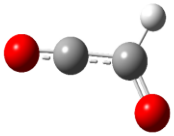
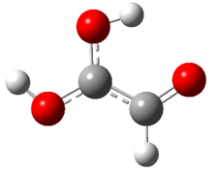
H-Abstraction from the CH2		E	E+ZPE	H	G
GDiol(.) rad 4 from C(OH)2	Gas phase				
	CBS-QB3	-304.493801	-304.417389	-304.410686	-304.446700
	M06-2X-D3	-304.837119	-304.759252	-304.752477	-304.788669
	PW6B95-D3	-305.298934	-305.221433	-305.214640	-305.250915
	B2PLYP	-304.744498	-304.667433	-304.660631	-304.696903
	CCSD(T)-freq//B2PLYP	-304.424837			
	CCSD(T)//B2PLYP+B2PLYP freq	-304.424837	-304.347772	-304.340970	-304.377242
	jChS	-304.819261	-304.741760	-304.734967	-304.771242
	SVECV-f12	-304.798325	-304.720458	-304.713683	-304.749875
	Bulk				
	CBS-QB3	-304.497002	-304.421946	-304.414606	-304.452183
	M06-2X-D3	-304.839985	-304.763379	-304.756031	-304.793621
	PW6B95-D3	-305.308243	-305.230940	-305.224190	-305.260233
	B2PLYP	-304.754142	-304.677299	-304.670516	-304.706639
	CCSD(T)-freq//B2PLYP	-304.434296			
	CCSD(T)//B2PLYP+B2PLYP freq	-304.434296	-304.357453	-304.350670	-304.386793
	jChS	-304.828695	-304.751392	-304.744642	-304.780685
	SVECV-f12				

Table SI4. Energies at different levels of calculation for the radical and closed-shell species related to glyoxal (**Gl**)

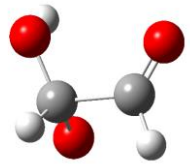
Gl	Gas phase	E	E+ZPE	H	G
	CBS-QB3	-227.558187	-227.521756	-227.516587	-227.548054
	M06-2X-D3	-227.821678	-227.783978	-227.778849	-227.810247
	PW6B95-D3	-228.174163	-228.136883	-228.131711	-228.163220
	B2PLYP	-227.757126	-227.720161	-227.714993	-227.746510
	CCSD(T)-freq//B2PLYP	-227.505053			
	CCSD(T)//B2PLYP+B2PLYP freq	-227.505053	-227.468088	-227.462920	-227.494437
	jChS	-227.807463	-227.770183	-227.765011	-227.796520
	SVECV-f12	-227.792833	-227.755133	-227.750004	-227.781402
	Bulk				
	CBS-QB3	-227.564705	-227.528210	-227.523020	-227.554555
	M06-2X-D3	-227.828523	-227.790787	-227.785633	-227.817118
	PW6B95-D3	-228.180736	-228.143391	-228.138197	-228.169788
	B2PLYP	-227.763782	-227.726728	-227.721538	-227.753135
	CCSD(T)-freq//B2PLYP	-227.511302			
	CCSD(T)//B2PLYP+B2PLYP freq	-227.511302	-227.474248	-227.469058	-227.500655
	jChS	-227.813663	-227.776318	-227.771124	-227.802715
	SVECV-f12				

GlDiol	Gas phase	E	E+ZPE	H	G
	CBS-QB3	-303.939026	-303.873655	-303.867236	-303.902173
	M06-2X-D3	-304.279898	-304.212940	-304.206533	-304.241442
	PW6B95-D3	-304.739696	-304.673115	-304.666726	-304.701571
	B2PLYP	-304.189988	-304.123909	-304.117489	-304.152418
	CCSD(T)-freq//B2PLYP	-303.869245			
	CCSD(T)//B2PLYP+B2PLYP freq	-303.869245	-303.803166	-303.796746	-303.831675
	jChS	-304.262721	-304.196140	-304.189751	-304.224596
	SVECV-f12	-304.242219	-304.175261	-304.168854	-304.203763
	Bulk				
	CBS-QB3	-303.948622	-303.883243	-303.876845	-303.911683
	M06-2X-D3	-304.289375	-304.222564	-304.216126	-304.251064
	PW6B95-D3	-304.748864	-304.682399	-304.675983	-304.710853
	B2PLYP	-304.199363	-304.133356	-304.126922	-304.161848
	CCSD(T)-freq//B2PLYP	-303.878295			
	CCSD(T)//B2PLYP+B2PLYP freq	-303.878295	-303.812288	-303.805854	-303.840780
	jChS	-304.271724	-304.205259	-304.198843	-304.233713
	SVECV-f12				

Radical H-abstraction from one equivalent CHO Gl(.)	Gas phase	E	E+ZPE	H	G
	CBS-QB3	-226.909261	-226.884767	-226.879645	-226.911574
	M06-2X-D3	-227.180341	-227.154961	-227.149957	-227.181594
	PW6B95-D3	-227.534301	-227.509152	-227.504097	-227.535858
	B2PLYP	-227.115770	-227.090888	-227.085792	-227.117657
	CCSD(T)-freq//B2PLYP	-226.855640			
	CCSD(T)//B2PLYP+B2PLYP freq	-226.855640	-226.830758	-226.825662	-226.857527
	jChS	-227.156108	-227.130959	-227.125904	-227.157665
	SVECV-f12	-227.143118	-227.117738	-227.112734	-227.144371
	Bulk				
	CBS-QB3	-226.916274	-226.891605	-226.886523	-226.918358
	M06-2X-D3	-227.188070	-227.162504	-227.157538	-227.189096
	PW6B95-D3	-227.541581	-227.516247	-227.511233	-227.542903
	B2PLYP	-227.123485	-227.098389	-227.093352	-227.125082
	CCSD(T)-freq//B2PLYP	-226.862524			
	CCSD(T)//B2PLYP+B2PLYP freq	-226.862524	-226.837428	-226.832391	-226.864121
	jChS	-227.163025	-227.137691	-227.132677	-227.164347
	SVECV-f12				

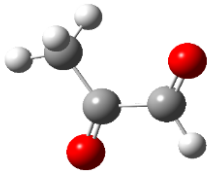
H-Abstraction from CH(OH)2 GlDiol(.)	Gas phase	E	E+ZPE	H	G
	CBS-QB3	-303.309908	-303.256215	-303.250268	-303.284610
	M06-2X-D3	-303.658573	-303.603387	-303.597522	-303.631712
	PW6B95-D3	-304.120153	-304.065263	-304.059398	-304.093583
	B2PLYP	-303.568358	-303.513939	-303.508028	-303.542318
	CCSD(T)-freq//B2PLYP	-303.238921			
	CCSD(T)//B2PLYP+B2PLYP freq	-303.238921	-303.184502	-303.178591	-303.212881
	jChS	-303.631393	-303.576503	-303.570638	-303.604823
	SVECV-f12	-303.612759	-303.557573	-303.551708	-303.585898
	Bulk				
	CBS-QB3	-303.319382	-303.265952	-303.259949	-303.294407
	M06-2X-D3	-303.668646	-303.613738	-303.607832	-303.642106
	PW6B95-D3	-304.129747	-304.075141	-304.069207	-304.103534
	B2PLYP	-303.578321	-303.524186	-303.518213	-303.552630
	CCSD(T)-freq//B2PLYP	-303.248235			
	CCSD(T)//B2PLYP+B2PLYP freq	-303.248235	-303.194100	-303.188127	-303.222544
	jChS	-303.640737	-303.586131	-303.580197	-303.614524
	SVECV-f12				

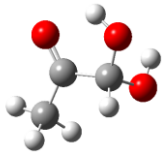
H-Abstraction from the exposed OH of C(OH)2

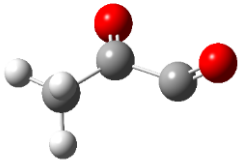


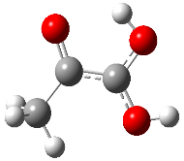
	E	E+ZPE	H	G
Gas phase				
CBS-QB3	-303.260134	-303.209460	-303.202921	-303.238701
M06-2X-D3	-303.603435	-303.551252	-303.544874	-303.580892
PW6B95-D3	-304.069920	-304.018078	-304.011611	-304.047217
B2PLYP				
CCSD(T)-freq//B2PLYP				
CCSD(T)//B2PLYP+B2PLYP freq				
jChS	-303.581227	-303.529385	-303.522918	-303.558524
SVECV-f12	-303.561964	-303.509781	-303.503403	-303.539421
Bulk				
CBS-QB3	-303.268273	-303.217802	-303.211176	-303.247179
M06-2X-D3	-303.612543	-303.560794	-303.554359	-303.590341
PW6B95-D3	-304.079419	-304.027860	-304.021295	-304.057137
B2PLYP				
CCSD(T)-freq//B2PLYP				
CCSD(T)//B2PLYP+B2PLYP freq				
jChS	-303.588863	-303.537304	-303.530739	-303.566581
SVECV-f12				

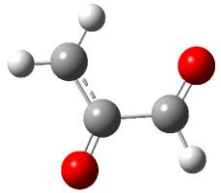
Table SI5. Energies at different levels of calculation for the radical and closed-shell species related to methylglyoxal (**MG**)

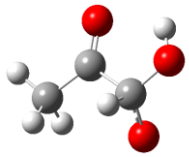
MG	Gas phase	E	E+ZPE	H	G
	CBS-QB3	-266.826029	-266.761842	-266.755183	-266.791052
	M06-2X-D3	-267.144322	-267.078342	-267.071838	-267.107120
	PW6B95-D3	-267.567323	-267.501879	-267.495209	-267.531195
	B2PLYP	-267.060674	-266.995465	-266.988855	-267.024543
	CCSD(T)-freq//B2PLYP	-266.761372			
	CCSD(T)//B2PLYP+B2PLYP freq	-266.761372	-266.696163	-266.689553	-266.725241
	jChS	-267.129824	-267.064380	-267.057710	-267.093696
	SVECV-f12	-267.111477	-267.045497	-267.038993	-267.074275
	Bulk				
	CBS-QB3	-266.832740	-266.768617	-266.761959	-266.797793
	M06-2X-D3	-267.151439	-267.085592	-267.079059	-267.114451
	PW6B95-D3	-267.574268	-267.508954	-267.502245	-267.538425
	B2PLYP	-267.067636	-267.002477	-266.995858	-267.031585
	CCSD(T)-freq//B2PLYP	-266.767833			
	CCSD(T)//B2PLYP+B2PLYP freq	-266.767833	-266.702674	-266.696055	-266.731782
	jChS	-267.136250	-267.070936	-267.064227	-267.100407
	SVECV-f12				

Mgdiol	Gas phase	E	E+ZPE	H	G
	CBS-QB3	-343.206756	-343.113775	-343.105798	-343.144762
	M06-2X-D3	-343.601862	-343.506931	-343.498902	-343.538197
	PW6B95-D3	-344.132255	-344.037644	-344.029653	-344.068705
	B2PLYP	-343.492941	-343.398823	-343.390800	-343.429960
	CCSD(T)-freq//B2PLYP	-343.125360			
	CCSD(T)//B2PLYP+B2PLYP freq	-343.125360	-343.031242	-343.023219	-343.062379
	jChS	-343.584790	-343.490179	-343.482188	-343.521240
	SVECV-f12	-343.560516	-343.465585	-343.457556	-343.496851
	Bulk				
	CBS-QB3	-343.216365	-343.123509	-343.115565	-343.154469
	M06-2X-D3	-343.611452	-343.516678	-343.508714	-343.547921
	PW6B95-D3	-344.137713	-344.043485	-344.035366	-344.074524
	B2PLYP	-343.502454	-343.408475	-343.400480	-343.439730
	CCSD(T)-freq//B2PLYP	-343.134472			
	CCSD(T)//B2PLYP+B2PLYP freq	-343.134472	-343.040493	-343.032498	-343.071748
	jChS	-343.590413	-343.496185	-343.488066	-343.527224
	SVECV-f12				

Radical H-abstraction from CHO					
MG rad 1	Gas phase	E	E+ZPE	H	G
	CBS-QB3	-266.173839	-266.121640	-266.114979	-266.151291
	M06-2X-D3	-266.497969	-266.444322	-266.437813	-266.473742
	PW6B95-D3	-266.923001	-266.869611	-266.863038	-266.899121
	B2PLYP	-266.415750	-266.363293	-266.356473	-266.393707
	CCSD(T)-freq//B2PLYP	-266.110419			
	CCSD(T)//B2PLYP+B2PLYP freq	-266.110419	-266.057962	-266.051142	-266.088376
	jChS	-266.474575	-266.421185	-266.414612	-266.450695
	SVECV-f12	-266.457823	-266.404176	-266.397667	-266.433596
	Bulk				
	CBS-QB3	-266.180858	-266.128624	-266.122003	-266.158227
	M06-2X-D3	-266.505732	-266.451995	-266.445554	-266.481307
	PW6B95-D3	-266.930399	-266.876940	-266.870421	-266.906373
	B2PLYP	-266.421988	-266.369614	-266.362801	-266.399877
	CCSD(T)-freq//B2PLYP	-266.115887			
	CCSD(T)//B2PLYP+B2PLYP freq	-266.115887	-266.063513	-266.056700	-266.093776
	jChS	-266.481590	-266.428131	-266.421612	-266.457564
	SVECV-f12				

abstraction from CH in CH(OH2)					
GlDiol(.)	Gas phase	E	E+ZPE	H	G
	CBS-QB3	-342.573923	-342.492881	-342.485219	-342.523935
	M06-2X-D3	-342.975731	-342.892637	-342.885089	-342.923668
	PW6B95-D3	-343.507893	-343.425182	-343.417615	-343.456153
	B2PLYP	-342.867100	-342.784806	-342.777223	-342.815795
	CCSD(T)-freq//B2PLYP	-342.491141			
	CCSD(T)//B2PLYP+B2PLYP freq	-342.491141	-342.408847	-342.401264	-342.439836
	jChS	-342.949457	-342.866746	-342.859179	-342.897717
	SVECV-f12	-342.926919	-342.843825	-342.836277	-342.874856
	Bulk				
	CBS-QB3	-342.582988	-342.502245	-342.494545	-342.533397
	M06-2X-D3	-342.985452	-342.902751	-342.895163	-342.933810
	PW6B95-D3	-343.517165	-343.434669	-343.427093	-343.465658
	B2PLYP	-342.876599	-342.794587	-342.786978	-342.825621
	CCSD(T)-freq//B2PLYP	-342.500128			
	CCSD(T)//B2PLYP+B2PLYP freq	-342.500128	-342.418116	-342.410507	-342.449150
	jChS	-342.958489	-342.875993	-342.868417	-342.906982
	SVECV-f12				

Radical H-abstraction from CH3		E	E+ZPE	H	G
MG rad 2	Gas phase				
	CBS-QB3	-266.164105	-266.112592	-266.106463	-266.141335
	M06-2X-D3	-266.485876	-266.432909	-266.426837	-266.461627
	PW6B95-D3	-266.907098	-266.854525	-266.848393	-266.883356
	B2PLYP	-266.401694	-266.349282	-266.343118	-266.378167
	CCSD(T)-freq//B2PLYP	-266.098824			
	CCSD(T)//B2PLYP+B2PLYP freq	-266.098824	-266.046412	-266.040248	-266.075297
	jChS	-266.463831	-266.411258	-266.405126	-266.440089
	SVECV-f12	-266.448586	-266.395619	-266.389547	-266.424337
	Bulk				
	CBS-QB3	-266.170566	-266.118988	-266.112838	-266.147809
	M06-2X-D3	-266.493545	-266.44053	-266.43443	-266.46938
	PW6B95-D3	-266.914388	-266.861756	-266.855589	-266.890733
	B2PLYP	-266.409168	-266.356709	-266.350506	-266.385770
	CCSD(T)-freq//B2PLYP	-266.105516			
	CCSD(T)//B2PLYP+B2PLYP freq	-266.105516	-266.053057	-266.046854	-266.082118
	jChS	-266.470521	-266.417889	-266.411722	-266.446866
	SVECV-f12				

H-Abstraction from the exposed OH of CH(OH)2		E	E+ZPE	H	G
GlDiol(.) rad 2 from C(OH)2	Gas phase				
	CBS-QB3	-342.551646	-342.474617	-342.464557	-342.512407
	M06-2X-D3	-342.926967	-342.846744	-342.838948	-342.878329
	PW6B95-D3	-343.462138	-343.382305	-343.374517	-343.413673
	B2PLYP	wrong (opens)			
	CCSD(T)-freq//B2PLYP				
	CCSD(T)//B2PLYP+B2PLYP freq				
	jChS	-342.903551	-342.823718	-342.815930	-342.855086
	SVECV-f12	-342.881567	-342.801344	-342.793548	-342.832929
	Bulk				
	CBS-QB3	-342.926967	-342.846744	-342.838948	-342.878329
mostly open structures at	M06-2X-D3	-342.954676	-342.875810	-342.866115	-342.911550
all levels	PW6B95-D3				
	B2PLYP	wrong (opens)			
	CCSD(T)-freq//B2PLYP				
	CCSD(T)//B2PLYP+B2PLYP freq				
	jChS				
	SVECV-f12				

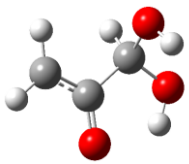
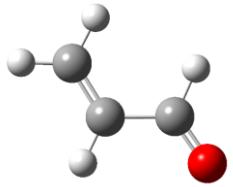
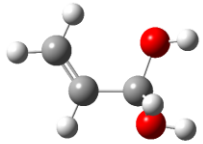
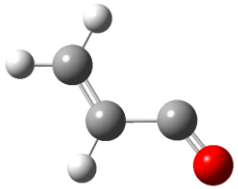
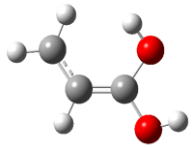
H-Abstraction from the CH3		E	E+ZPE	H	G
GlDiol(.) rad 2 from COH	Gas phase				
	CBS-QB3	-342.543029	-342.463015	-342.455431	-342.494025
	M06-2X-D3	-342.941951	-342.860126	-342.852562	-342.891042
	PW6B95-D3	-343.470091	-343.388486	-343.380979	-343.419333
	B2PLYP	-342.833116	-342.751884	-342.744323	-342.782802
	CCSD(T)-freq//B2PLYP	-342.462047			
	CCSD(T)//B2PLYP+B2PLYP freq	-342.462047	-342.380815	-342.373254	-342.411733
	jChS	-342.918354	-342.836749	-342.829242	-342.867596
	SVECV-f12	-342.896206	-342.814381	-342.806817	-342.845297
	Bulk				
	CBS-QB3	-342.553148	-342.473122	-342.465559	-342.504074
	M06-2X-D3	-342.952213	-342.870426	-342.862878	-342.901326
	PW6B95-D3	-343.479974	-343.398381	-343.390891	-343.429187
	B2PLYP	-342.843286	-342.762089	-342.754549	-342.793009
	CCSD(T)-freq//B2PLYP	-342.471733			
	CCSD(T)//B2PLYP+B2PLYP freq	-342.471733	-342.390536	-342.382996	-342.421456
	jChS	-342.928007	-342.846414	-342.838924	-342.877220
	SVECV-f12				

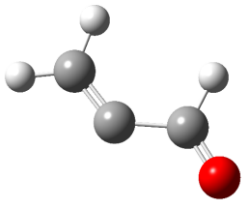
Table SI6. Energies at different levels of calculation for the radical and closed-shell species related to acrolein (**AC**)

