- Supporting Information -

Difficulties of Popular Density Functionals to Describe the Conformational Isomerism in Iodoacetic Acid

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Table of Contents

1. Additional Infrared Spectra

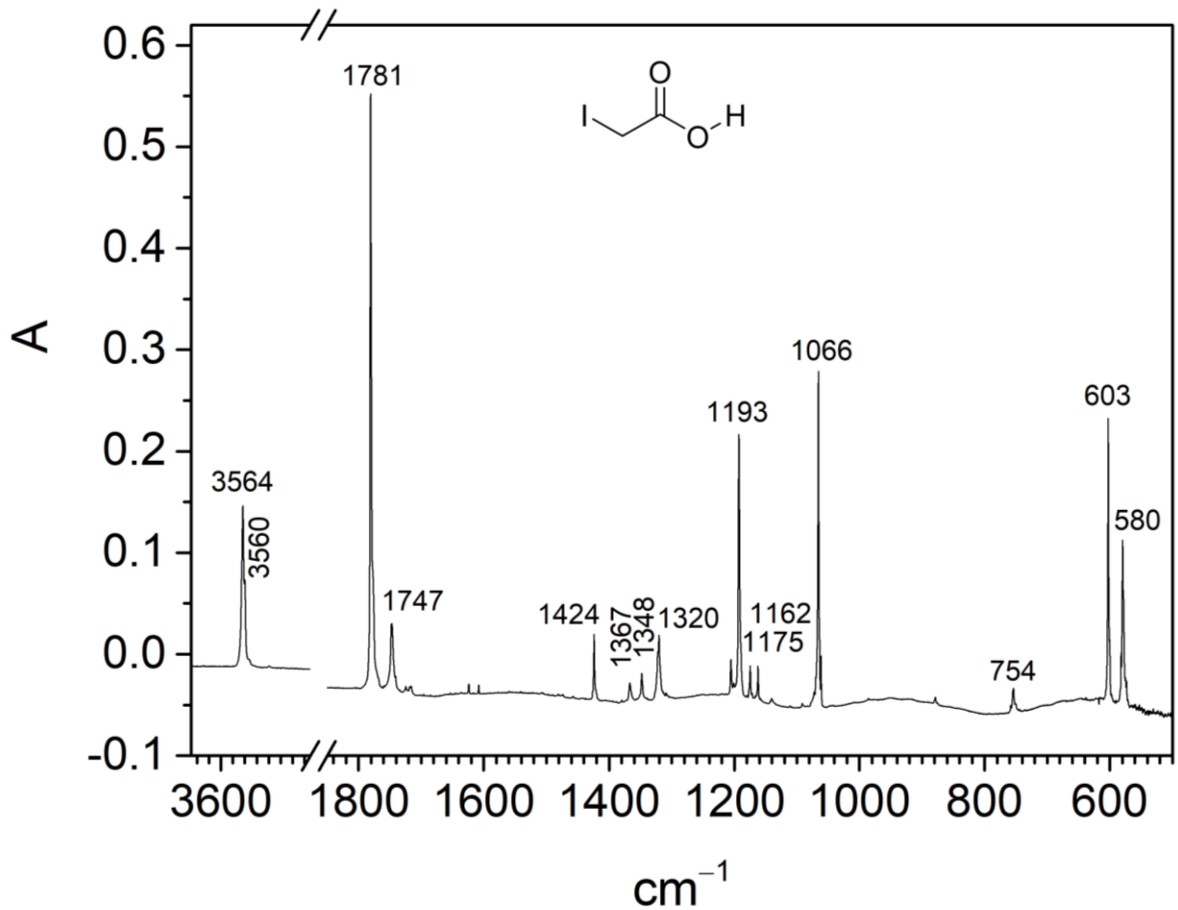

Figure S1. Infrared spectrum of matrix isolated iodoacetic acid in solid argon at 4 K.