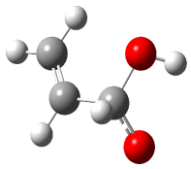
ACROLEINE	Gas phase				
	CBS-QB3	-191.660234	-191.599762	-191.594432	-191.626061
	M06-2X-D3	-191.901529	-191.839600	-191.834309	-191.865882
	PW6B95-D3	-192.218849	-192.157089	-192.151785	-192.183367
	B2PLYP	-191.836269	-191.774868	-191.769556	-191.801166
	CCSD(T)-freq//B2PLYP	-191.610947			
	CCSD(T)//B2PLYP+B2PLYP freq	-191.610947	-191.549546	-191.544234	-191.575844
	jChS	-191.892961	-191.831201	-191.825897	-191.857479
	SVECV-f12	-191.878585	-191.816656	-191.811365	-191.842938
	Bulk				
	CBS-QB3	-191.666399	-191.605898	-191.600562	-191.632207
	M06-2X-D3	-191.908317	-191.846340	-191.841051	-191.872622
	PW6B95-D3	-192.225525	-192.163684	-192.158387	-192.189956
	B2PLYP	-191.842916	-191.781414	-191.776107	-191.807711
	CCSD(T)-freq//B2PLYP	-191.616921			
	CCSD(T)//B2PLYP+B2PLYP freq	-191.616921	-191.555419	-191.550112	-191.581716
	jChS	-191.898937	-191.837096	-191.831799	-191.863368
	SVECV-f12				

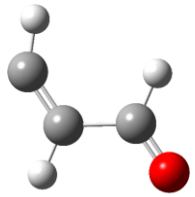
Acdiol	Gas phase				
	CBS-QB3	-268.025431	-267.937025	-267.930018	-267.966061
	M06-2X-D3	-268.342723	-268.252319	-268.245361	-268.281329
	PW6B95-D3	-268.766157	-268.676148	-268.669105	-268.705299
	B2PLYP	-268.252159	-268.162624	-268.155567	-268.191814
	CCSD(T)-freq//B2PLYP	-267.959808			
	CCSD(T)//B2PLYP+B2PLYP freq	-267.959808	-267.870273	-267.863216	-267.899463
	jChS	-268.332397	-268.242388	-268.235345	-268.271539
	SVECV-f12	-268.312061	-268.221657	-268.214699	-268.250667
	Bulk				
	CBS-QB3	-268.036587	-267.948025	-267.941171	-267.976804
	M06-2X-D3	-268.353938	-268.263408	-268.256615	-268.292159
	PW6B95-D3	-268.776840	-268.686590	-268.679760	-268.715359
	B2PLYP	-268.262929	-268.173180	-268.166326	-268.202008
	CCSD(T)-freq//B2PLYP	-267.970263			
	CCSD(T)//B2PLYP+B2PLYP freq	-267.970263	-267.880514	-267.873660	-267.909342
	jChS	-268.343112	-268.252862	-268.246032	-268.281631
	SVECV-f12				

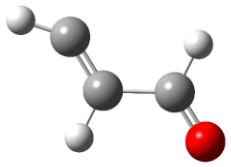
Radical H-abstraction from CHO		E	E+ZPE	H	G
AC rad 1	Gas phase				
	CBS-QB3	-191.005891	-190.957601	-190.952240	-190.984514
	M06-2X-D3	-191.249605	-191.200201	-191.194864	-191.227126
	PW6B95-D3	-191.566167	-191.516844	-191.511499	-191.543765
	B2PLYP	-191.186869	-191.137842	-191.132501	-191.164760
	CCSD(T)-freq//B2PLYP	-190.957629			
	CCSD(T)//B2PLYP+B2PLYP freq	-190.957629	-190.908602	-190.903261	-190.935520
	jChS	-191.237027	-191.187704	-191.182359	-191.214625
	SVECV-f12	-191.224077	-191.174673	-191.169336	-191.201598
	Bulk				
	CBS-QB3	-191.009601	-190.961302	-190.955955	-190.988190
	M06-2X-D3	-191.254293	-191.204901	-191.199580	-191.231799
	PW6B95-D3	-191.570826	-191.521497	-191.516170	-191.548384
	B2PLYP	-191.191302	-191.142254	-191.136928	-191.169145
	CCSD(T)-freq//B2PLYP	-190.961403			
	CCSD(T)//B2PLYP+B2PLYP freq	-190.961403	-190.912355	-190.907029	-190.939246
	jChS	-191.240806	-191.191477	-191.186150	-191.218364
	SVECV-f12				

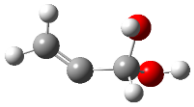
abstraction from CH in CH(OH2)		E	E+ZPE	H	G
ACDiol(.)	Gas phase				
	CBS-QB3	-267.390377	-267.315418	-267.308490	-267.344547
	M06-2X-D3	-267.713503	-267.637061	-267.630038	-267.666705
	PW6B95-D3	-268.138454	-268.062304	-268.055086	-268.093771
	B2PLYP	-267.622959	-267.547169	-267.539999	-267.577486
	CCSD(T)-freq//B2PLYP	-267.323357			
	CCSD(T)//B2PLYP+B2PLYP freq	-267.323357	-267.247567	-267.240397	-267.277884
	jChS	-267.695022	-267.618872	-267.611654	-267.650339
	SVECV-f12	-267.676361	-267.599919	-267.592896	-267.629563
	Bulk				
	CBS-QB3	-267.394729	-267.320147	-267.313248	-267.349295
	M06-2X-D3	-267.720523	-267.644421	-267.637398	-267.673948
	PW6B95-D3	-268.145124	-268.069339	-268.063008	-268.097964
	B2PLYP	-267.629699	-267.554116	-267.547017	-267.583802
	CCSD(T)-freq//B2PLYP	-267.329843			
	CCSD(T)//B2PLYP+B2PLYP freq	-267.329843	-267.254260	-267.247161	-267.283946
	jChS	-267.701472	-267.625687	-267.619356	-267.654312
	SVECV-f12				

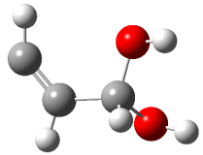
Radical H-abstraction from CH		E	E+ZPE	H	G
AC rad 2	Gas phase				
	CBS-QB3	-190.969713	-190.923555	-190.917836	-190.951094
	M06-2X-D3	-191.214758	-191.167015	-191.161428	-191.194283
	PW6B95-D3	-191.529332	-191.482167	-191.476462	-191.509777
	B2PLYP	-191.149132	-191.101841	-191.096219	-191.129168
	CCSD(T)-freq//B2PLYP	-190.920127			
	CCSD(T)//B2PLYP+B2PLYP freq	-190.920127	-190.872836	-190.867214	-190.900163
	jChS	-191.198218	-191.151053	-191.145348	-191.178663
	SVECV-f12	-191.187474	-191.139731	-191.134144	-191.166999
	Bulk				
	CBS-QB3	-190.976089	-190.929804	-190.924106	-190.957266
	M06-2X-D3	-191.221728	-191.173936	-191.168351	-191.201186
	PW6B95-D3	-191.536235	-191.488958	-191.483267	-191.516502
	B2PLYP	-191.155904	-191.108068	-191.102733	-191.134977
	CCSD(T)-freq//B2PLYP	-190.926753			
	CCSD(T)//B2PLYP+B2PLYP freq	-190.926753	-190.878917	-190.873582	-190.905826
	jChS	-191.204900	-191.157623	-191.151932	-191.185167
	SVECV-f12				

H-Abstraction from the exposed OH of CH(OH)2		E	E+ZPE	H	G
ACDiol(.) rad 2 from C(OH)2	Gas phase				
	CBS-QB3	-267.348091	-267.274300	-267.267372	-267.304337
	M06-2X-D3	-267.669901	-267.593673	-267.587044	-267.623037
	PW6B95-D3	-268.095934	-268.020519	-268.013735	-268.050157
	B2PLYP	-267.580811	-267.505406	-267.498665	-267.534965
	CCSD(T)-freq//B2PLYP	-267.284886			
	CCSD(T)//B2PLYP+B2PLYP freq	-267.284886	-267.209481	-267.202740	-267.239040
	jChS	-267.653056	-267.577641	-267.570857	-267.607279
	SVECV-f12	-267.634822	-267.558594	-267.551965	-267.587958
	Bulk				
	CBS-QB3	-267.354153	-267.280437	-267.273586	-267.310185
	M06-2X-D3	-267.676564	-267.600317	-267.593685	-267.629758
	PW6B95-D3	-268.102016	-268.026560	-268.019762	-268.056423
	B2PLYP	-267.587260	-267.511704	-267.504945	-267.541512
	CCSD(T)-freq//B2PLYP	-267.291296			
	CCSD(T)//B2PLYP+B2PLYP freq	-267.291296	-267.215740	-267.208981	-267.245548
	jChS	-267.659389	-267.583933	-267.577135	-267.613796
	SVECV-f12				

Radical H-abstraction from CH2 cis		E	E+ZPE	H	G
AC rad3	Gas phase				
	CBS-QB3	-190.970813	-190.923999	-190.918624	-190.950929
	M06-2X-D3	-191.216055	-191.167856	-191.162555	-191.194730
	PW6B95-D3	-191.529549	-191.481726	-191.476373	-191.508642
	B2PLYP	-191.149630	-191.101867	-191.096516	-191.128801
	CCSD(T)-freq//B2PLYP	-190.921611			
	CCSD(T)//B2PLYP+B2PLYP freq	-190.921611	-190.873848	-190.868497	-190.900782
	jChS	-191.199733	-191.151910	-191.146557	-191.178826
	SVECV-f12	-191.188676	-191.140477	-191.135176	-191.167351
	Bulk				
	CBS-QB3	-190.976508	-190.929624	-190.924260	-190.956538
	M06-2X-D3	-191.222510	-191.174256	-191.168967	-191.201114
	PW6B95-D3	-191.535743	-191.487839	-191.482500	-191.514735
	B2PLYP	-191.155904	-191.108068	-191.102733	-191.134977
	CCSD(T)-freq//B2PLYP	-190.927616			
	CCSD(T)//B2PLYP+B2PLYP freq	-190.927616	-190.879780	-190.874445	-190.906689
	jChS	-191.205779	-191.157875	-191.152536	-191.184771
	SVECV-f12				

Radical H-abstraction from CH2 trans		E	E+ZPE	H	G
AC rad4	Gas phase				
	CBS-QB3	-190.970852	-190.924214	-190.918853	-190.951044
	M06-2X-D3	-191.216228	-191.168228	-191.162916	-191.195034
	PW6B95-D3	-191.529498	-191.481870	-191.476529	-191.508687
	B2PLYP	-191.149767	-191.102200	-191.096860	-191.129037
	CCSD(T)-freq//B2PLYP	-190.921721			
	CCSD(T)//B2PLYP+B2PLYP freq	-190.921721	-190.874154	-190.868814	-190.900991
	jChS	-191.199788	-191.152160	-191.146819	-191.178977
	SVECV-f12	-191.188696	-191.140696	-191.135384	-191.167502
	Bulk				
	CBS-QB3	-190.976470	-190.929801	-190.924445	-190.956624
	M06-2X-D3	-191.222622	-191.174611	-191.169302	-191.201415
	PW6B95-D3	-191.535708	-191.488027	-191.482695	-191.514834
	B2PLYP	-191.156005	-191.108399	-191.103069	-191.135223
	CCSD(T)-freq//B2PLYP	-190.927652			
	CCSD(T)//B2PLYP+B2PLYP freq	-190.927652	-190.880046	-190.874716	-190.906870
	jChS	-191.205754	-191.158073	-191.152741	-191.184880
	SVECV-f12				

H-Abstraction from the intermediate CH		E	E+ZPE	H	G
ACDiol(.) rad 3 from CH	Gas phase				
	CBS-QB3	-267.337992	-267.263323	-267.256230	-267.292960
	M06-2X-D3	-267.659776	-267.583130	-267.576121	-267.612684
	PW6B95-D3	-268.080246	-268.004157	-267.997059	-268.033807
	B2PLYP	-267.568966	-267.493144	-267.486058	-267.522787
	CCSD(T)-freq//B2PLYP	-267.273454			
	CCSD(T)//B2PLYP+B2PLYP freq	-267.273454	-267.197632	-267.190546	-267.227275
	jChS	-267.642601	-267.566512	-267.559414	-267.596162
	SVECV-f12	-267.624399	-267.547753	-267.540744	-267.577307
	Bulk				
	CBS-QB3	-267.348780	-267.274267	-267.267090	-267.304042
	M06-2X-D3	-267.670556	-267.594078	-267.587025	-267.623715
	PW6B95-D3	-268.090415	-268.014545	-268.007309	-268.044529
	B2PLYP	-267.580129	-267.504676	-267.497482	-267.534635
	CCSD(T)-freq//B2PLYP	-267.284249			
	CCSD(T)//B2PLYP+B2PLYP freq	-267.284249	-267.208796	-267.201602	-267.238755
	jChS	-267.652672	-267.576802	-267.569566	-267.606786
	SVECV-f12				

H-Abstraction from the final CH2 cis		E	E+ZPE	H	G
ACDiol(.) rad 4 from CH2 cis	Gas phase				
	CBS-QB3	-267.335800	-267.261115	-267.254042	-267.290875
	M06-2X-D3	-267.657519	-267.580969	-267.573955	-267.610742
	PW6B95-D3	-268.076773	-268.000741	-267.993626	-268.030689
	B2PLYP	-267.565971	-267.490248	-267.483136	-267.520184
	CCSD(T)-freq//B2PLYP	-267.271384			
	CCSD(T)//B2PLYP+B2PLYP freq	-267.271384	-267.195661	-267.188549	-267.225597
	jChS	-267.640461	-267.564429	-267.557314	-267.594377
	SVECV-f12	-267.621508	-267.544958	-267.537944	-267.574731
	Bulk				
	CBS-QB3	-267.347427	-267.272551	-267.265629	-267.302017
	M06-2X-D3	-267.669053	-267.592388	-267.585536	-267.621817
	PW6B95-D3	-268.087919	-268.011617	-268.004724	-268.041056
	B2PLYP	-267.577201	-267.501221	-267.494326	-267.530686
	CCSD(T)-freq//B2PLYP	-267.282548			
	CCSD(T)//B2PLYP+B2PLYP freq	-267.282548	-267.206568	-267.199673	-267.236033
	jChS	-267.651646	-267.575344	-267.568451	-267.604783
	SVECV-f12				

H-Abstraction from the final CH2 trans		E	E+ZPE	H	G
ACDiol(.) rad 4 from CH2 cis	Gas phase				
	CBS-QB3	-267.335800	-267.261115	-267.254042	-267.290875
	M06-2X-D3	-267.656468	-267.580377	-267.573148	-267.610644
	PW6B95-D3	-268.079174	-268.003324	-267.996308	-268.032899
	B2PLYP	-267.568595	-267.493014	-267.486021	-267.522564
	CCSD(T)-freq//B2PLYP	-267.273691			
	CCSD(T)//B2PLYP+B2PLYP freq	-267.273691	-267.198110	-267.191117	-267.227660
	jChS	-267.642838	-267.566988	-267.559972	-267.596563
	SVECV-f12	-267.620902	-267.544811	-267.537582	-267.575078
	Bulk				
	CBS-QB3	-267.346966	-267.272377	-267.265401	-267.301925
	M06-2X-D3	-267.668975	-267.592497	-267.585603	-267.621971
	PW6B95-D3	-268.087781	-268.012052	-268.005016	-268.041662
	B2PLYP	-267.577869	-267.502569	-267.495420	-267.532507
	CCSD(T)-freq//B2PLYP	-267.282892			
	CCSD(T)//B2PLYP+B2PLYP freq	-267.282892	-267.207592	-267.200443	-267.237530
	jChS	-267.651451	-267.575722	-267.568686	-267.605332
	SVECV-f12				

Table SI7. Cartesian coordinates for the optimized geometries of the molecules considered in this study. See Figs. 1-3 in the main text for the structure of the species.

Formaldehyde (**F**)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C 0.00000000 -0.52550500 0.00000000 O 0.00000000 0.67051600 0.00000000 H 0.93836000 -1.10554800 0.00000000 H -0.93835900 -1.10554900 0.00000000	C 0.00000000 -0.52904400 0.00000000 O 0.00000000 0.67296300 0.00000000 H 0.93711400 -1.10472200 0.00000000 H -0.93711300 -1.10472100 0.00000000
PW6B95-D3/jun-cc-pVTZ	C 0.00000000 0.00000000 -0.52476400 O 0.00000000 0.00000000 0.67010800 H 0.00000000 -0.93518000 -1.10613900 H 0.00000000 0.93518000 -1.10613900	C 0.00000000 0.00000000 -0.52821900 O 0.00000000 0.00000000 0.67242300 H 0.00000000 0.93381200 -1.10503300 H 0.00000000 -0.93381200 -1.10503300
B2PLYP/aug-cc-pVTZ	C 0.00000000 -0.53011400 0.00000000 O 0.00000000 0.67551100 0.00000000 H 0.93628500 -1.11170300 0.00000000 H -0.93628400 -1.11170300 0.00000000	C 0.00000000 -0.55070600 0.00000000 O 0.00000000 0.70369200 0.00000000 H 0.93936500 -1.16265100 0.00000000 H -0.93936500 -1.16265000 0.00000000

Formaldehyde radical (*F rad*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C 0.06171500 0.58080600 0.00000000 O 0.06171500 -0.58705600 0.00000000 H -0.86401600 1.21161200 0.00000000	C 0.06091300 0.58177400 0.00000000 O 0.06091300 -0.58911500 0.00000000 H -0.85278100 1.22227900 0.00000000
PW6B95-D3/jun-cc-pVTZ	C 0.06151300 0.58080900 0.00000000 O 0.06151300 -0.58705500 0.00000000 H -0.86118300 1.21158600 0.00000000	C 0.06075700 0.58179000 0.00000000 O 0.06075700 -0.58890400 0.00000000 H -0.85060300 1.22049500 0.00000000
B2PLYP/aug-cc-pVTZ	C 0.06143400 0.58629800 0.00000000 O 0.06143400 -0.59220400 0.00000000 H -0.86008000 1.21984500 0.00000000	C 0.06426700 0.61988400 0.00000000 O 0.06426700 -0.61768600 0.00000000 H -0.89973900 1.22218100 0.00000000

Methanediol (*Fdiol*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C 0.00000300 0.53130000 0.00000200 O 1.15953500 -0.24679200 -0.09416300 H 0.00415300 1.15780500 0.89270500 H -0.00412800 1.15786500 -0.89266000	C -0.00000100 0.52888900 -0.00000700 O 1.16088300 -0.25113900 -0.10185200 H 0.01827200 1.15219700 0.89328000 H -0.01827000 1.15217800 -0.89330900

	O -1.15953700 -0.24679200 0.09415900 H 1.23502500 -0.77742400 0.70422900 H -1.23505600 -0.77737400 -0.70425900	O -1.16089100 -0.25112800 0.10185400 H 1.28334300 -0.72973500 0.72440300 H -1.28327600 -0.72983900 -0.72434500
PW6B95-D3/jun-cc-pVTZ	C 0.00000200 0.52708900 -0.00000100 O 1.16048600 -0.24610800 -0.09489900 H 0.00182200 1.15237300 0.88967000 H -0.00182900 1.15236400 -0.88967700 O -1.16048800 -0.24610800 0.09490000 H 1.24442500 -0.76476700 0.70668900 H -1.24441600 -0.76477900 -0.70668200	C 0.00000000 0.52437300 0.00000000 O -1.16187100 -0.25082800 0.10300100 H -0.01703700 1.14618500 -0.89024700 H 0.01703700 1.14618500 0.89024700 O 1.16187100 -0.25082800 -0.10300100 H -1.29599900 -0.71267800 -0.72702700 H 1.29600000 -0.71267800 0.72702700
B2PLYP/aug-cc-pVTZ	C 0.00000200 0.53071400 0.00000000 O 1.16850200 -0.24756800 -0.09532900 H 0.00120600 1.15423000 0.89309700 H -0.00120600 1.15423100 -0.89309700 O -1.16850300 -0.24756800 0.09532900 H 1.25022200 -0.76583100 0.71192000 H -1.25022800 -0.76582500 -0.71192300	C -0.00000500 0.54813800 -0.00000400 O 1.21204200 -0.25771900 -0.09415300 H -0.00933800 1.19944400 0.90798300 H 0.00933800 1.19942000 -0.90800300 O -1.21204500 -0.25771700 0.09415400 H 1.18099500 -0.78206700 0.78025200 H -1.18093900 -0.78213300 -0.78020700

Methanediol radical on C (*Fdiol rad1*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -0.00389000 0.50629400 -0.14765400 O 1.07752800 -0.30969300 0.07999300 H 1.87223600 0.11885900 -0.24735300 O -1.17477500 -0.14000400 0.05386900 H -1.07914400 -1.04793600 -0.25369500 H 0.00822900 1.48889100 0.31607600	C 0.00217700 0.49956400 -0.15639100 O 1.07734300 -0.31971600 0.06770900 H 1.88825200 0.15302600 -0.14670800 O -1.17723600 -0.13273500 0.07010800 H -1.13597900 -1.02081300 -0.30463600 H 0.03380600 1.49000900 0.28715500
PW6B95-D3/jun-cc-pVTZ	C -0.00426200 0.50468600 -0.14851500 O 1.07636100 -0.30937100 0.07949800 H 1.86666500 0.12415600 -0.24306900 O -1.17238900 -0.13973800 0.05471700 H -1.07886100 -1.04331200 -0.25645700 H 0.00599700 1.48392200 0.31690100	C -0.00165300 0.49814800 0.15632500 O -1.07618200 -0.31883100 -0.06718100 H -1.88186100 0.15706400 0.14531400 O 1.17525000 -0.13234500 -0.06880100 H 1.13039900 -1.02078800 0.29583700 H -0.03116000 1.48424300 -0.29124200
B2PLYP/aug-cc-pVTZ	C -0.00454600 0.50764500 -0.15075300 O 1.08361200 -0.31149200 0.08032100 H 1.87481100 0.12943400 -0.24346700 O -1.17927900 -0.14090300 0.05719400 H -1.08738100 -1.04329500 -0.27035700 H 0.00518000 1.48715400 0.31822600	C 0.00199000 0.52419000 -0.17228500 O 1.11360300 -0.34224300 0.06002900 H 1.90954900 0.27705600 -0.07427100 O -1.22776800 -0.13879500 0.06775300 H -1.03017400 -1.08444400 -0.25916800 H 0.02200800 1.51054800 0.34488800

Methanediol radical on O (*Fdiol rad2*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -0.10016300 0.45686500 0.04332700 O -1.17069700 -0.34240300 -0.04095000 H -0.15274800 1.24115800 -0.72537300 H -0.20442800 0.97197500 1.02105100 O 1.14660600 -0.15711200 -0.08450600 H 1.15088500 -0.95820400 0.44801400	C -0.10112700 0.45232000 0.04669300 O -1.17921700 -0.34389800 -0.03389100 H -0.17763800 1.22955300 -0.72738000 H -0.17418900 0.97192300 1.02004700 O 1.13703000 -0.17518400 -0.11640100 H 1.29608200 -0.76273300 0.62951000
PW6B95-D3/jun-cc-pVTZ	C -0.10673700 0.44849300 0.02829000 O -1.16140600 -0.33959300 -0.03265300 H -0.15247700 1.22760900 -0.74859000 H -0.21237100 1.00558700 0.98642900 O 1.15219900 -0.14612700 -0.05460500 H 1.07892600 -1.03839000 0.29048300	C -0.10699900 0.44281600 0.04594000 O -1.17212700 -0.34087800 -0.04002800 H -0.16797400 1.24619500 -0.70150100 H -0.19180100 0.95906300 1.02402900 O 1.14302900 -0.15988800 -0.10361600 H 1.23455800 -0.85602400 0.55098000
B2PLYP/aug-cc-pVTZ	C -0.10465100 0.45310000 0.04321400 O -1.17635300 -0.34153100 -0.04209100 H -0.15020400 1.24353700 -0.71879100 H -0.21140900 0.96375000 1.02399000 O 1.15495600 -0.15479500 -0.08480500 H 1.16070400 -0.95528400 0.45068500	C -0.07381500 0.50133200 0.05232900 O -1.24984100 -0.34850100 -0.04155700 H -0.11080400 1.26854900 -0.75741200 H -0.14186100 1.02531900 1.04168300 O 1.19027600 -0.20672700 -0.11654100 H 1.17207800 -0.86003800 0.66653900

Acetaldehyde (**A**)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C 0.23324900 0.39800100 -0.00001900 C -1.16258200 -0.14774500 0.00012700 H 0.31442500 1.50205200 0.00000300 O 1.22509800 -0.27720200 -0.00014600 H -1.14795100 -1.23394000 0.00005000 H -1.69550400 0.22391800 0.87708300 H -1.69575600 0.22405100 -0.87661800	C 0.22697900 0.39826100 -0.00001400 C -1.16042600 -0.15042600 0.00012900 H 0.30741000 1.49867100 0.00002100 O 1.22840700 -0.27545400 -0.00015400 H -1.15243700 -1.23668300 0.00006000 H -1.69065000 0.22725500 0.87600400 H -1.69089700 0.22737600 -0.87554300
PW6B95-D3/jun-cc-pVTZ	C 0.23082000 0.39553100 -0.00001500 C -1.15923600 -0.14808400 0.00013100 H 0.30632800 1.49797700 0.00001600 O 1.22502700 -0.27496300 -0.00015400 H -1.15064000 -1.23092800 0.00005800 H -1.69258200 0.22392700 0.87313600	C 0.22448800 0.39562300 -0.00001100 C -1.15699400 -0.15069800 0.00013600 H 0.29947500 1.49411400 0.00003600 O 1.22833100 -0.27311300 -0.00016500 H -1.15518800 -1.23353600 0.00007100 H -1.68783300 0.22733500 0.87186200

	H -1.69282300 0.22404900 -0.87267300	H -1.68806500 0.22744200 -0.87140200
B2PLYP/aug-cc-pVTZ	C 0.22983800 0.39875100 -0.00002900	C 0.22368500 0.39910000 -0.00004300
	C -1.16564800 -0.14938300 0.00011600	C -1.16338300 -0.15183000 0.00009600
	H 0.30438600 1.50296900 -0.00003800	H 0.29860400 1.49915300 -0.00010200
	O 1.23318900 -0.27603100 -0.00012200	O 1.23605600 -0.27441400 -0.00008400
	H -1.15479600 -1.23525600 0.00002200	H -1.15835200 -1.23770100 -0.00002300
	H -1.69998500 0.22208200 0.87632400	H -1.69510500 0.22501200 0.87528700
	H -1.70025700 0.22224900 -0.87585400	H -1.69540800 0.22523000 -0.87481100

Acetaldehyde radical on C (*A rad1*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C 0.24752300 -0.43038800 -0.00001200	C 0.24122300 -0.42320800 -0.00001200
	C -1.16482900 0.09823100 -0.00000700	C -1.16544600 0.09797700 -0.00000700
	O 1.25320700 0.17345600 0.00000200	O 1.25847400 0.16925500 0.00000300
	H -1.17004900 1.18835300 -0.00042200	H -1.17428500 1.18770700 -0.00039100
	H -1.67569900 -0.29117600 0.87845400	H -1.67391600 -0.29485300 0.87848600
	H -1.67606400 -0.29188400 -0.87793400	H -1.67425800 -0.29551100 -0.87799900
PW6B95-D3/jun-cc-pVTZ	C 0.24320100 -0.42641900 0.00002500	C 0.23713100 -0.41960800 0.00003700
	C -1.16064200 0.09772100 0.00000700	C -1.16105400 0.09751200 0.00001200
	O 1.25320900 0.17139400 -0.00002800	O 1.25810900 0.16739900 -0.00004100
	H -1.17517400 1.18512700 -0.00014300	H -1.17885900 1.18436500 -0.00013900
	H -1.67288400 -0.29192100 0.87396300	H -1.67120400 -0.29536500 0.87384100
	H -1.67297300 -0.29217000 -0.87378400	H -1.67127400 -0.29561300 -0.87366500
B2PLYP/aug-cc-pVTZ	C 0.24293600 -0.43093900 -0.00000400	C 0.23719400 -0.42428400 -0.00001200
	C -1.16739300 0.09852700 -0.00000300	C -1.16778700 0.09828800 -0.00000600
	O 1.26083400 0.17300900 0.00000100	O 1.26533100 0.16913500 0.00000200
	H -1.17708200 1.18874300 -0.00015200	H -1.18029500 1.18794500 -0.00036600
	H -1.68136000 -0.28904000 0.87720300	H -1.67923900 -0.29221800 0.87738400
	H -1.68148800 -0.28929500 -0.87701700	H -1.67955400 -0.29283100 -0.87693200

Acetaldehyde radical on CH_3 (*A rad2*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C 0.13833600 0.40651100 -0.00003400	C 0.13370000 0.40673700 -0.00003600
	H 0.19901800 1.50611400 -0.00009100	H 0.19363800 1.50337600 -0.00012900
	O 1.16016500 -0.26659000 -0.00007000	O 1.16475600 -0.26530900 -0.00005900
	C -1.16614000 -0.16966100 0.00009500	C -1.16627800 -0.17126500 0.00008900
	H -1.26388500 -1.24512700 0.00017200	H -1.26976000 -1.24633700 0.00012600

	H -2.04962600 0.45063500 0.00011600	H -2.04646100 0.45260300 0.00015000
PW6B95-D3/jun-cc-pVTZ	C 0.13045700 0.40588100 -0.00003700 H 0.18859400 1.50260500 -0.00009200 O 1.16015400 -0.26374300 -0.00006700 C -1.15886000 -0.17118200 0.00009300 H -1.25580000 -1.24410300 0.00016100 H -2.04361100 0.44324500 0.00012700	C 0.12732300 0.40595700 -0.00004100 H 0.18515800 1.49961400 -0.00008900 O 1.16428000 -0.26288200 -0.00006500 C -1.15988100 -0.17229700 0.00009400 H -1.26318300 -1.24468500 0.00016300 H -2.04086500 0.44616900 0.00012800
B2PLYP/aug-cc-pVTZ	C 0.13758400 0.40513600 -0.00003000 H 0.19317000 1.50528700 -0.00009000 O 1.16556200 -0.26540200 -0.00007500 C -1.16992800 -0.17028000 0.00009800 H -1.27280900 -1.24469800 0.00016500 H -2.05079700 0.45349400 0.00012000	C 0.13259500 0.40586200 -0.00004300 H 0.18839200 1.50236900 -0.00014100 O 1.17025700 -0.26428100 -0.00004700 C -1.17007800 -0.17197700 0.00008400 H -1.27758400 -1.24598900 0.00011000 H -2.04797000 0.45455900 0.00016400

Ethanediol (*Adiol*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C 0.05566400 -0.01183200 0.37354000 O 0.89894400 -1.04224600 -0.03462900 C -1.36937100 -0.21139000 -0.10715200 H 0.10065300 -0.01999000 1.46554200 O 0.59975400 1.19567800 -0.12454600 H 1.02960500 -0.95482500 -0.98484400 H -0.07518600 1.87844900 -0.11987400 H -2.02146500 0.58355500 0.25804200 H -1.39035200 -0.21109100 -1.19819600 H -1.75059400 -1.16422100 0.25440100	C 0.05952000 -0.00350100 0.37099300 O 0.88837600 -1.05531400 -0.02604000 C -1.36838800 -0.18590700 -0.09728400 H 0.11469500 0.01068800 1.46146900 O 0.62373000 1.18892100 -0.15076500 H 0.81690300 -1.15310100 -0.98263900 H -0.01319000 1.90447100 -0.06160600 H -1.99246200 0.64174800 0.23915500 H -1.39409100 -0.22398200 -1.18756200 H -1.77549600 -1.11223400 0.30337600
PW6B95-D3/jun-cc-pVTZ	C 0.05738000 -0.01370200 0.37114300 O 0.92510800 -1.01968200 -0.04033600 C -1.36103300 -0.24017700 -0.10382300 H 0.10427000 -0.03185300 1.45954800 O 0.56977900 1.21283900 -0.11016100 H 1.04684100 -0.93012700 -0.98810300 H -0.14670600 1.84011200 -0.20309200 H -2.02699600 0.53449400 0.27005100 H -1.39352300 -0.23552800 -1.19105100 H -1.72106000 -1.19907900 0.25270400	C 0.06883300 0.00000000 0.36953200 O 0.74154000 -1.16400900 -0.04665300 C -1.37325000 0.00001800 -0.07348500 H 0.14954600 -0.00000100 1.45115500 O 0.74157300 1.16399000 -0.04665300 H 0.50357100 -1.35521200 -0.95677000 H 0.50361300 1.35519700 -0.95677200 H -1.88273400 0.88273000 0.29708200 H -1.42965500 0.00003300 -1.16159500 H -1.88274300 -0.88269800 0.29706100
B2PLYP/aug-cc-pVTZ	C 0.05381800 -0.01380900 0.37220100 O 0.91168100 -1.04070300 -0.03651400 C -1.37263600 -0.21967700 -0.10617200	C 0.05649500 -0.00541500 0.36956100 O 0.88926400 -1.06286600 -0.02561400 C -1.37397200 -0.18055500 -0.09748500

	H 0.10162700 -0.02765000 1.46286600 O 0.59589700 1.20801100 -0.11877300 H 1.03121400 -0.95811600 -0.98956700 H -0.09981700 1.87078700 -0.15216300 H -2.02709200 0.57133200 0.26263600 H -1.40386100 -0.22134100 -1.19612700 H -1.74978500 -1.17256200 0.25847900	H 0.11401700 0.00725200 1.45869500 O 0.63280400 1.19333800 -0.15133500 H 0.80613400 -1.17145000 -0.98082000 H -0.00431600 1.90957200 -0.05557800 H -1.99170000 0.65239100 0.23627900 H -1.40773300 -0.22569200 -1.18629100 H -1.78808200 -1.10003400 0.31086000

Ethanediol radical on C (*Adiol rad1*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -0.03666300 -0.00836700 -0.28472100 C 1.41619700 -0.04798900 0.04626900 O -0.75753500 1.10008200 0.11170700 H 1.56118800 -0.07148400 1.13269300 H 1.92571500 0.82777900 -0.35287200 H 1.86768900 -0.93877000 -0.38383500 H -0.35744300 1.88781000 -0.26467900 O -0.69655700 -1.14719500 0.05564900 H -1.64162200 -0.99029800 -0.03944100	C -0.03916400 -0.00784200 -0.28272200 C 1.41175300 -0.10331500 0.04214200 O -0.70993600 1.13201000 0.10321200 H 1.56071100 -0.14432600 1.12784100 H 1.94648200 0.76156000 -0.34613500 H 1.83506000 -1.00214900 -0.40024900 H -0.22560700 1.90528800 -0.20368200 O -0.74856200 -1.11893400 0.06758600 H -1.68420200 -0.95803900 -0.10068300
PW6B95-D3/jun-cc-pVTZ	C -0.03482500 -0.00865400 -0.28135400 C 1.41368600 -0.04016500 0.04563300 O -0.76467900 1.09337300 0.11124100 H 1.56857000 -0.06312400 1.12856200 H 1.91760000 0.83451300 -0.35336800 H 1.87001500 -0.92418200 -0.38470200 H -0.36956600 1.87922100 -0.26616700 O -0.68893800 -1.14844300 0.05514700 H -1.63084700 -0.99295300 -0.04109600	C -0.03723100 -0.00806200 -0.27958700 C 1.40968700 -0.09198500 0.04202300 O -0.71984600 1.12362800 0.10324000 H 1.56739300 -0.13243100 1.12431000 H 1.93715300 0.77315300 -0.34549100 H 1.84016900 -0.98337100 -0.40004800 H -0.24647600 1.89700200 -0.20967500 O -0.73780300 -1.12271800 0.06526300 H -1.67178100 -0.96135100 -0.09173200
B2PLYP/aug-cc-pVTZ	C -0.03454600 -0.00816400 -0.28753300 C 1.41959200 -0.03069100 0.04657100 O -0.77650700 1.09473500 0.11450700 H 1.56642700 -0.05427200 1.13273600 H 1.91929300 0.85128800 -0.34943000 H 1.88460600 -0.91332600 -0.38473600 H -0.39140000 1.88451300 -0.27641800 O -0.68115800 -1.15998000 0.05700200 H -1.62788200 -1.01311300 -0.04845000	C -0.03683200 -0.00766600 -0.28563200 C 1.41586800 -0.08554200 0.04296600 O -0.72951600 1.12679100 0.10597400 H 1.56586100 -0.12641000 1.12848800 H 1.94113000 0.78552700 -0.34226800 H 1.85281300 -0.97694000 -0.39992600 H -0.26073500 1.90451400 -0.21686000 O -0.73326000 -1.13290900 0.06735700 H -1.67107700 -0.97850500 -0.10008400

Ethanediol radical on O (*Adiol rad2*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -0.00344100 0.01672000 0.37115500 O -0.69506200 1.15507200 -0.06019800 C 1.40818800 0.00245300 -0.10213300 H -0.05075800 0.05826300 1.46178600 O -0.71288100 -1.10607000 -0.11454700 H -0.73484800 1.12741500 -1.02257700 H -0.17006800 -1.89104700 -0.00018700 H 1.61276500 -0.30486500 -1.11871900 H 2.17797100 0.50318800 0.46353200	C -0.00504600 0.01187700 0.36928300 O -0.69940600 1.15799300 -0.05657400 C 1.40510400 -0.00164000 -0.09792000 H -0.05794100 0.03941200 1.45922000 O -0.72160800 -1.10604400 -0.12622300 H -0.58525200 1.24077300 -1.01093300 H -0.18683000 -1.89668000 0.00056500 H 1.61750400 -0.31697800 -1.10988100 H 2.18029200 0.45645500 0.49522400
PW6B95-D3/jun-cc-pVTZ	C 0.00211300 -0.01466200 0.37062100 O 0.68930700 -1.15622400 -0.06077400 C -1.40073900 -0.00016200 -0.10208700 H 0.05041500 -0.06284500 1.45751300 O 0.71830400 1.10470700 -0.10925800 H 0.71027900 -1.13867800 -1.02074400 H 0.15545900 1.87748500 -0.04587400 H -1.60750500 0.29087400 -1.12019800 H -2.17778000 -0.46575300 0.47835900	C 0.00311000 -0.01096500 0.36794700 O 0.70914900 -1.15031900 -0.05738400 C -1.39875700 -0.01382800 -0.09842400 H 0.05641300 -0.04423700 1.45433500 O 0.71196100 1.11344400 -0.12109000 H 0.58782600 -1.23865400 -1.00686600 H 0.15187800 1.88756400 -0.03298600 H -1.61820500 0.29308400 -1.10846800 H -2.17290600 -0.45400300 0.50464500
B2PLYP/aug-cc-pVTZ	C 0.00074300 0.01556100 0.37150200 O -0.69814500 1.16052900 -0.05958400 C 1.40947000 0.00418200 -0.10359200 H -0.04944600 0.06198200 1.46027400 O -0.71924900 -1.11288800 -0.11166400 H -0.71919100 1.14287200 -1.02390900 H -0.15774600 -1.89058500 -0.03027200 H 1.61871300 -0.28706200 -1.12321600 H 2.18555200 0.47320100 0.47965200	C -0.00017200 0.01131600 0.36938700 O -0.70878400 1.15983200 -0.05562400 C 1.40716800 0.00707600 -0.09995600 H -0.05560500 0.04203900 1.45750600 O -0.72161400 -1.11605500 -0.12466400 H -0.58322600 1.25099400 -1.00869000 H -0.16997700 -1.89936500 -0.01682600 H 1.62508800 -0.29392800 -1.11425000 H 2.18492500 0.43969600 0.50797200