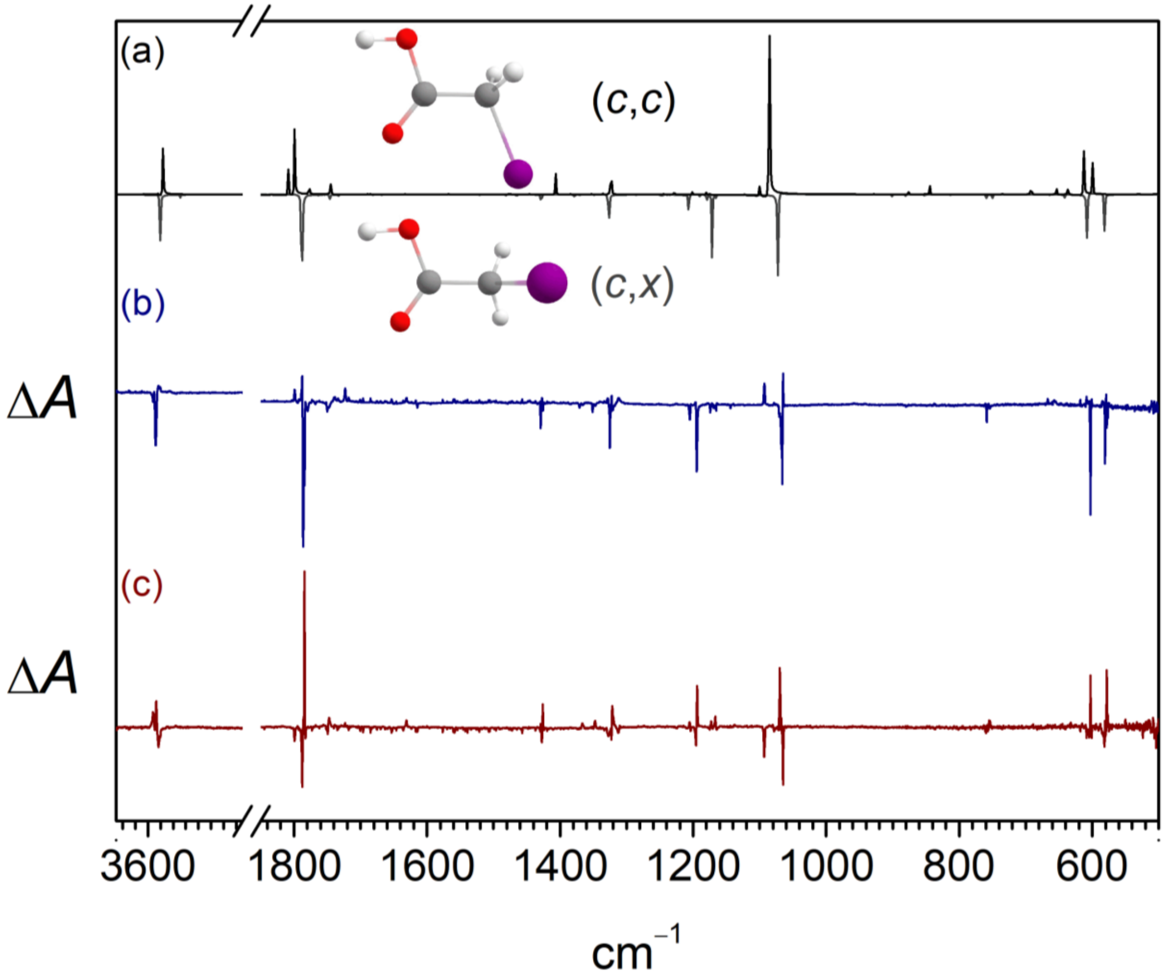

Figure S2. The top trace in (a) displays the anharmonic infrared spectra of conformers (*c*,*x*) and (*c*,*c*) pointing upwards and downwards, respectively, computed within the VPT2 approximation at the MP2/def2-TZVPP level of theory. The blue trace in (b) corresponds to the difference IR spectrum after UV irradiation (240−255 nm) of a neon matrix doped with iodoacetic acid for 1.5 minutes. The red trace shows the difference after annealing of the irradiated matrix for ten minutes at 6.2 K.