Ethanediol radical on CH_3 (*Adiol rad3*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C 0.08924200 0.08634600 0.35114400 O 1.13584000 -0.76922400 -0.02385000 C -1.28471100 -0.45671000 -0.09784600 H 0.11301700 0.12999300 1.44835400 O 0.18190200 1.33269400 -0.14965400 H 1.30835000 -0.63888200 -0.96192600	C 0.09180200 0.09951600 0.34174500 O 1.14433000 -0.75841300 -0.01722400 C -1.28142500 -0.45454500 -0.07908700 H 0.12763100 0.17880600 1.43669000 O 0.19586500 1.34419900 -0.17244600 H 1.07971200 -0.95899400 -0.95782300

	H -2.08707000 0.15541400 0.30409500 H -1.33452900 -0.45376800 -1.18568400 H -1.36889000 -1.47833100 0.26339600	H -2.07804600 0.17481900 0.30629400 H -1.33928300 -0.49051600 -1.16620800 H -1.37382900 -1.46022800 0.32245600
PW6B95-D3/jun-cc-pVTZ	C 0.08183000 0.09204000 0.29488000 O 0.91125700 -0.97265400 -0.08861400 C -1.35791800 -0.26537400 -0.08774200 H 0.10962300 0.19939100 1.40237700 O 0.44067900 1.28806300 -0.14647100 H 1.79313000 -0.61935000 -0.21938300 H -2.03910800 0.47704700 0.30754800 H -1.43099500 -0.29742100 -1.16849100 H -1.59160700 -1.24293600 0.31579600	C 0.08336800 0.09288300 0.29405100 O 0.94316100 -0.93628600 -0.12337300 C -1.34787600 -0.30770500 -0.07645000 H 0.12377700 0.18931900 1.39922400 O 0.38746700 1.30623300 -0.15258600 H 1.84858600 -0.64142600 -0.00264100 H -2.04661300 0.41642100 0.32082700 H -1.43203700 -0.34907400 -1.15630700 H -1.55168600 -1.28588100 0.34096700
B2PLYP/aug-cc-pVTZ	C 0.08735600 0.08871400 0.34797700 O 1.13344700 -0.78490900 -0.02775800 C -1.29516800 -0.45430700 -0.10463300 H 0.10014800 0.12065200 1.44641700 O 0.18553600 1.33217400 -0.14222200 H 1.41328300 -0.53619600 -0.91568000 H -2.09484600 0.15112100 0.31127300 H -1.35172000 -0.44145900 -1.19050900 H -1.37185800 -1.47868000 0.24827900	C 0.09021800 0.10439200 0.33868900 O 1.16343900 -0.74640800 -0.01612900 C -1.28051500 -0.47423500 -0.07966500 H 0.12442700 0.17570300 1.43365700 O 0.17264900 1.34986900 -0.17085800 H 1.11249300 -0.93274100 -0.96130500 H -2.08516700 0.14030900 0.31138300 H -1.34592400 -0.51159700 -1.16512600 H -1.35274700 -1.48030600 0.32314100

Glycolaldehyde (**G**)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -0.82646800 0.48388700 -0.00000200 C 0.66707000 0.64716700 0.00000000 H -1.42533500 1.41034600 0.00000900 O -1.34636100 -0.59920700 0.00000000 H 0.93739300 1.24415000 0.88000700 O 1.32849600 -0.57809300 0.00000000 H 0.93740000 1.24414600 -0.88000800 H 0.64984700 -1.26656900 0.00000800	C -0.82576600 0.48682500 0.00000900 C 0.66388000 0.65256100 -0.00000600 H -1.42490100 1.40863900 0.00002600 O -1.34167200 -0.60348900 -0.00000400 H 0.93240800 1.24730800 0.87978500 O 1.32739800 -0.58062200 0.00000800 H 0.93236400 1.24727000 -0.87984300 H 0.64564200 -1.26663600 -0.00001100
PW6B95-D3/jun-cc-pVTZ	C -0.82127700 0.48572200 0.00000200 C 0.66561200 0.64493700 0.00000000 H -1.41768300 1.41038200 0.00000300 O -1.34028900 -0.59777600 -0.00000200 H 0.93806600 1.24221100 0.87607200 O 1.32065100 -0.58000700 0.00000000 H 0.93806600 1.24221000 -0.87607200	C -0.82033600 0.48870000 -0.00000200 C 0.66247100 0.65050300 0.00000000 H -1.41714000 1.40838900 0.00000100 O -1.33542800 -0.60186700 0.00000200 H 0.93353800 1.24518500 0.87574600 O 1.31918000 -0.58288400 -0.00000100 H 0.93354100 1.24518500 -0.87574600

	H 0.63264300 -1.25649800 0.00000300	H 0.62723400 -1.25596700 0.00000000
B2PLYP/aug-cc-pVTZ	C 0.82637700 0.48788100 0.00000000	C 0.82559600 0.49094600 -0.00000300
	C -0.66734400 0.64938600 0.00000000	C -0.66414600 0.65539100 0.00000300
	H 1.42071300 1.41648100 -0.00000400	H 1.42105300 1.41396500 -0.00000800
	O 1.35463000 -0.60167600 0.00000000	O 1.34893100 -0.60594100 0.00000100
	H -0.94083400 1.24494000 -0.87944500	H -0.93647100 1.24787900 -0.87929800
	O -1.33514000 -0.58144900 0.00000000	O -1.33316400 -0.58447400 -0.00000400
	H -0.94083600 1.24494100 0.87944400	H -0.93646000 1.24786800 0.87931600
	H -0.64915400 -1.26496000 -0.00000400	H -0.64295500 -1.26441200 0.00001500

Glycolaldehyde radical on C (*G rad1*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C 0.85630700 0.54680300 -0.04669700	C 0.86956700 0.52624100 0.00140100
	C -0.66047900 0.63818100 0.03825800	C -0.64825200 0.63804800 0.02770700
	O 1.49235000 -0.43767800 0.00244000	O 1.52070900 -0.45114200 -0.01476800
	H -1.00686500 1.28608200 -0.76489300	H -0.93218300 1.27812500 -0.80567700
	O -1.30791400 -0.59622300 -0.07003700	O -1.31537600 -0.58582500 -0.10844500
	H -0.86362800 1.14618400 0.98824100	H -0.89570700 1.16523900 0.95278500
	H -0.77996900 -1.27096800 0.36806400	H -1.14266400 -1.13336500 0.66395100
PW6B95-D3/jun-cc-pVTZ	C 0.85295500 0.54186100 -0.04422200	C 0.86756300 0.51894500 0.00490700
	C -0.65334600 0.63485700 0.03708400	C -0.64046000 0.63343200 0.02599800
	O 1.49815500 -0.43798100 0.00126900	O 1.53028000 -0.45135900 -0.01527100
	H -0.99654800 1.28315500 -0.76304800	H -0.91715800 1.27306500 -0.80622000
	O -1.31646500 -0.59021900 -0.06952100	O -1.32658800 -0.57891200 -0.10928700
	H -0.85626300 1.14868100 0.98129000	H -0.88886000 1.16829900 0.94301700
	H -0.79836900 -1.26654100 0.37060000	H -1.18613600 -1.11345200 0.67423400
B2PLYP/aug-cc-pVTZ	C 0.85981700 0.54111000 -0.04424700	C 0.87105700 0.52233400 0.00560100
	C -0.65331100 0.63937600 0.04017300	C -0.64299300 0.63933600 0.02579900
	O 1.51552700 -0.44313200 0.00017000	O 1.54061400 -0.45452600 -0.01531400
	H -0.99646300 1.28938000 -0.76133400	H -0.92185800 1.27460800 -0.81196700
	O -1.33152000 -0.58940200 -0.07857000	O -1.33440300 -0.58361800 -0.11037700
	H -0.85825400 1.14746800 0.98919400	H -0.89622600 1.17200600 0.94508800
	H -0.85638000 -1.25948900 0.42378600	H -1.19998800 -1.11147700 0.68400900

Glycolaldehyde radical on O (*G rad2*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C 0.67586700 -0.36404800 0.11192900	C -0.67212900 0.36433300 0.11236000

	C -0.60419300 0.46360200 0.10595000 H 0.53033600 -1.43091700 0.36206800 O 1.74793600 0.10404700 -0.13066900 H -0.49823500 1.35533200 -0.52245700 O -1.71474900 -0.27236400 -0.15591100 H -0.72764500 0.82479800 1.14575300	C 0.60224700 -0.46268400 0.10559700 H -0.53278500 1.42955200 0.36251300 O -1.74913200 -0.10412700 -0.13090200 H 0.50449100 -1.35555000 -0.52159800 O 1.71418300 0.27210800 -0.15579000 H 0.72717700 -0.82774200 1.14487800
PW6B95-D3/jun-cc-pVTZ	C 0.67536900 -0.35227400 0.16102800 C -0.62867800 0.47191400 0.14767600 H 0.54574600 -1.38605900 0.51390800 O 1.71888300 0.10150600 -0.18378900 H -0.48804100 1.39909800 -0.41311500 O -1.66953300 -0.28293400 -0.21295400 H -0.73266000 0.72054700 1.22093000	C 0.67402500 -0.35652700 0.15694800 C -0.62259700 0.46570100 0.14701900 H 0.55237000 -1.39292700 0.49800400 O 1.72104100 0.10521200 -0.18156500 H -0.49195400 1.40113100 -0.40071600 O -1.67593500 -0.27656400 -0.21141100 H -0.72983300 0.70756800 1.22270800
B2PLYP/aug-cc-pVTZ	C 0.67679500 -0.36166900 0.12798800 C -0.60967400 0.46197300 0.11990000 H 0.53699700 -1.42079900 0.40734700 O 1.75182900 0.10446000 -0.14752800 H -0.49727400 1.37243600 -0.47939800 O -1.71335800 -0.27227200 -0.17559000 H -0.75021600 0.78904000 1.16966800	C -0.67317800 0.36231200 0.12731500 C 0.60690700 -0.46063700 0.11858800 H -0.53978400 1.42019700 0.40426400 O -1.75320200 -0.10471800 -0.14656800 H 0.50355100 -1.37108500 -0.48106500 O 1.71378000 0.27165200 -0.17410400 H 0.74922800 -0.79463300 1.16676000

Glycolaldehyde radical on CH_2 (*G rad3*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -0.77792500 0.52081400 0.00000300 C 0.63592500 0.62750600 0.00000500 H -1.36877300 1.44312500 -0.00000900 O -1.30237800 -0.59749000 -0.00000200 H 1.19623000 1.54911900 -0.00001400 O 1.34362400 -0.48580800 -0.00000200 H 0.69457900 -1.21578300 0.00000700	C -0.77687200 0.51992500 0.00000000 C 0.63440500 0.62355200 -0.00000100 H -1.35676500 1.44706500 0.00000000 O -1.31797400 -0.59707300 0.00000000 H 1.18409300 1.55124900 0.00000200 O 1.35502300 -0.48144500 0.00000100 H 0.73107600 -1.23103300 -0.00000400
PW6B95-D3/jun-cc-pVTZ	C 0.77099900 0.52536700 -0.00002400 C -0.63649100 0.62804300 -0.00000600 H 1.36442800 1.44201000 -0.00004900 O 1.29162800 -0.59637500 -0.00000300 H -1.20533900 1.54032700 -0.00001700 O -1.32992900 -0.49126500 0.00002900 H -0.65973400 -1.20167800 0.00003400	C 0.77049000 0.52383900 -0.00002400 C -0.63478700 0.62400200 -0.00000600 H 1.35254100 1.44564800 -0.00004800 O 1.30807300 -0.59582400 -0.00000300 H -1.19264300 1.54261800 -0.00001700 O -1.34247000 -0.48634600 0.00002900 H -0.69894300 -1.21795000 0.00003600
B2PLYP/aug-cc-pVTZ	C -0.77666900 0.52480200 0.00001000 C 0.64010400 0.63108300 -0.00003400	C -0.77579300 0.52365000 -0.00000100 C 0.63783900 0.62647600 0.00000300

	H -1.36649800 1.44742600 0.00005800 O -1.30465600 -0.59759000 -0.00000400 H 1.20718000 1.54704000 -0.00000500 O 1.34285300 -0.49255900 0.00002600 H 0.67313700 -1.20858600 -0.00008400	H -1.35391800 1.45119500 -0.00000900 O -1.32223400 -0.59732400 0.00000100 H 1.19326300 1.54917400 -0.00000100 O 1.35638900 -0.48712500 -0.00000100 H 0.71513400 -1.22553300 -0.00000200

Glycolaldehyde geminal diol (*Gdiol*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -0.49937100 0.00279100 0.36153100 C 0.71066500 -0.70978500 -0.22673600 H -0.44528400 0.00663100 1.45645000 O -1.67862800 -0.66114900 0.03703000 H 0.57434400 -0.78712600 -1.30671100 O 1.89147800 0.04800500 -0.01991200 H 0.78761000 -1.71590100 0.18897000 H 2.20034700 -0.07929600 0.88024100 O -0.56550000 1.31479800 -0.13087400 H -1.90266000 -0.42404600 -0.86936000 H 0.33908400 1.62846700 -0.24831300	C -0.50315600 0.01588700 0.36151900 C 0.69956200 -0.72412100 -0.20645300 H -0.46009300 0.03840400 1.45421500 O -1.69559200 -0.62946100 0.04160700 H 0.56017400 -0.83868600 -1.28325300 O 1.88526500 0.03143200 -0.02679800 H 0.77280200 -1.71291500 0.24764400 H 2.18085500 -0.05443000 0.88463400 O -0.54242600 1.32849300 -0.14897600 H -1.78133600 -0.65427600 -0.91893200 H 0.37118200 1.62760500 -0.24137000
PW6B95-D3/jun-cc-pVTZ	C -0.50513900 0.00485500 0.36306200 C 0.70348400 -0.72039500 -0.20723300 H -0.47067300 0.00583300 1.45521800 O -1.68719200 -0.64308700 0.02669300 H 0.56613000 -0.82962700 -1.28022400 O 1.88519700 0.04256600 -0.03138800 H 0.78603100 -1.71128100 0.23364000 H 2.19768400 -0.05930500 0.86741100 O -0.54292900 1.31634100 -0.12746700 H -1.87837300 -0.43206700 -0.89014300 H 0.36852800 1.59312700 -0.26357500	C -0.50973000 0.01797600 0.36379200 C 0.69121500 -0.73623300 -0.18318900 H -0.48958500 0.03804300 1.45344600 O -1.70412400 -0.61010300 0.02679300 H 0.54871000 -0.88874900 -1.25068100 O 1.87701200 0.02569900 -0.04090100 H 0.77175800 -1.70592100 0.30070000 H 2.18246700 -0.03502600 0.86570100 O -0.51579300 1.33062200 -0.14318700 H -1.76499100 -0.65256100 -0.93150400 H 0.40596400 1.58400900 -0.26291400
B2PLYP/aug-cc-pVTZ	C -0.50377400 0.00278700 0.36281500 C 0.70962900 -0.71746300 -0.21614700 H -0.46446300 0.00421600 1.45681900 O -1.69094500 -0.65756000 0.03125000 H 0.57801800 -0.81536100 -1.29338700 O 1.90057200 0.04833400 -0.02712600 H 0.79288900 -1.71388700 0.21866000 H 2.21996600 -0.08302800 0.87007100 O -0.56198100 1.32345500 -0.12904200	C -0.50757800 0.01490600 0.36296000 C 0.69803400 -0.73306500 -0.19507600 H -0.48008600 0.03554100 1.45453900 O -1.70840100 -0.62456600 0.03377800 H 0.56291000 -0.86963800 -1.26803100 O 1.89312300 0.03127400 -0.03480200 H 0.77871800 -1.71049700 0.27914100 H 2.19774600 -0.05518600 0.87463600 O -0.53575400 1.33737900 -0.14597200

	H -1.89185000 -0.44037900 -0.88659100 H 0.34914700 1.62266200 -0.24623500	H -1.77902000 -0.66050200 -0.92842000 H 0.38525700 1.61654100 -0.24320200

Glycolaldehyde geminal diol radical on C (*Gdiol rad1*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C 0.48689900 -0.01369000 -0.23688500 C -0.75068200 -0.69118500 0.25821500 O 1.62022200 -0.73682300 -0.06369900 H -0.74539700 -0.73770800 1.35260200 O -1.88988700 0.07696700 -0.09101700 H -0.79405500 -1.70954300 -0.13043000 H -1.98354700 0.05551200 -1.04817700 O 0.63995300 1.29501700 0.12795000 H 2.37895500 -0.16197900 -0.20867000 H -0.23556200 1.70167700 0.12082600	C 0.49065000 -0.00917400 -0.23837700 C -0.74700900 -0.70078800 0.24091300 O 1.62514500 -0.72890300 -0.04601800 H -0.73167400 -0.78302100 1.33326000 O -1.89033900 0.07374900 -0.07790500 H -0.79383000 -1.70554900 -0.18035000 H -2.00645700 0.06551100 -1.03389200 O 0.63049900 1.30053600 0.13324200 H 2.38944900 -0.19380400 -0.28996400 H -0.24176700 1.71358200 0.08117400
PW6B95-D3/jun-cc-pVTZ	C 0.48766300 -0.01521200 -0.23305100 C -0.74422800 -0.69829700 0.25180600 O 1.62659600 -0.72439400 -0.06185200 H -0.74762200 -0.75795400 1.34285300 O -1.88281600 0.07477400 -0.08858300 H -0.79000900 -1.70980900 -0.14446300 H -1.97610700 0.05881600 -1.04274200 O 0.62339000 1.29396900 0.12824700 H 2.37524100 -0.14309400 -0.21139600 H -0.25947300 1.67829800 0.12072300	C 0.49192700 -0.01064500 -0.23567900 C -0.74002300 -0.70806900 0.23330200 O 1.63167300 -0.71619600 -0.04374900 H -0.73159200 -0.80521600 1.32171000 O -1.88296700 0.07156500 -0.07386300 H -0.78985400 -1.70488900 -0.19698100 H -2.00329100 0.06631100 -1.02590900 O 0.61316500 1.29981400 0.13179200 H 2.38666200 -0.17256300 -0.28380600 H -0.26832100 1.68717200 0.08581100
B2PLYP/aug-cc-pVTZ	C 0.48869700 -0.01351300 -0.24028400 C -0.74900700 -0.69342600 0.25507200 O 1.62551800 -0.74105700 -0.05975600 H -0.74676000 -0.74457900 1.34839900 O -1.89982800 0.07920300 -0.08639500 H -0.79745200 -1.70868900 -0.13804700 H -2.01005000 0.03853900 -1.04208900 O 0.64501800 1.30138400 0.12849400 H 2.38272800 -0.16628000 -0.21907400 H -0.23227400 1.70640100 0.10333300	C 0.49257700 -0.00944800 -0.24203700 C -0.74538900 -0.70318800 0.23782000 O 1.63077500 -0.73271700 -0.04256200 H -0.73274800 -0.78972700 1.32892000 O -1.89988100 0.07597100 -0.07326400 H -0.79776500 -1.70448200 -0.18786400 H -2.03145100 0.04863000 -1.02763200 O 0.63485000 1.30696800 0.13263300 H 2.39296000 -0.19588700 -0.29246200 H -0.24007500 1.71550300 0.06988600

Glycolaldehyde geminal diol radical on diol O (*Gdiol rad2*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -0.59242900 -0.01174500 0.30545600 C 0.69114600 -0.71864400 -0.22523000 H -0.54456600 -0.03786400 1.41470600 O -1.64496400 -0.73717400 -0.05110300 H 0.58723900 -0.82440000 -1.30268200 O 1.81845300 0.09217400 0.00485500 H 0.77219700 -1.70130900 0.23694400 H 2.10458200 -0.00013800 0.91724900 O -0.64486800 1.30853300 -0.14597000 H 0.25928000 1.63777400 -0.20983600	C -0.60471300 -0.01610100 0.31082600 C 0.70944600 -0.72666300 -0.22443500 H -0.50642600 -0.03158800 1.41555600 O -1.63396000 -0.74185400 -0.04932900 H 0.59139800 -0.84584500 -1.29811100 O 1.80799400 0.10865600 -0.00203700 H 0.79526300 -1.69323300 0.26583000 H 2.11108900 0.01449200 0.90695800 O -0.65582600 1.30099500 -0.16202100 H 0.23461500 1.67037700 -0.10147600
PW6B95-D3/jun-cc-pVTZ	C -0.60888900 -0.01264800 0.30184900 C 0.69753100 -0.72060800 -0.22543800 H -0.52199100 -0.03081900 1.40808400 O -1.63557600 -0.73805800 -0.04831900 H 0.59081500 -0.82792500 -1.29734500 O 1.81090500 0.09763700 0.00464600 H 0.77595400 -1.69410500 0.24609100 H 2.10865800 -0.00777700 0.90866800 O -0.64351800 1.30601900 -0.15199100 H 0.26022200 1.63538000 -0.15864400	C -0.62686200 -0.01609700 0.31287800 C 0.72617700 -0.72711600 -0.22306300 H -0.48357100 -0.02049200 1.40950300 O -1.62506100 -0.74752700 -0.04985300 H 0.59693000 -0.84766100 -1.29007100 O 1.80302600 0.11749300 -0.00386600 H 0.80695700 -1.68145800 0.28167000 H 2.12461300 0.01290600 0.89435600 O -0.66046100 1.29569300 -0.16887800 H 0.21916000 1.67071100 -0.05357400
B2PLYP/aug-cc-pVTZ	C -0.60027600 -0.01540500 0.30383000 C 0.69531100 -0.72420400 -0.22021100 H -0.55218800 -0.04095900 1.41304100 O -1.64832100 -0.74001000 -0.05404900 H 0.59696500 -0.84235300 -1.29507600 O 1.82635000 0.09765800 0.00054400 H 0.78203500 -1.69850400 0.25580500 H 2.11880100 -0.00014300 0.91167900 O -0.64980600 1.31469800 -0.14660500 H 0.25838600 1.64084900 -0.18628500	C -0.61468600 -0.01878700 0.31282000 C 0.71557800 -0.73367700 -0.21688900 H -0.51474800 -0.03145900 1.41606800 O -1.63559600 -0.74582100 -0.05548900 H 0.60035900 -0.86889200 -1.28697700 O 1.81497300 0.11420100 -0.00829300 H 0.80644700 -1.68897500 0.29140000 H 2.12035400 0.02599000 0.90163900 O -0.66084700 1.30784500 -0.16186000 H 0.23398900 1.66831700 -0.09258600

Glycolaldehyde geminal diol radical on hydroxyl O(*Gdiol rad3*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -0.46929800 0.00751500 0.37558400 C 0.79467000 -0.69824000 -0.13154700 H -0.47750900 0.01340400 1.46942200 O -1.61170700 -0.67882100 -0.01795400 H 0.69184900 -0.80813100 -1.22794600	C -0.47026100 0.01894400 0.37030200 C 0.78682200 -0.70024200 -0.12623700 H -0.47786800 0.04190300 1.46255600 O -1.62341600 -0.66080700 -0.00459400 H 0.70024900 -0.82961500 -1.22259500

	O 1.92554500 0.04664500 0.03687400 H 0.89552400 -1.71047200 0.27663600 O -0.51857800 1.30898300 -0.13506400 H -1.80129200 -0.43212900 -0.92985500 H 0.37711700 1.66722600 -0.12332100	O 1.92356900 0.03506100 0.04374900 H 0.88070500 -1.70694200 0.29625200 O -0.51308800 1.32195100 -0.15208900 H -1.68159000 -0.66882000 -0.96769000 H 0.38261400 1.68162200 -0.12944800
PW6B95-D3/jun-cc-pVTZ	C -0.46850600 0.01553000 0.36787500 C 0.84768200 -0.72802900 -0.20999800 H -0.38855500 -0.01303900 1.45148000 O -1.59959800 -0.66574800 0.01796600 H 0.63352600 -0.77431600 -1.28481000 O 1.85961600 0.06949100 0.09346100 H 0.86859900 -1.72194500 0.24301400 O -0.50565400 1.29614200 -0.14380600 H -1.82789600 -0.42035600 -0.88285100 H 0.40435600 1.60556700 -0.21506100	C -0.48104800 0.01952800 0.37148500 C 0.78600200 -0.71825200 -0.09527900 H -0.51155800 0.02323800 1.46027200 O -1.63633700 -0.63356500 -0.02865500 H 0.67531200 -0.88045500 -1.18405500 O 1.90289500 0.03233700 0.02066300 H 0.88086400 -1.70910000 0.35542500 O -0.47184900 1.32450700 -0.12989700 H -1.68256800 -0.62403500 -0.98884700 H 0.45054100 1.59647200 -0.19692200
B2PLYP/aug-cc-pVTZ	C -0.47395200 0.00706700 0.37606500 C 0.79769500 -0.70410800 -0.11767000 H -0.49753200 0.00610800 1.46858200 O -1.62358400 -0.67470100 -0.02694800 H 0.69776800 -0.84066100 -1.21128700 O 1.92965000 0.04636400 0.02683200 H 0.90211600 -1.70758500 0.31038700 O -0.51260800 1.31856800 -0.12786000 H -1.78853200 -0.44490200 -0.94904700 H 0.39606800 1.64743500 -0.14519700	C -0.47468900 0.01774000 0.37105100 C 0.78938900 -0.70645300 -0.11226100 H -0.49835400 0.03462800 1.46186700 O -1.63504600 -0.65665500 -0.01497400 H 0.70540200 -0.86230300 -1.20521500 O 1.92735300 0.03467300 0.03354700 H 0.88704300 -1.70394800 0.32974600 O -0.50611400 1.33211200 -0.14403200 H -1.67572300 -0.67620400 -0.97951200 H 0.40388800 1.65907100 -0.15594800

Glycolaldehyde geminal diol radical on CH_2 (*Gdiol rad4*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -0.49604200 -0.00288100 0.37408500 C 0.71799900 -0.75022900 -0.07830600 H -0.57801800 0.04789000 1.46347200 O -1.65987100 -0.61645100 -0.08624900 H 0.79407900 -1.81693700 0.07760000 O 1.89685000 -0.09744900 -0.05531300 H 1.70350700 0.85090600 -0.04393800 O -0.38966500 1.34972800 -0.02918300 H -1.46700200 -1.04174000 -0.92934300 H -0.56282500 1.39191900 -0.97650200	C -0.45470900 -0.00609400 0.33643500 C 0.76724400 -0.60788100 -0.27051800 H -0.34467200 0.06327000 1.42347100 O -1.58472100 -0.78627200 0.11171100 H 0.72261900 -1.01538200 -1.27198700 O 1.97798600 -0.07141000 0.03979800 H 1.98469800 0.25468200 0.94790000 O -0.72111600 1.29471600 -0.18542900 H -1.72782000 -0.84914700 -0.84018000 H 0.11277600 1.73415900 -0.38334700
PW6B95-D3/jun-cc-pVTZ	C -0.49751100 -0.00714100 0.37750700	C -0.49348200 0.00189300 0.36455400

	C 0.71288700 -0.76084500 -0.05170800 H -0.60379100 0.04444200 1.46189100 O -1.65893200 -0.60243900 -0.10796500 H 0.80381300 -1.81787500 0.13538700 O 1.88156200 -0.09650400 -0.07368200 H 1.66322300 0.84524800 -0.07930600 O -0.36531400 1.34812100 -0.01778500 H -1.43708400 -1.05829300 -0.92423600 H -0.57694200 1.40096600 -0.95307100	C 0.70772400 -0.74430000 -0.09256300 H -0.56628500 0.05664100 1.45130100 O -1.66503700 -0.62073700 -0.06805500 H 0.76554900 -1.81480900 0.00647400 O 1.89918500 -0.11451900 -0.03767600 H 1.72882000 0.83511600 0.00322600 O -0.39778400 1.35518100 -0.03696100 H -1.51581100 -0.96735700 -0.95254800 H -0.38863900 1.38545100 -0.99886100
B2PLYP/aug-cc-pVTZ	C -0.49726600 -0.00643800 0.37519800 C 0.71633600 -0.75922700 -0.06600600 H -0.59412700 0.04766100 1.46199700 O -1.66946300 -0.61310700 -0.09645100 H 0.80264900 -1.82115400 0.10868000 O 1.89976300 -0.09969800 -0.06390200 H 1.68965500 0.84728000 -0.06545400 O -0.37794200 1.35872000 -0.02263000 H -1.46132300 -1.05309400 -0.92957800 H -0.57013900 1.40598200 -0.96693000	C -0.49263400 0.00149400 0.36344800 C 0.71391200 -0.74005100 -0.10620300 H -0.55711700 0.05645000 1.45235000 O -1.67175000 -0.63557900 -0.05818700 H 0.77052700 -1.81389900 -0.01789500 O 1.91797300 -0.11414000 -0.02977800 H 1.75407500 0.83995900 0.01232100 O -0.41572700 1.36459300 -0.04044400 H -1.53644700 -0.96380200 -0.95634000 H -0.40266700 1.39363900 -1.00663600

Glyoxal (**Gl**)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -0.00001600 0.76136700 0.00000000 C 0.00000000 -0.76135000 0.00000000 O -1.02438700 -1.37921700 0.00000000 O 1.02439800 1.37919500 0.00000000 H -0.99833600 1.23076800 0.00000000 H 0.99834600 -1.23070100 0.00000000	C -0.00001600 0.76154000 0.00000000 C 0.00000000 -0.76152100 0.00000000 O -1.02951800 -1.37564200 0.00000000 O 1.02952900 1.37561900 0.00000000 H -0.99289600 1.23685200 0.00000000 H 0.99290500 -1.23678500 0.00000000
PW6B95-D3/jun-cc-pVTZ	C -0.00001000 0.75809700 0.00000000 C 0.00000000 -0.75808600 0.00000000 O -1.02136000 -1.38125200 0.00000000 O 1.02136700 1.38123900 0.00000000 H -0.99710500 1.22396900 0.00000000 H 0.99711100 -1.22392900 0.00000000	C -0.00001800 0.75820500 0.00000000 C 0.00000000 -0.75818300 0.00000000 O -1.02628000 -1.37775600 0.00000000 O 1.02629200 1.37773100 0.00000000 H -0.99155400 1.22988300 0.00000000 H 0.99156300 -1.22981100 0.00000000
B2PLYP/aug-cc-pVTZ	C -0.00001500 0.75980800 0.00000000 C 0.00000000 -0.75979000 0.00000000 O -1.02994800 -1.38943100 0.00000000 O 1.02995800 1.38941000 0.00000000 H -0.99837600 1.22701200 0.00000000	C -0.00000800 0.75980500 0.00000000 C 0.00000000 -0.75979600 0.00000000 O -1.03496600 -1.38551900 0.00000000 O 1.03497100 1.38550900 0.00000000 H -0.99256100 1.23311000 0.00000000

	H 0.99838400 -1.22694800 0.00000000	H 0.99256500 -1.23308000 0.00000000

Glyoxal radical (*Gl rad*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C 0.64095900 0.11147800 -0.00006400 C -0.70863800 0.45302000 0.00001800 O -1.58489400 -0.42995500 0.00000300 O 1.74758300 -0.18477300 0.00002800 H -0.89543700 1.53083900 0.00002900	C 0.64283200 0.10913300 0.00000200 C -0.70487400 0.45397000 0.00000100 O -1.59017100 -0.42818200 -0.00000100 O 1.74739800 -0.18546400 -0.00000100 H -0.88556200 1.53055400 -0.00000500
PW6B95-D3/jun-cc-pVTZ	C 0.63505500 0.12809900 -0.00000600 C -0.70807200 0.46058300 0.00000300 O -1.56696100 -0.44150600 0.00000000 O 1.73655900 -0.19141200 0.00000300 H -0.91867900 1.53126000 0.00000000	C 0.63794700 0.12039500 -0.00000800 C -0.70327700 0.45831400 0.00000200 O -1.57811700 -0.43517800 0.00000000 O 1.73960300 -0.19003200 0.00000300 H -0.89990800 1.52943000 0.00000500
B2PLYP/aug-cc-pVTZ	C 0.63765400 0.13644500 -0.00000100 C -0.71618200 0.46465800 0.00000000 O -1.56959800 -0.44815600 0.00000000 O 1.74525900 -0.19466800 0.00000000 H -0.93412000 1.53597000 0.00000000	C 0.64065900 0.12872700 -0.00000600 C -0.71010900 0.46357500 0.00000400 O -1.58119400 -0.44227100 0.00000000 O 1.74763800 -0.19382800 0.00000200 H -0.91485400 1.53498500 -0.00000200

Glyoxal gem diol (*Gldiol*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -0.50402100 0.01071900 0.42265600 C 0.86761500 -0.62686300 0.20637500 O 1.78510500 -0.00884400 -0.25789900 O -1.45701000 -0.76205700 -0.25910500 H -0.77593300 -0.05132100 1.48005900 H 0.94551200 -1.69599000 0.45938600 O -0.49084600 1.32524600 -0.00381800 H -1.43943800 -0.49902800 -1.18574800 H 0.39029500 1.50843900 -0.36130500	C -0.50886300 0.01885900 0.41961400 C 0.86630700 -0.61753700 0.23362800 O 1.77767800 -0.01184300 -0.26348200 O -1.45572700 -0.76140000 -0.26423100 H -0.79516400 -0.03190100 1.47117400 H 0.95587100 -1.66937300 0.53975500 O -0.49261400 1.33864800 -0.00197100 H -1.27507600 -0.71834000 -1.21108700 H 0.33500600 1.48844600 -0.48181900
PW6B95-D3/jun-cc-pVTZ	C -0.50646000 0.01636300 0.42304300 C 0.85948300 -0.62603800 0.21954500 O 1.77348500 -0.01857000 -0.26503600 O -1.45728400 -0.75452000 -0.26418600 H -0.79254000 -0.04350600 1.47319900 H 0.93959300 -1.68616500 0.49441400	C -0.50939500 0.02341000 0.41823800 C 0.85715000 -0.62102600 0.23836500 O 1.76955400 -0.02357900 -0.26636200 O -1.46242200 -0.74898000 -0.26512800 H -0.80202200 -0.02482200 1.46467300 H 0.94344900 -1.66696400 0.55308500

	O -0.47509500 1.32693400 -0.00331100 H -1.40084400 -0.52504100 -1.19487900 H 0.40680100 1.48201200 -0.36799500	O -0.47328800 1.33961100 -0.00452800 H -1.26635400 -0.72774200 -1.20607900 H 0.36764400 1.46881400 -0.46314500
B2PLYP/aug-cc-pVTZ	C -0.50785400 0.01520800 0.42583900 C 0.86615000 -0.62378900 0.22654800 O 1.78613000 -0.01550000 -0.27026400 O -1.45885400 -0.76758500 -0.26851100 H -0.80188100 -0.04464600 1.47559200 H 0.95054100 -1.68170100 0.51590600 O -0.48879000 1.33528700 -0.00187600 H -1.39775500 -0.53627900 -1.20308100 H 0.39143000 1.49649700 -0.37753200	C -0.51130100 0.02181100 0.42210800 C 0.86562600 -0.61509800 0.24945600 O 1.78060900 -0.01815200 -0.27423100 O -1.45925700 -0.76654500 -0.27186400 H -0.81551500 -0.02631500 1.46692500 H 0.96062600 -1.65549500 0.58586300 O -0.49130500 1.34750900 -0.00204000 H -1.25238200 -0.74350200 -1.21511400 H 0.34094800 1.48253700 -0.48197500

Glyoxal gem diol radical on C (*Gldiol rad1*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -0.41741400 -0.04985300 0.00000200 C 0.82971000 -0.69807300 0.00000300 O 1.85816500 0.00777600 -0.00000200 O -1.57978700 -0.68400700 -0.00000500 H 0.84417700 -1.79065600 0.00000800 O -0.46449900 1.27163000 0.00000000 H -2.29953800 -0.04121400 0.00002100 H 0.47054100 1.55623300 -0.00000200	C -0.41875600 -0.04223900 0.00000000 C 0.83138200 -0.68502800 0.00000100 O 1.87388600 0.01029500 -0.00000100 O -1.55720100 -0.70585300 -0.00000200 H 0.83751700 -1.77704300 0.00000500 O -0.49504400 1.27448100 -0.00000800 H -2.30835700 -0.09605900 0.00002600 H 0.42195600 1.60531400 0.00005100
PW6B95-D3/jun-cc-pVTZ	C -0.55050300 0.01951900 0.44393400 C 0.99088800 -0.23461000 0.57830100 O 1.73509900 -0.04813100 -0.31014400 O -1.08018200 -1.06763600 -0.23777700 H -1.02037000 0.03818400 1.41591100 O -0.76177900 1.24849200 -0.15174800 H -0.62787700 -1.17767400 -1.07785000 H -0.13916300 1.36824000 -0.87412100	C -0.52223000 0.02323900 0.43261400 C 0.95641600 -0.48132700 0.43846400 O 1.80479900 -0.08430700 -0.26721700 O -1.28434500 -0.92665900 -0.23956100 H -0.88623600 0.05048600 1.45030000 O -0.60809000 1.30502500 -0.07793000 H -0.96162500 -1.04223600 -1.13765100 H -0.05616500 1.38781700 -0.86144300
B2PLYP/aug-cc-pVTZ	C -0.42120700 -0.05003400 -0.00000100 C 0.82507500 -0.70571400 0.00000700 O 1.86007100 0.00222200 -0.00000400 O -1.59415600 -0.67533300 -0.00001300 H 0.84038900 -1.79749500 0.00002500 O -0.44851300 1.27622000 -0.00000200 H -2.30377100 -0.02003700 0.00007500 H 0.50095600 1.52714400 0.00001800	C -0.42210400 -0.04253600 0.00000000 C 0.82736200 -0.69175900 0.00000000 O 1.87759100 0.00549100 0.00000000 O -1.56984100 -0.69946800 0.00000000 H 0.83409300 -1.78275000 -0.00000200 O -0.48280800 1.27958300 0.00000000 H -2.31245500 -0.07832200 0.00000300 H 0.44727400 1.58199600 -0.00000100

Glyoxal gem diol radical on O (*Gldiol rad2*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -0.59103500 -0.05499500 0.34388900 C 0.88642400 -0.56929200 0.22194900 O 1.73062300 0.13241100 -0.23432000 O -1.29705500 -0.91269400 -0.39171500 H -0.85741900 -0.19234600 1.40821900 H 1.05104900 -1.60298700 0.55556100 O -0.68763500 1.28205600 0.02230000 H 0.06656100 1.52687600 -0.52893100	C -0.58788600 -0.05724200 0.33924100 C 0.88552800 -0.59771800 0.19398800 O 1.73777300 0.12070600 -0.22043700 O -1.34250500 -0.87869100 -0.37569500 H -0.81315000 -0.19944800 1.41375500 H 1.02857600 -1.64491300 0.48370100 O -0.66284500 1.28728800 0.01663500 H 0.13933400 1.53969100 -0.46085700
PW6B95-D3/jun-cc-pVTZ	C 0.41958100 -0.05127400 -0.00000100 C -0.81825500 -0.70654800 0.00000200 O -1.84656900 0.00200400 -0.00000100 O 1.59012600 -0.66463800 0.00000000 H -0.83799200 -1.79538800 0.00000100 O 0.43717000 1.26789100 0.00000100 H 2.29456700 -0.01013300 -0.00000400 H -0.51034000 1.51039600 0.00000300	C -0.42080900 -0.04369800 0.00000200 C 0.82045700 -0.69336900 0.00000300 O 1.86273400 0.00380000 -0.00000600 O -1.56756400 -0.68729100 0.00000200 H 0.83075800 -1.78170900 0.00000000 O -0.46836900 1.27197200 0.00000000 H -2.30450500 -0.06618500 0.00000000 H 0.46145200 1.56244900 0.00000100
B2PLYP/aug-cc-pVTZ (suffers decomposition in the calculation in gas phase)	C -1.45192700 -0.09038200 0.39204200 C 2.16800800 -0.37055900 0.07870800 O 3.02089300 0.43486100 -0.03745000 O -1.54221600 -1.15849400 -0.17138400 H -1.01757000 0.04491200 1.38667200 H 1.96816200 -1.19784900 -0.65033800 O -1.85671600 1.09664100 -0.11211300 H -2.22276000 0.93451100 -0.99324800	C -0.55989000 -0.03107100 0.37538500 C 0.85360300 -0.60543000 0.23347700 O 1.74979400 0.03987400 -0.25637200 O -1.43572800 -0.83537500 -0.39815100 H -0.91316000 -0.14018400 1.40371400 H 0.98254300 -1.65540900 0.54640400 O -0.57484200 1.31231400 0.01215600 H 0.25454600 1.48009400 -0.46434600

Glyoxal gem diol radical on C(=O)H (*Gldiol rad3*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C 0.41417000 -0.00000200 0.33739800 C -0.97158100 -0.00000300 -0.38855800 O -2.03277400 -0.00000900 0.09329600 O 1.07637000 1.16750800 0.00322900 H 0.26630400 -0.00000400 1.41501400 O 1.07639500 -1.16749700 0.00322600 H 1.05910300 1.29042700 -0.95302700	C -0.40841700 -0.00000500 0.33542500 C 0.97459100 -0.00014000 -0.39641300 O 2.03626100 -0.00003400 0.09182000 O -1.07567700 -1.16675400 0.00778900 H -0.24608100 -0.00001200 1.41115500 O -1.07542500 1.16688800 0.00777000 H -1.11621300 -1.26592900 -0.95212200

	H 1.05913700 -1.29040600 -0.95303100	H -1.11601200 1.26601700 -0.95214400
PW6B95-D3/jun-cc-pVTZ	C 0.41277200 0.00000000 0.33352600	C 0.40693400 0.00000000 0.33056200
	C -0.96328200 0.00000600 -0.38457000	C -0.96735600 -0.00002600 -0.39335600
	O -2.02780800 0.00000200 0.09362700	O -2.03162800 -0.00000400 0.09250000
	O 1.07375600 1.16863300 0.00276900	O 1.07309800 1.16796500 0.00799100
	H 0.27412500 0.00000000 1.40890800	H 0.25230100 0.00000000 1.40386400
	O 1.07374600 -1.16863800 0.00276800	O 1.07313600 -1.16794400 0.00799600
	H 1.03569700 1.30270600 -0.94798000	H 1.09667000 1.27857300 -0.94750000
	H 1.03568900 -1.30270900 -0.94798200	H 1.09671500 -1.27855400 -0.94749600
B2PLYP/aug-cc-pVTZ	C -0.41062600 -0.00000500 0.33267500	C 0.40523900 -0.00001100 0.33039200
	C 0.96654800 -0.00003000 -0.38827900	C -0.96976400 -0.00003200 -0.39586800
	O 2.04052000 -0.00001300 0.09435000	O -2.04353800 -0.00000900 0.09322000
	O -1.08059400 -1.17619000 0.00439800	O 1.07987400 1.17559100 0.00888600
	H -0.27424400 -0.00000700 1.41081700	H 0.25452200 -0.00000500 1.40667700
	O -1.08052700 1.17622600 0.00439700	O 1.07993300 -1.17555400 0.00888600
	H -1.04827300 -1.30782500 -0.95117600	H 1.10119300 1.28704700 -0.95088000
	H -1.04821000 1.30785400 -0.95117800	H 1.10128800 -1.28701300 -0.95087900

Methylglyoxal (**MG**)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -0.96127200 -0.55844200 -0.00003600	C -0.96253500 -0.55652900 -0.00003800
	C 0.52380800 -0.17942400 -0.00004000	C 0.52328700 -0.17625000 -0.00003600
	O 1.32632000 -1.07528700 -0.00015200	O 1.32188500 -1.07990900 -0.00014400
	C 0.85139000 1.27975700 0.00010500	C 0.85783100 1.27649500 0.00011100
	H 1.92780200 1.41689600 0.00004800	H 1.93414600 1.41332600 -0.00002100
	H 0.40053300 1.75284200 -0.87285200	H 0.41055900 1.74912000 -0.87499800
	H 0.40065900 1.75263300 0.87324000	H 0.41082600 1.74885900 0.87550100
	O -1.83467400 0.25940400 0.00009700	O -1.83640300 0.26346700 0.00007500
	H -1.14570800 -1.64665100 -0.00016400	H -1.15087900 -1.64206000 -0.00015000
PW6B95-D3/jun-cc-pVTZ	C 0.84949800 1.27652400 -0.00000200	C 0.85742800 1.27271800 0.00000000
	C -0.95660000 -0.55579000 -0.00000800	C -0.95806200 -0.55287200 -0.00001000
	C 0.52243900 -0.17706500 0.00000000	C 0.52194200 -0.17378500 -0.00001800
	H 1.92188100 1.41717800 -0.00002000	H 1.92981600 1.41204000 0.00000500
	H 0.40034700 1.75144300 0.86879900	H 0.41232500 1.74773400 0.87083700
	H 0.40032400 1.75143500 -0.86879800	H 0.41232800 1.74775600 -0.87082500
	O 1.32626900 -1.07265100 0.00000600	O 1.32062900 -1.07820700 0.00000400
	O -1.83633400 0.25519700 0.00000700	O -1.83849300 0.25981900 0.00001200
	H -1.13405300 -1.64244300 -0.00002600	H -1.13941100 -1.63678900 0.00001600
B2PLYP/aug-cc-pVTZ	C -0.96185100 -0.55510400 -0.00004700	C -0.96295900 -0.55268200 -0.00004700

	C 0.52160900 -0.17691400 -0.00002600 O 1.32975800 -1.08263000 -0.00011400 C 0.86278300 1.28099700 0.00012900 H 1.94012000 1.40825700 -0.00005500 H 0.42063500 1.76218300 -0.87226700 H 0.42100000 1.76188200 0.87288100 O -1.85212900 0.25985000 0.00001800 H -1.13803800 -1.64396100 -0.00012600	C 0.52109700 -0.17366200 -0.00003100 O 1.32447200 -1.08756300 -0.00013300 C 0.86975000 1.27742600 0.00012300 H 1.94699500 1.40386500 -0.00002900 H 0.43127300 1.75808200 -0.87435800 H 0.43157500 1.75779700 0.87491600 O -1.85369700 0.26411400 0.00005200 H -1.14337100 -1.63865000 -0.00015300

Methylglyoxal radical on C (*MG rad1*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -0.93192400 -0.05664900 -0.00000100 C 0.44419300 0.18970700 0.00000000 O 0.82752100 1.37126100 0.00000000 C 1.34876200 -1.01319200 0.00000000 H 1.98474400 -0.97357800 -0.88339800 H 1.98470500 -0.97360900 0.88342800 H 0.79226200 -1.94945600 -0.00002900 O -2.06850900 -0.22408100 0.00000000	C 0.93086600 -0.05466400 -0.00000100 C -0.44447000 0.18646000 0.00000000 O -0.83266300 1.37348400 0.00000000 C -1.34187300 -1.01733700 0.00000000 H -1.97606400 -0.98226200 0.88504400 H -1.97606200 -0.98226900 -0.88504600 H -0.77896700 -1.94848300 0.00000500 O 2.06565700 -0.22020300 0.00000100
PW6B95-D3/jun-cc-pVTZ	C 1.39226800 -0.97421100 -0.00000100 C -0.92213100 -0.09479400 -0.00000100 C 0.43900400 0.18115400 0.00000000 H 2.02613100 -0.91329700 -0.87997000 H 0.87803600 -1.93068600 0.00000600 H 2.02613400 -0.91329600 0.87996800 O 0.76401400 1.38288200 0.00000000 O -2.06215700 -0.24733400 0.00000000	C -1.37504900 -0.98642800 -0.00000100 C 0.92199500 -0.08494900 0.00000000 C -0.44034400 0.17980900 -0.00000200 H -2.00765300 -0.93584000 0.88159800 H -0.84524000 -1.93302100 -0.00000400 H -2.00765800 -0.93583700 -0.88159600 O -0.78235300 1.38276200 0.00000100 O 2.05997100 -0.23849900 0.00000100
B2PLYP/aug-cc-pVTZ	C -0.98237400 -0.11091400 0.38488900 C 0.44735600 0.20586900 0.02110000 O 0.78699800 1.36709800 -0.05083400 C 1.35869400 -0.98609000 -0.04815400 H 2.30887900 -0.67792800 -0.47411900 H 1.52228200 -1.37530100 0.95688400 H 0.91217700 -1.78057500 -0.64552600 O -1.99767300 -0.21952100 -0.19719700	C -0.97376200 -0.12581300 0.37075800 C 0.44790000 0.19890000 0.01792700 O 0.76287200 1.37407900 -0.04688500 C 1.37647700 -0.97201200 -0.04835700 H 2.30874900 -0.65941800 -0.50903000 H 1.57503400 -1.32763400 0.96295800 H 0.92791300 -1.79055500 -0.60898400 O -2.00229400 -0.22768500 -0.18897900

Methylglyoxal radical on CH_3 (*MG rad2*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -0.90679200 -0.55889000 0.00000000 C 0.54527900 -0.08810300 0.00000000 O 1.42566600 -0.94281600 0.00000100 C 0.78762200 1.31289200 0.00001200 H 1.80709400 1.66591200 -0.00003800 H -0.03830100 2.00705300 -0.00002900 O -1.83965100 0.19140100 0.00000100 H -1.01355900 -1.65704900 -0.00001900	C -0.90692200 -0.55652200 0.00000000 C 0.54405200 -0.08482800 0.00000100 O 1.42177400 -0.94883900 -0.00000100 C 0.79485700 1.31071300 0.00000000 H 1.81452500 1.66308000 0.00000100 H -0.02448500 2.01193600 -0.00000100 O -1.84237200 0.19401200 0.00000000 H -1.01718300 -1.65257800 0.00000200
PW6B95-D3/jun-cc-pVTZ	C -0.78181500 1.30730900 0.00000700 C 0.90095500 -0.55655900 -0.00000800 C -0.54225800 -0.08198100 0.00000200 H -1.79644400 1.66572000 -0.00002100 H 0.04348000 1.99823900 -0.00002800 O -1.43005400 -0.93699900 0.00000200 O 1.84162800 0.18404800 0.00000500 H 0.99908100 -1.65296500 -0.00001000	C -0.79087400 1.30530300 -0.00000200 C 0.90126700 -0.55337200 0.00000400 C -0.54096200 -0.07954400 0.00000100 H -1.80621500 1.66127600 -0.00000500 H 0.02658600 2.00463300 -0.00000400 O -1.42442800 -0.94423000 0.00000200 O 1.84438900 0.18764400 -0.00000400 H 1.00335500 -1.64753900 0.00001300
B2PLYP/aug-cc-pVTZ	C -0.90771600 -0.55773300 -0.00004700 C 0.54748000 -0.08838900 -0.00001100 O 1.42870200 -0.94706700 0.00003500 C 0.79577100 1.31562900 -0.00002000 H 1.81621900 1.66417800 -0.00000100 H -0.02499400 2.01481200 -0.00003100 O -1.85314500 0.19202900 0.00004600 H -1.00889500 -1.65572400 -0.00015100	C -0.90754600 -0.55545500 0.00000200 C 0.54590300 -0.08499300 0.00000000 O 1.42478300 -0.95304000 -0.00000100 C 0.80264500 1.31364500 0.00000000 H 1.82320300 1.66146800 0.00000000 H -0.01198000 2.01916700 0.00000400 O -1.85538100 0.19444800 -0.00000200 H -1.01245000 -1.65108800 0.00000500

Methylglyoxal geminal diol (*MGdiol*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C 0.68745800 -0.25191500 0.39944600 C -0.70617400 0.28634200 0.02160300 O -0.80162300 1.40837000 -0.41053200 C -1.86195600 -0.64819300 0.19174100 H -2.76805400 -0.20430000 -0.20826600 H -1.64010400 -1.59508600 -0.29876900 H -1.99126600 -0.85962300 1.25504900 O 0.98170000 -1.35087800 -0.43107900 H 0.67485000 -0.64505000 1.41920400 O 1.62765700 0.75129500 0.27957800 H 1.37129200 -0.99980800 -1.23900000	C 0.69574600 -0.24414600 0.39159400 C -0.70240100 0.29490900 0.03357700 O -0.80233300 1.42841700 -0.37427900 C -1.85190300 -0.64576300 0.18410900 H -2.78991300 -0.12634900 0.01649300 H -1.73927200 -1.45744300 -0.53536200 H -1.83364000 -1.09533300 1.17703400 O 0.98091400 -1.37668700 -0.38917800 H 0.69555000 -0.59868600 1.42358500 O 1.64306300 0.75552400 0.23585400 H 1.04210400 -1.11037200 -1.31441600

	H 1.17544200 1.51616400 -0.10869600	H 1.20337600 1.50015400 -0.20219200
PW6B95-D3/jun-cc-pVTZ	C -1.85810900 0.64620000 0.19077500 C 0.68843400 0.25219100 0.40011300 C -0.70394100 -0.28018400 0.02251300 H -2.75491100 0.21754700 -0.23661200 H -1.62934900 1.60474800 -0.26488600 H -2.01207600 0.82920000 1.25292200 O -0.79529400 -1.40187900 -0.41270800 O 1.61385800 -0.75978500 0.28039000 H 0.68145200 0.64807300 1.41496200 H 1.14025700 -1.51002200 -0.10857000 O 0.98985500 1.35000200 -0.42927100 H 1.34897500 0.99451100 -1.24551600	C -1.29475300 1.08177300 0.51943500 C 0.72314300 -0.30571600 -0.30803800 C -0.78986100 -0.16676900 -0.12499600 H -2.33039200 0.95999500 0.80773500 H -1.20365400 1.89815900 -0.19309300 H -0.69116600 1.35618800 1.38006500 O -1.50825300 -1.06864000 -0.48144500 O 1.22851700 0.94642800 -0.64611400 H 0.91317900 -1.05166200 -1.07382500 H 2.14353300 0.84998700 -0.91969800 O 1.29633500 -0.81587800 0.86671900 H 1.20452800 -0.16367300 1.56713800
B2PLYP/aug-cc-pVTZ	C 0.68837200 -0.25880300 0.40154700 C -0.70698200 0.27738800 0.01884700 O -0.79638600 1.40072700 -0.43864300 C -1.87308200 -0.64202800 0.20881600 H -2.76996800 -0.20966500 -0.22281600 H -1.65720300 -1.61183100 -0.23567900 H -2.02438000 -0.80515900 1.27757200 O 0.99923200 -1.34817000 -0.45306000 H 0.67954700 -0.67688900 1.40912600 O 1.62277700 0.76049600 0.31169400 H 1.35628900 -0.97252100 -1.26645100 H 1.16088100 1.51230400 -0.09694600	C 0.68789200 -0.27025200 0.39428700 C -0.70448900 0.27297500 0.01322800 O -0.77901300 1.38805000 -0.47271800 C -1.87942400 -0.61975700 0.24210100 H -2.77489700 -0.19349900 -0.19797700 H -1.68383400 -1.60923600 -0.16663400 H -2.02078100 -0.73990600 1.31767000 O 1.01856500 -1.33975100 -0.47461900 H 0.67250900 -0.71052800 1.38921800 O 1.62286800 0.75977000 0.35608900 H 1.07768300 -0.99701200 -1.37555100 H 1.20607800 1.48783400 -0.13443600

Methylglyoxal geminal diol radical on C (*MGdiol rad1*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -0.66591700 -0.10860100 0.00000100 C 0.71232400 0.20603100 0.00000100 O 0.99423100 1.42331200 0.00000100 O -1.16031100 -1.34163000 0.00000200 C 1.75206100 -0.87509200 -0.00000100 H 2.38499000 -0.75906800 -0.87923700 H 2.38502000 -0.75904000 0.87920900 H 1.31148400 -1.86862800 0.00002000 O -1.55152900 0.87592700 -0.00000100 H -2.12407000 -1.29724500 -0.00000500 H -1.00735800 1.68908400 -0.00000100	C -0.66914900 -0.10577000 -0.00000300 C 0.70871800 0.21001100 0.00000100 O 1.00391600 1.43076700 0.00000200 O -1.13869400 -1.34116600 0.00000100 C 1.74420900 -0.87363700 0.00000400 H 2.37736300 -0.76361800 -0.88035800 H 2.37741200 -0.76357800 0.88031700 H 1.30149900 -1.86556900 0.00000500 O -1.56527800 0.86606400 -0.00000300 H -2.10589500 -1.33253400 0.00002700 H -1.05260500 1.69635500 0.00000000

PW6B95-D3/jun-cc-pVTZ	C -1.74941400 0.87391700 0.00000000 C 0.66505200 0.11189800 -0.00000100 C -0.70899300 -0.19776800 0.00000100 H -2.38266800 0.76170400 -0.87571900 H -1.31389100 1.86621200 0.00002400 H -2.38270100 0.76167300 0.87569000 O -0.98244400 -1.41897900 0.00000100 O 1.53209600 -0.88452300 -0.00000100 H 0.95330700 -1.67529400 -0.00000100 O 1.16989600 1.33783900 0.00000100 H 2.12970100 1.28272900 0.00000200	C -1.74109900 0.87238600 0.00000000 C 0.66793200 0.10939900 0.00000000 C -0.70574300 -0.20261000 0.00000000 H -2.37454200 0.76673800 -0.87682500 H -1.30182800 1.86234500 0.00002000 H -2.37457000 0.76671300 0.87680100 O -0.99177200 -1.42698100 0.00000100 O 1.54659400 -0.87459100 -0.00000100 H 0.99935800 -1.68299500 -0.00000100 O 1.14701400 1.33811900 0.00000000 H 2.11035400 1.31977500 0.00000400
B2PLYP/aug-cc-pVTZ	C 0.66915900 -0.11089400 -0.00000200 C -0.71313600 0.19724600 -0.00000700 O -0.99463100 1.42319800 0.00000700 O 1.17897600 -1.34332100 0.00000400 C -1.75676200 -0.88069900 -0.00000200 H -2.39058900 -0.76527900 0.87844800 H -2.39061700 -0.76525800 -0.87842700 H -1.32181900 -1.87645400 -0.00001900 O 1.54124500 0.89125500 -0.00000200 H 2.14273800 -1.28151200 0.00000700 H 0.95999800 1.68553000 -0.00001100	C 0.67176100 -0.10826400 0.00000000 C -0.70953800 0.20175400 -0.00000100 O -1.00414100 1.43202500 -0.00000100 O 1.15524000 -1.34345200 -0.00000100 C -1.74881400 -0.87878500 0.00000100 H -2.38273200 -0.76971200 0.87963200 H -2.38275200 -0.76969500 -0.87961400 H -1.31088500 -1.87251400 -0.00001300 O 1.55685700 0.88001900 0.00000100 H 2.12281300 -1.31824800 0.00000000 H 1.00946500 1.69321100 0.00000200

Methylglyoxal geminal diol radical on O (*MGdiol rad2*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C 0.74879400 -0.34882400 0.31148000 C -0.66919900 0.33756100 0.03094800 O -0.66953100 1.49382600 -0.25886600 C -1.86357200 -0.55048300 0.13996300 H -2.76833000 0.04836800 0.17782500 H -1.87547300 -1.19917100 -0.73712900 H -1.77850300 -1.19576400 1.01260400 O 0.77788300 -1.43195700 -0.44004700 H 0.67982600 -0.63591400 1.38039700 O 1.77248400 0.56030800 0.13604200 H 1.39965100 1.37553600 -0.22507100	C 0.74879400 -0.34882400 0.31148100 C -0.66919900 0.33756100 0.03094800 O -0.66953100 1.49382600 -0.25886600 C -1.86357200 -0.55048200 0.13996300 H -2.76833000 0.04836800 0.17782500 H -1.87547200 -1.19917100 -0.73712900 H -1.77850300 -1.19576400 1.01260400 O 0.77788300 -1.43195700 -0.44004700 H 0.67982600 -0.63591400 1.38039700 O 1.77248400 0.56030800 0.13604100 H 1.39965100 1.37553600 -0.22507100
PW6B95-D3/jun-cc-pVTZ (suffers decomposition in the calculation in bulk	C 0.76023300 -0.33090700 0.30134800 C -0.68362700 0.33836300 0.02990000 O -0.70463500 1.50868400 -0.18194000	C 1.75179000 -0.06446300 0.35742100 C -1.63081200 0.28449200 0.06306900 O -2.42323400 1.15023800 -0.03195400

solvent)	C -1.84101700 -0.58842600 0.07585200 H -2.76896000 -0.03251100 0.10615900 H -1.79871500 -1.21095500 -0.81511600 H -1.75153000 -1.25816500 0.92490500 O 0.80182500 -1.45854200 -0.33654600 H 0.68593800 -0.49983400 1.39826100 O 1.76135500 0.58061500 0.02583800 H 1.35136000 1.44123100 -0.11563700	C -1.80638100 -1.19151700 -0.04115500 H -2.84806900 -1.45434300 -0.20629100 H -1.18475900 -1.55068200 -0.85552600 H -1.43268200 -1.64760100 0.87018300 O 1.85847500 -1.13538800 -0.16451900 H 1.37550100 0.08349900 1.37246800 O 2.09796200 1.05710400 -0.27176500 H 1.93679700 1.82242400 0.28905600
B2PLYP/aug-cc-pVTZ (suffers decomposition in the calculation in gas phase)	C 1.76744700 -0.41014400 0.36372500 C -1.63325100 0.40188100 0.44748300 O -1.27160600 1.39848800 -0.08170700 C -2.38734300 -0.76001300 -0.12719500 H -2.87740100 -0.48731800 -1.06276200 H -1.64409400 -1.53628200 -0.31495100 H -3.10084500 -1.14193400 0.59564200 O 1.01231600 -1.12688100 -0.23972300 H 2.06935400 -0.54411600 1.40733600 O 2.38307100 0.67023300 -0.13807000 H 2.08161400 0.78459000 -1.05334400	C 0.74879400 -0.34882400 0.31148100 C -0.66919900 0.33756100 0.03094800 O -0.66953100 1.49382600 -0.25886600 C -1.86357200 -0.55048200 0.13996300 H -2.76833000 0.04836800 0.17782500 H -1.87547200 -1.19917100 -0.73712900 H -1.77850300 -1.19576400 1.01260400 O 0.77788300 -1.43195700 -0.44004700 H 0.67982600 -0.63591400 1.38039700 O 1.77248400 0.56030800 0.13604100 H 1.39965100 1.37553600 -0.22507100

Methylglyoxal geminal diol radical on CH_3 (*MGdiol rad3*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -0.68241600 0.18888300 0.39256500 C 0.77106900 -0.18915900 0.05363900 O 1.02610500 -1.33387500 -0.30241100 C 1.76440800 0.83306500 0.15062600 H 2.78909700 0.58900100 -0.08315100 H 1.49600000 1.83496100 0.44722400 O -1.06905100 1.31337900 -0.35485000 H -0.74569000 0.50310600 1.43829400 O -1.50830000 -0.89386500 0.15854100 H -1.30343400 1.00838500 -1.23812500 H -0.94437400 -1.61730200 -0.15546500	C -0.67843700 0.21933700 0.38807600 C 0.76432400 -0.19547900 0.05164600 O 0.97598400 -1.33413900 -0.36056500 C 1.79087600 0.78047700 0.20699400 H 2.80771800 0.52061300 -0.04326000 H 1.56128000 1.76723500 0.57730300 O -1.05939800 1.30768600 -0.41530500 H -0.73165600 0.58967700 1.41257200 O -1.52314500 -0.86977300 0.23911000 H -1.03463900 1.03746500 -1.34106700 H -1.01080800 -1.57119200 -0.19176600
PW6B95-D3/jun-cc-pVTZ	C -1.75870700 0.82958700 0.15777800 C 0.68350100 0.19075500 0.39217800 C -0.76876200 -0.17821400 0.05524700 H -2.78069800 0.58656900 -0.07649000 H -1.49829500 1.82803500 0.46284400 O -1.02049500 -1.32438700 -0.31271400	C -1.78162300 0.78508000 0.20557200 C 0.67971300 0.21619200 0.38746200 C -0.76298800 -0.18318200 0.05179700 H -2.79727000 0.52753900 -0.03977000 H -1.55475000 1.77033700 0.57293700 O -0.97753100 -1.32446900 -0.36202000

	O 1.49121800 -0.90393600 0.16980600 H 0.75345400 0.51603200 1.43010100 H 0.90854000 -1.60777800 -0.15093700 O 1.08043000 1.30637100 -0.36264900 H 1.27159000 0.99999200 -1.25227200	O 1.50361400 -0.88536700 0.23638200 H 0.74053600 0.58550500 1.40792000 H 0.96234100 -1.57225500 -0.17957400 O 1.07523200 1.30211700 -0.41126200 H 1.02800800 1.04208700 -1.33530600
B2PLYP/aug-cc-pVTZ	C -0.68131100 0.20488600 0.39495700 C 0.77016300 -0.18634600 0.05122300 O 1.00355500 -1.32980200 -0.34313000 C 1.78740700 0.81135700 0.18081100 H 2.80647800 0.55130900 -0.05827400 H 1.54561200 1.80996500 0.50728500 O -1.07377200 1.31217000 -0.39374000 H -0.74371700 0.55940600 1.42548900 O -1.50930600 -0.89172000 0.20849500 H -1.28848100 0.97615800 -1.27205400 H -0.94125600 -1.60141400 -0.13738600	C -0.67680300 0.23086100 0.39034400 C 0.76518800 -0.18839900 0.04754600 O 0.96208600 -1.32448400 -0.39720200 C 1.80931500 0.76664100 0.23125500 H 2.82164300 0.49447600 -0.02199100 H 1.60000000 1.74729800 0.62656100 O -1.07317100 1.30178600 -0.44620400 H -0.73043600 0.63290800 1.40042800 O -1.51809400 -0.87323400 0.28180800 H -1.04443500 1.00347800 -1.36423200 H -0.99952700 -1.56532700 -0.16284300

Acrolein (**AC**)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	H 2.09555000 0.64892700 0.00000000 C 1.20796100 1.27161700 0.00000000 H 1.35626700 2.34236300 0.00000000 C 0.00000000 0.72332000 0.00000000 H -0.91167100 1.30720600 0.00000000 C -0.15098200 -0.74349400 0.00000000 O -1.21032600 -1.31221600 0.00000000 H 0.80059100 -1.30942300 0.00000000	H 2.09704000 0.63163200 0.00000000 C 1.21484500 1.26135300 0.00000000 H 1.36963900 2.33114900 0.00000000 C 0.00000000 0.72388900 0.00000000 H -0.90489900 1.31834600 0.00000000 C -0.15130200 -0.73609200 0.00000000 O -1.21711900 -1.30874900 0.00000000 H 0.79391500 -1.30603300 0.00000000
PW6B95-D3/jun-cc-pVTZ	H 2.09176600 0.64824100 0.00000000 C 1.20699800 1.26797600 0.00000000 H 1.35585700 2.33474000 0.00000000 C 0.00000000 0.71944700 0.00000000 H -0.90627500 1.30492900 0.00000000 C -0.15165400 -0.73749200 0.00000000 O -1.20915900 -1.31103500 0.00000000 H 0.79986700 -1.29921000 0.00000000	H 2.09320600 0.63109300 0.00000000 C 1.21391700 1.25775700 0.00000000 H 1.36914500 2.32346200 0.00000000 C 0.00000000 0.71997900 0.00000000 H -0.89934200 1.31608600 0.00000000 C -0.15200500 -0.72988100 0.00000000 O -1.21591300 -1.30778900 0.00000000 H 0.79282300 -1.29545600 0.00000000
B2PLYP/aug-cc-pVTZ	H 2.10298100 0.66836500 0.00000000 C 1.21041200 1.28099500 0.00000000 H 1.34757900 2.35195600 0.00000000 C 0.00000000 0.71986300 0.00000000	H 2.10433000 0.65108100 0.00000000 C 1.21720600 1.27083200 0.00000000 H 1.36065000 2.34082400 0.00000000 C 0.00000000 0.72029700 0.00000000

	H -0.91058900 1.30360800 0.00000000 C -0.14820600 -0.74226600 0.00000000 O -1.21466500 -1.32118800 0.00000000 H 0.80411900 -1.30597800 0.00000000	H -0.90392400 1.31430800 0.00000000 C -0.14844900 -0.73486900 0.00000000 O -1.22130500 -1.31762400 0.00000000 H 0.79684200 -1.30278600 0.00000000

Acrolein radical on C (*AC rad1*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	H 2.08975600 0.62580100 0.00000000 C 1.20627000 1.25116100 0.00000000 H 1.34128500 2.32381500 0.00000000 C 0.00000000 0.70151700 0.00000000 H -0.91669600 1.28287800 0.00000000 C -0.13465400 -0.77049500 0.00000000 O -1.11800500 -1.41569800 0.00000000	H 2.09366500 0.61611500 0.00000000 C 1.21228600 1.24432100 0.00000000 H 1.35233600 2.31612500 0.00000000 C 0.00000000 0.70356400 0.00000000 H -0.91243100 1.29091800 0.00000000 C -0.14050200 -0.76026600 0.00000000 O -1.12053500 -1.41860900 0.00000000
PW6B95-D3/jun-cc-pVTZ	H 2.08859700 0.64411100 0.00000000 C 1.20025700 1.25494900 0.00000000 H 1.32382200 2.32511800 0.00000000 C 0.00000000 0.69382100 0.00000000 H -0.91464000 1.27328900 0.00000000 C -0.13179700 -0.76620300 0.00000000 O -1.11356800 -1.41724000 0.00000000	H 2.09247300 0.63597400 0.00000000 C 1.20581100 1.24894900 0.00000000 H 1.33336800 2.31833900 0.00000000 C 0.00000000 0.69549400 0.00000000 H -0.91062300 1.28033500 0.00000000 C -0.13708100 -0.75664500 0.00000000 O -1.11595000 -1.42017900 0.00000000
B2PLYP/aug-cc-pVTZ	H 2.09850500 0.65781000 0.00000000 C 1.20483700 1.26529500 0.00000000 H 1.32129000 2.33879600 0.00000000 C 0.00000000 0.69543200 0.00000000 H -0.91763200 1.27471700 0.00000000 C -0.12914400 -0.77019800 0.00000000 O -1.11954000 -1.42681300 0.00000000	H 2.10215200 0.64916800 0.00000000 C 1.21033200 1.25913000 0.00000000 H 1.33095700 2.33187500 0.00000000 C 0.00000000 0.69714800 0.00000000 H -0.91378300 1.28156400 0.00000000 C -0.13447600 -0.76099900 0.00000000 O -1.12180700 -1.42928500 0.00000000

Acrolein radical on Cα (*AC rad2*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	H 2.06485000 1.00855300 0.00000000 C 1.07274700 1.45979600 0.00000000 H 1.02586500 2.54188800 0.00000000 C 0.00000000 0.70894100 0.00000000 C -0.14697500 -0.74763300 0.00000000 O -1.18402600 -1.34948700 0.00000000	H 2.06176400 1.01904000 0.00000000 C 1.06703200 1.46374800 0.00000000 H 1.01167900 2.54564400 0.00000000 C 0.00000000 0.70340800 0.00000000 C -0.13836200 -0.74792500 0.00000000 O -1.18421700 -1.34927700 0.00000000

	H 0.82686000 -1.28117100 0.00000000	H 0.82826900 -1.28584400 0.00000000
PW6B95-D3/jun-cc-pVTZ	H 2.05536700 1.05646100 0.00000000 C 1.05249200 1.47641800 0.00000000 H 0.98143400 2.55378000 0.00000000 C 0.00000000 0.70174700 0.00000000 C -0.14322600 -0.74447500 0.00000000 O -1.16645800 -1.36892100 0.00000000 H 0.83926700 -1.26101400 0.00000000	H 2.05084200 1.06855200 0.00000000 C 1.04539300 1.48122600 0.00000000 H 0.96539500 2.55805500 0.00000000 C 0.00000000 0.69571300 0.00000000 C -0.13353100 -0.74512800 0.00000000 O -1.16607000 -1.36890200 0.00000000 H 0.84115400 -1.26625300 0.00000000
B2PLYP/aug-cc-pVTZ	H 2.05760200 1.07031600 0.00000000 C 1.05115100 1.48799800 0.00000000 H 0.97248200 2.56703100 0.00000000 C 0.00000000 0.70329000 0.00000000 C -0.13690100 -0.75027500 0.00000000 O -1.17021500 -1.37685700 0.00000000 H 0.84613500 -1.26857200 0.00000000	H 2.05356100 1.08061000 0.00000000 C 1.04495200 1.49196300 0.00000000 H 0.95804100 2.57045500 0.00000000 C 0.00000000 0.69726800 0.00000000 C -0.12767600 -0.75035100 0.00000000 O -1.17031000 -1.37633800 0.00000000 H 0.84722300 -1.27364000 0.00000000

Acrolein radical on Cβ cis (*AC rad3*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C 1.02356900 -1.51782100 0.00000000 H 2.08485800 -1.32289800 0.00000000 C -0.06595100 -0.79374600 0.00000000 C 0.00000000 0.69168600 0.00000000 O -0.97360300 1.39399500 0.00000000 H 1.01880900 1.11785500 0.00000000 H -1.06054600 -1.22762600 0.00000000	C 1.03091500 -1.50812300 0.00000000 H 2.09177000 -1.30988800 0.00000000 C -0.06703400 -0.79364200 0.00000000 C 0.00000000 0.68481700 0.00000000 O -0.97895500 1.39189800 0.00000000 H 1.01395900 1.11399800 0.00000000 H -1.05737500 -1.23761300 0.00000000
PW6B95-D3/jun-cc-pVTZ	C 1.02203500 -1.51700100 0.00000000 H 2.08551600 -1.35840100 0.00000000 C -0.05958900 -0.78801100 0.00000000 C 0.00000000 0.69332200 0.00000000 O -0.97742800 1.38995800 0.00000000 H 1.01301700 1.12359300 0.00000000 H -1.05378600 -1.21471300 0.00000000	C 1.02909600 -1.50728700 0.00000000 H 2.09236800 -1.34648000 0.00000000 C -0.06091600 -0.78768300 0.00000000 C 0.00000000 0.68623100 0.00000000 O -0.98236700 1.38811700 0.00000000 H 1.00820900 1.11893200 0.00000000 H -1.05072200 -1.22494800 0.00000000
B2PLYP/aug-cc-pVTZ	C 1.02901400 -1.52162500 0.00000000 H 2.09449800 -1.36170200 0.00000000 C -0.05874100 -0.79243100 0.00000000 C 0.00000000 0.69462600 0.00000000 O -0.98479400 1.39712100 0.00000000 H 1.01510800 1.12620400 0.00000000 H -1.05289300 -1.22489700 0.00000000	C 1.03657000 -1.51168800 0.00000000 H 2.10174900 -1.34875600 0.00000000 C -0.05974100 -0.79179600 0.00000000 C 0.00000000 0.68747200 0.00000000 O -0.99035000 1.39459700 0.00000000 H 1.00959100 1.12262600 0.00000000 H -1.04951700 -1.23457400 0.00000000

Acrolein radical on Cβ trans (*AC rad4*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C 1.10609500 -1.43270400 0.00000000 H 1.41718500 -2.46397300 0.00000000 C -0.00863500 -0.74856500 0.00000000 C 0.00000000 0.73362900 0.00000000 O -1.00185500 1.39701900 0.00000000 H 1.00157300 1.19689400 0.00000000 H -0.98867900 -1.22322700 0.00000000	C 1.10962900 -1.42496600 0.00000000 H 1.43210100 -2.45315500 0.00000000 C -0.01253600 -0.74920600 0.00000000 C 0.00000000 0.72540500 0.00000000 O -1.00332900 1.39897300 0.00000000 H 0.99879900 1.18923900 0.00000000 H -0.98682500 -1.23526600 0.00000000
PW6B95-D3/jun-cc-pVTZ	C 1.10130500 -1.43916600 0.00000000 H 1.42120300 -2.46403400 0.00000000 C 0.00028600 -0.74065000 0.00000000 C 0.00000000 0.73475900 0.00000000 O -1.00572600 1.39274500 0.00000000 H 0.99507600 1.20323500 0.00000000 H -0.98001600 -1.21081500 0.00000000	C 1.10475600 -1.43143800 0.00000000 H 1.43476100 -2.45351500 0.00000000 C -0.00387800 -0.74108800 0.00000000 C 0.00000000 0.72625100 0.00000000 O -1.00683300 1.39504900 0.00000000 H 0.99243400 1.19468100 0.00000000 H -0.97780000 -1.22391000 0.00000000
B2PLYP/aug-cc-pVTZ	C 1.10885800 -1.44329700 0.00000000 H 1.42895900 -2.47049100 0.00000000 C 0.00167700 -0.74465900 0.00000000 C 0.00000000 0.73649700 0.00000000 O -1.01381200 1.39912500 0.00000000 H 0.99661200 1.20712000 0.00000000 H -0.97828600 -1.22087400 0.00000000	C 1.11282400 -1.43531200 0.00000000 H 1.44305700 -2.45969200 0.00000000 C -0.00203100 -0.74480300 0.00000000 C 0.00000000 0.72812900 0.00000000 O -1.01564200 1.40057900 0.00000000 H 0.99314200 1.19999600 0.00000000 H -0.97581700 -1.23302100 0.00000000

Acrolein geminal diol (*ACdiol*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -1.94222200 0.03471200 -0.15049000 H -2.89247600 -0.46585100 -0.27335500 C -0.85473700 -0.64297100 0.16901000 C 0.49665300 -0.02245300 0.35976100 O 1.41469100 -0.84397000 -0.31959200 H 0.74806700 -0.00645000 1.42859600 H -0.87691700 -1.71566900 0.31589400 H -1.90582000 1.10395200 -0.30591800 O 0.49460700 1.29126200 -0.13163100 H 2.30666300 -0.52444200 -0.16163400	C -1.94380500 0.03476000 -0.16217500 H -2.89587400 -0.46659000 -0.26885100 C -0.85844600 -0.63538900 0.18544200 C 0.49964700 -0.02439400 0.36263900 O 1.40873400 -0.83215400 -0.35305400 H 0.77521000 -0.03160300 1.42250100 H -0.89442700 -1.70152900 0.37482000 H -1.90906200 1.09947200 -0.34786500 O 0.49054400 1.29575900 -0.10832100 H 2.30447900 -0.62746500 -0.06728500

	H 1.14793700 1.81439400 0.33651400	H 1.24106800 1.76900600 0.26223800
PW6B95-D3/jun-cc-pVTZ	C -1.93959400 0.02663400 -0.14569000 H -2.88444300 -0.47635400 -0.26743100 C -0.84769700 -0.64429600 0.16489700 C 0.49502300 -0.01955200 0.35534900 O 1.41829200 -0.83871700 -0.31796400 H 0.74403300 0.00081500 1.42160600 H -0.86393400 -1.71381200 0.30653200 H -1.91195700 1.09302200 -0.29488100 O 0.48678100 1.29335300 -0.13615300 H 2.30629600 -0.53665600 -0.12607200 H 1.12303100 1.81918300 0.34584900	C -1.94252600 0.02695400 -0.15564700 H -2.88853600 -0.47763400 -0.26233300 C -0.85161900 -0.63703000 0.17829900 C 0.49711600 -0.02114800 0.35780400 O 1.41472900 -0.82840000 -0.34701800 H 0.76714700 -0.02259300 1.41574700 H -0.88001000 -1.70112400 0.35715100 H -1.91819700 1.08982300 -0.32998100 O 0.48400100 1.29691300 -0.11577500 H 2.30155400 -0.62819400 -0.04243900 H 1.21037200 1.77895900 0.28146300
B2PLYP/aug-cc-pVTZ	C -1.95150100 0.02738400 -0.14654100 H -2.89503200 -0.48356900 -0.26879600 C -0.85080500 -0.64459000 0.16660000 C 0.49685700 -0.01914500 0.35971600 O 1.42299700 -0.84711200 -0.31987300 H 0.75156600 0.00322900 1.42629500 H -0.86932900 -1.71686800 0.30792400 H -1.92984500 1.09615100 -0.29609000 O 0.49232600 1.30162500 -0.13810600 H 2.31463600 -0.54030300 -0.12909800 H 1.13812200 1.82335700 0.34495100	C -1.95378500 0.02812500 -0.15798500 H -2.89910200 -0.48361900 -0.26359300 C -0.85519900 -0.63683400 0.18199400 C 0.49908100 -0.02105200 0.36244300 O 1.41836000 -0.83705500 -0.35054100 H 0.77642400 -0.02108500 1.42030400 H -0.88712400 -1.70289100 0.36501200 H -1.93386900 1.09258800 -0.33703600 O 0.49015700 1.30509900 -0.11672900 H 2.30963800 -0.63286800 -0.04684400 H 1.22531400 1.78208600 0.28160600

Acrolein geminal diol radical on C (*ACdiol rad1*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -2.02168600 0.05257700 0.01617300 H -2.96369600 -0.47104200 -0.00121100 C -0.83235600 -0.64313700 -0.01789300 C 0.41011800 -0.06151800 -0.00824000 O 1.54795200 -0.79508600 0.08512100 H -0.83121700 -1.72389100 -0.05831700 H -2.03408700 1.13097100 0.05638800 O 0.57987900 1.28084900 -0.07708500 H 2.20098600 -0.46201600 -0.54180400 H 1.26891500 1.55234300 0.54041500	C -2.02408800 0.05522000 0.01714300 H -2.96520800 -0.47080700 -0.00692400 C -0.83159700 -0.64025600 -0.02103200 C 0.41394500 -0.06005400 -0.00738700 O 1.53987400 -0.80247900 0.07796300 H -0.83304200 -1.72094700 -0.07022800 H -2.04159500 1.13357700 0.07035200 O 0.56975200 1.27854200 -0.06039100 H 2.24064300 -0.42592900 -0.47028200 H 1.37262900 1.54614300 0.40416700
PW6B95-D3/jun-cc-pVTZ	C -2.00442400 0.00028600 -0.00000300 H -2.93005200 -0.54443600 0.00000600 C -0.79497300 -0.66233800 0.00000300	C 2.01090400 0.00267700 0.00072900 H 2.93166400 -0.55161600 -0.00111100 C 0.79730300 -0.65566200 -0.00082900

	C 0.43533000 -0.06265500 0.00000000 O 1.57413700 -0.76748200 -0.00000300 H -0.77564100 -1.73980900 0.00001100 H -2.08490800 1.07684400 -0.00001900 O 0.65677700 1.26546200 0.00000000 H 2.31250800 -0.15427100 0.00000800 H -0.18481800 1.72607400 0.00002300	C -0.43577100 -0.05707900 -0.00014700 O -1.56527700 -0.77728100 0.00101100 H 0.77699200 -1.73377100 -0.00295100 H 2.09393800 1.07824900 0.00420700 O -0.66945600 1.26486000 0.00031600 H -2.32001300 -0.18166200 -0.00296600 H 0.16066200 1.74855000 -0.00631400
B2PLYP/aug-cc-pVTZ	C -2.01662800 0.00244700 -0.00000100 H -2.94162500 -0.54846200 0.00000400 C -0.79924400 -0.66111500 0.00000400 C 0.43473400 -0.06234400 0.00000000 O 1.57665900 -0.77721500 -0.00000700 H -0.78019700 -1.74125600 0.00001000 H -2.09984500 1.08098400 -0.00001000 O 0.66856900 1.27181500 0.00000000 H 2.31971400 -0.16295600 0.00003700 H -0.17304100 1.74096100 0.00000300	C -2.02288800 0.00491300 -0.00923600 H -2.94295600 -0.55511200 0.01413700 C -0.80156200 -0.65452400 0.01089700 C 0.43517700 -0.05689500 0.00218700 O 1.56819700 -0.78643300 -0.01370700 H -0.78197200 -1.73498800 0.03793900 H -2.10849400 1.08163800 -0.05396600 O 0.68042400 1.27103400 -0.00417500 H 2.32644100 -0.19088300 0.04230100 H -0.14635500 1.76157400 0.07955800

Acrolein geminal diol radical on O (*ACdiol rad2*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -1.86942600 0.13870500 -0.18803500 H -2.86506300 -0.27479200 -0.27065100 C -0.85852500 -0.61851300 0.19307600 C 0.56084500 -0.10278800 0.32775700 O 1.40409900 -0.87825900 -0.38333900 H -0.97108700 -1.66802400 0.42999800 H -1.72650300 1.18396200 -0.42163800 O 0.61573200 1.25942700 0.01900800 H 1.52665200 1.47484000 -0.20022500 H 0.87998800 -0.26975300 1.38036900	C -1.86309900 0.14713900 -0.18708800 H -2.86150500 -0.26339600 -0.25026000 C -0.85556100 -0.60312000 0.21969600 C 0.57047900 -0.09596600 0.33135100 O 1.36655300 -0.91384200 -0.39910700 H -0.97847600 -1.64229000 0.49315600 H -1.72096700 1.18413300 -0.45636800 O 0.63477200 1.25142200 -0.03280100 H 1.53327600 1.56667100 0.10749600 H 0.90615400 -0.23407000 1.37748100
PW6B95-D3/jun-cc-pVTZ	C -1.86780900 0.14185900 -0.19026500 H -2.86167300 -0.26697300 -0.27122800 C -0.86135800 -0.61867100 0.18695200 C 0.56252300 -0.10796700 0.31703300 O 1.40089100 -0.87209800 -0.37590300 H -0.97233900 -1.66408700 0.42365200 H -1.72446800 1.18327100 -0.42134100 O 0.62676200 1.26131400 0.04729100 H 1.47790500 1.42687000 -0.36166500	C -1.86344400 0.14613800 -0.18879400 H -2.85930700 -0.26183400 -0.24656500 C -0.85780600 -0.60510600 0.21223100 C 0.56937100 -0.10240800 0.31687800 O 1.37388300 -0.90135600 -0.39177000 H -0.97713300 -1.64024100 0.48553000 H -1.72448700 1.17913000 -0.45813900 O 0.63009800 1.25418100 -0.00751700 H 1.55051700 1.52473400 0.00255800

	H 0.85920400 -0.28414100 1.37715300	H 0.88983700 -0.25614100 1.36902400
B2PLYP/aug-cc-pVTZ	C -1.87604300 0.13980300 -0.19367700	C -1.85797500 0.16200000 -0.20544300
	H -2.87006400 -0.27673000 -0.26573400	H -2.86179500 -0.23516700 -0.24383300
	C -0.86015600 -0.61459000 0.20142600	C -0.86041700 -0.58399100 0.25171900
	C 0.56446500 -0.10678900 0.32498900	C 0.57867400 -0.10369100 0.33746700
	O 1.40103600 -0.88520800 -0.38883200	O 1.32587900 -0.93910600 -0.42572000
	H -0.97900600 -1.65818200 0.45546100	H -1.00720500 -1.60227800 0.58063900
	H -1.73733100 1.17932800 -0.44613200	H -1.70129000 1.17749700 -0.53450700
	O 0.62306000 1.26719500 0.02675000	O 0.66145800 1.25432100 -0.02155200
	H 1.53211800 1.46751200 -0.21851400	H 1.57265000 1.54233400 0.10059400
	H 0.89192700 -0.27836300 1.37515700	H 0.93725700 -0.25000900 1.37282900

Acrolein geminal diol radical on Cα (*ACdiol rad3*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -2.00864300 -0.09475500 -0.17682700	C -2.03910700 -0.09213200 -0.12129700
	H -2.92686500 -0.66708600 -0.12642400	H -2.92588200 -0.71354100 -0.16015600
	C -0.88038400 -0.55829100 0.28128500	C -0.87159500 -0.57059400 0.20518800
	C 0.50957800 -0.05064400 0.39489600	C 0.50103000 -0.03499300 0.36674600
	O 1.34869800 -0.91051000 -0.30277600	O 1.37635600 -0.90626300 -0.30416500
	H -2.05634800 0.88566100 -0.64760000	H -2.15527700 0.96174100 -0.36783600
	O 0.64601600 1.24108100 -0.17350400	O 0.53435600 1.26368700 -0.17532800
	H 0.27685600 1.89043700 0.43167700	H 1.21344300 1.77814600 0.27210400
	H 0.79372400 -0.00355400 1.45431900	H 0.76010200 0.00478700 1.42845100
	H 2.23161100 -0.52789100 -0.29785000	H 2.27995200 -0.70420300 -0.04044000
PW6B95-D3/jun-cc-pVTZ	C -2.02045800 -0.08999700 -0.16796700	C -2.03510400 -0.10219200 -0.14165300
	H -2.92809200 -0.67213500 -0.10836200	H -2.92293100 -0.71746200 -0.12942100
	C -0.88178200 -0.53663000 0.26885400	C -0.87275400 -0.55286000 0.22589400
	C 0.50655500 -0.05215700 0.38915100	C 0.50441800 -0.04049100 0.37481000
	O 1.33941400 -0.92302300 -0.29690000	O 1.36460700 -0.91124300 -0.29145300
	H -2.09570400 0.88925600 -0.63162100	H -2.15602600 0.92227800 -0.48149700
	O 0.66293600 1.23860700 -0.18268800	O 0.63100500 1.24676300 -0.20339000
	H 0.36996000 1.89439500 0.45151100	H 0.50844800 1.90825700 0.48004700
	H 0.78127600 0.00001900 1.44769900	H 0.75992200 0.02050100 1.43348700
	H 2.22787200 -0.56350100 -0.26275200	H 2.26633300 -0.64448100 -0.09816900
B2PLYP/aug-cc-pVTZ	C -2.02929100 -0.08620400 -0.17049600	C -2.16347000 -0.00000200 0.06927700
	H -2.93886700 -0.66899800 -0.10641300	H -3.00582700 -0.00001500 -0.61040300
	C -0.88744600 -0.53354800 0.27636800	C -0.92657400 -0.00001600 -0.34763100
	C 0.50775100 -0.05181600 0.39365000	C 0.42188700 0.00000000 0.25557000
	O 1.33625200 -0.93524000 -0.30024800	O 1.09074200 -1.17322200 -0.16450400

	H -2.09998600 0.89105700 -0.64396200 O 0.67204600 1.24534600 -0.18653600 H 0.40380400 1.90587700 0.46061900 H 0.79106700 0.00139900 1.45140800 H 2.23150800 -0.58077800 -0.26451100	H -2.39337000 0.00002000 1.13439900 O 1.09072300 1.17322600 -0.16451700 H 1.81319400 1.34981100 0.44842300 H 0.32997500 0.00000500 1.34804600 H 1.81325300 -1.34975300 0.44840400

Acrolein geminal diol radical on Cβ cis (*ACdiol rad4*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -1.99149000 -0.08692300 -0.17950600 C -0.89257100 -0.70402200 0.14801600 C 0.43131700 -0.01223800 0.35978100 O 1.39570800 -0.76487100 -0.33105300 H -2.28115200 0.93041900 -0.38141600 O 0.33741900 1.30538600 -0.10642800 H 1.04866600 1.83197200 0.26485100 H 0.67312100 -0.00631600 1.43018300 H 2.27572500 -0.48105800 -0.07095400 H -0.86491900 -1.78003700 0.28743800	C -1.99301400 -0.08125100 -0.19032300 C -0.89913300 -0.69372500 0.16480800 C 0.43503000 -0.01389000 0.36290200 O 1.38485300 -0.76560100 -0.35391200 H -2.29445600 0.92659700 -0.42262200 O 0.34976500 1.30643700 -0.09612200 H 1.08482700 1.81341200 0.26159800 H 0.69539300 -0.02081700 1.42577700 H 2.26682700 -0.54829500 -0.03587100 H -0.88683000 -1.76438500 0.34706200
PW6B95-D3/jun-cc-pVTZ	C -1.98732300 -0.09549500 -0.17296300 C -0.88622800 -0.70531300 0.14386500 C 0.43137000 -0.00858800 0.35548400 O 1.39990900 -0.76003000 -0.32775300 H -2.31196300 0.90816100 -0.37033100 O 0.33144700 1.30651100 -0.11282800 H 1.02049400 1.83926600 0.28258600 H 0.66806000 0.00132200 1.42382600 H 2.27346500 -0.48609600 -0.04750500 H -0.84781400 -1.77812800 0.27776400	C -1.98967400 -0.09031900 -0.18318000 C -0.89295100 -0.69567400 0.15910700 C 0.43471700 -0.01028200 0.35808400 O 1.39111300 -0.75883700 -0.35064500 H -2.32535300 0.90436600 -0.40787300 O 0.34227500 1.30775900 -0.10132400 H 1.06191600 1.81908400 0.27196600 H 0.68890600 -0.01487000 1.41903500 H 2.26327800 -0.55871500 -0.00578900 H -0.86840200 -1.76359600 0.33434600
B2PLYP/aug-cc-pVTZ	C -1.99932200 -0.09383600 -0.17333700 C -0.89112400 -0.70337000 0.14520800 C 0.43207300 -0.00805400 0.35959000 O 1.40206600 -0.77385100 -0.32632700 H -2.33089400 0.90942300 -0.37232700 O 0.34292100 1.31460400 -0.11852000 H 1.02497700 1.84768100 0.29900700 H 0.67254200 0.00699600 1.42878400 H 2.27983700 -0.47972700 -0.06420400 H -0.85611700 -1.77883600 0.27874600	C -2.00124600 -0.08900700 -0.18471100 C -0.89788200 -0.69348400 0.16218500 C 0.43567500 -0.01002200 0.36234300 O 1.39323900 -0.77058700 -0.35264600 H -2.34376900 0.90437100 -0.41462900 O 0.35155800 1.31615200 -0.10382200 H 1.07709300 1.82285300 0.27600800 H 0.69614700 -0.01202600 1.42365500 H 2.27044400 -0.56121700 -0.01310800 H -0.87757800 -1.76343000 0.34091900

Acrolein geminal diol radical on Cβ trans (*ACdiol rad5*)

Method	Gas-Phase	Bulk water solvent
M06-2X-D3/aug-cc-pVTZ	C -1.97689200 0.13254300 -0.15139700 C -0.93028700 -0.58543800 0.14046200 C 0.44386800 -0.01132100 0.35615300 O 1.34139800 -0.88716500 -0.27697100 H -3.02000200 -0.04989000 -0.34647200 O 0.51322000 1.28446000 -0.17273500 H 1.06353300 1.83557100 0.38648600 H 0.66205600 0.02302700 1.43123900 H 2.23162300 -0.53507300 -0.19498400 H -0.99428500 -1.66669200 0.25007500	C -1.96973000 0.12574700 -0.18843900 C -0.93365500 -0.57299800 0.18093200 C 0.45192500 -0.01500300 0.36037900 O 1.32864600 -0.86494900 -0.34175000 H -3.01604900 -0.05640700 -0.36962400 O 0.48766600 1.29851000 -0.12623100 H 1.27222700 1.73873400 0.21466400 H 0.71763900 -0.02254500 1.42207500 H 2.22786500 -0.71701400 -0.03266100 H -1.02341700 -1.63773000 0.39216600
PW6B95-D3/jun-cc-pVTZ	C 2.10712900 -0.00340800 -0.25326600 C 0.97082600 -0.14226200 0.35826500 C -0.36755100 -0.00889300 -0.30832300 O -1.13351900 -1.10652500 0.05423600 H 3.15613100 -0.02414500 -0.02674100 O -1.05225300 1.14157400 0.14924300 H -0.58260800 1.91941000 -0.15552400 H -0.24143100 0.04941200 -1.39168600 H -2.02713500 -0.95946200 -0.26128700 H 0.91879000 -0.33821700 1.42735500	C 2.10781300 -0.00689900 -0.26188500 C 0.97359900 -0.10083300 0.36266400 C -0.36985000 -0.00497500 -0.30062500 O -1.10456100 -1.12428800 0.07783500 H 3.15865200 -0.01703100 -0.04104500 O -1.07628100 1.13430600 0.15447000 H -0.72060000 1.91013600 -0.28409800 H -0.25601400 0.04621800 -1.38271600 H -1.94009500 -1.11134400 -0.39447900 H 0.93542200 -0.23187500 1.44297500
B2PLYP/aug-cc-pVTZ	C 2.11654500 -0.00167300 -0.25545800 C 0.97460000 -0.13383000 0.36127000 C -0.36616500 -0.00901300 -0.30987200 O -1.12971400 -1.11829600 0.05668100 H 3.16704700 -0.02148500 -0.02472300 O -1.06637000 1.14431500 0.14946900 H -0.60576400 1.92723500 -0.17049500 H -0.24313800 0.04946200 -1.39566500 H -2.02561800 -0.97818600 -0.26890600 H 0.92627000 -0.31807400 1.43494300	C 2.11397600 -0.00000200 -0.28734500 C 0.98177300 0.00000100 0.36040500 C -0.37052000 0.00000000 -0.29286000 O -1.03928100 -1.17123900 0.13818500 H 3.16778600 0.00001000 -0.06901400 O -1.03928400 1.17123700 0.13818700 H -1.78610300 1.33664300 -0.44789300 H -0.28185000 0.00000200 -1.37889400 H -1.78611400 -1.33663300 -0.44788100 H 0.96343200 0.00000000 1.45149800