2. Additional Potential Energy Curves

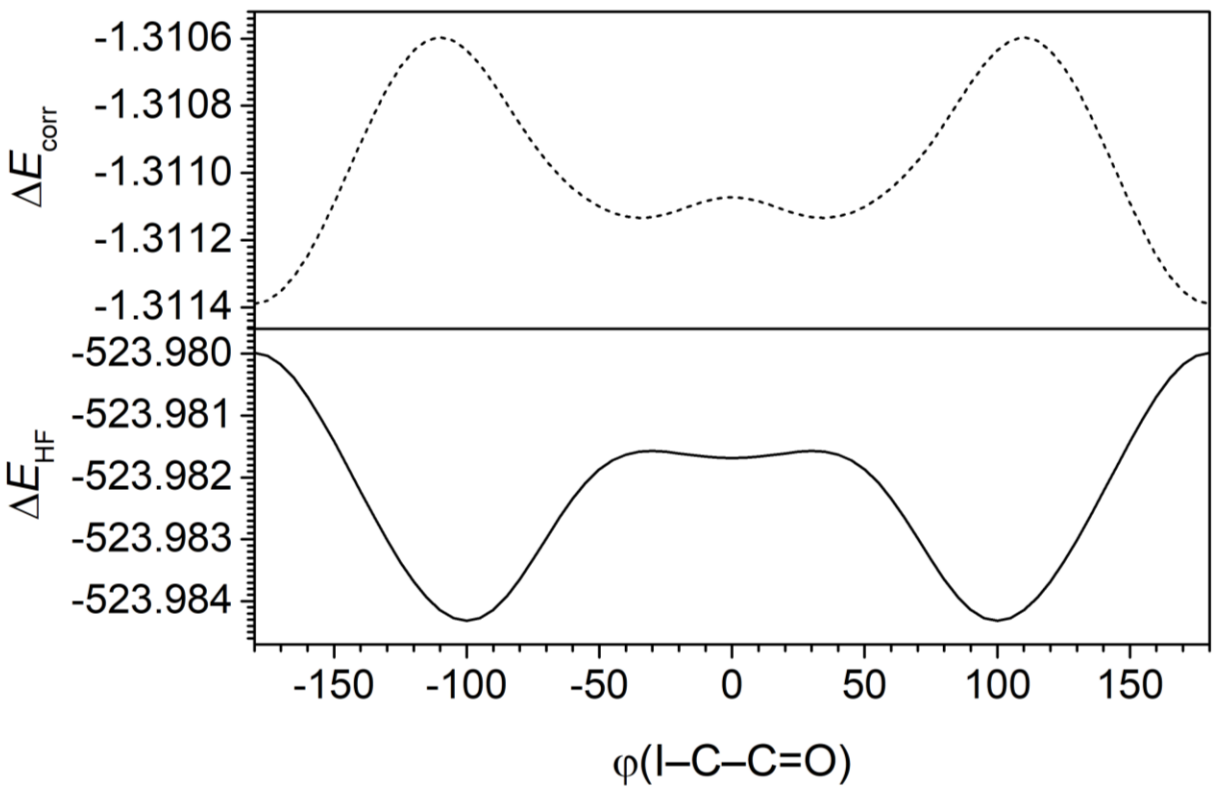

Figure S3. Absolute self-consistent field and correlation energies along the relaxed CCSD(T)/def2-TZVPP//MP2/def2-TZVPP potential energy curves of *cis*-iodoacetic acid.

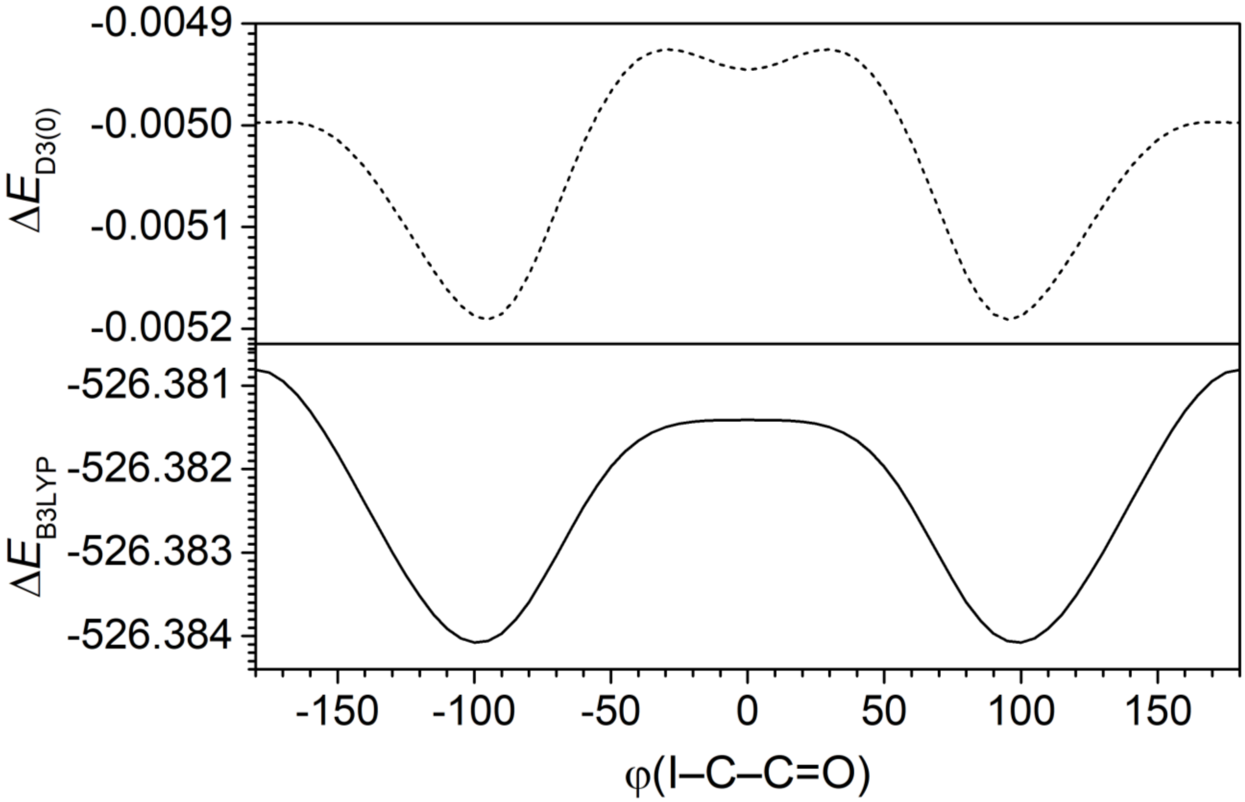

Figure S4. Absolute DFT electronic and D3(0)-dispersion correction energies along the relaxed B3LYP-D3(0)/def2-TZVPP potential energy curves of *cis*-iodoacetic acid.

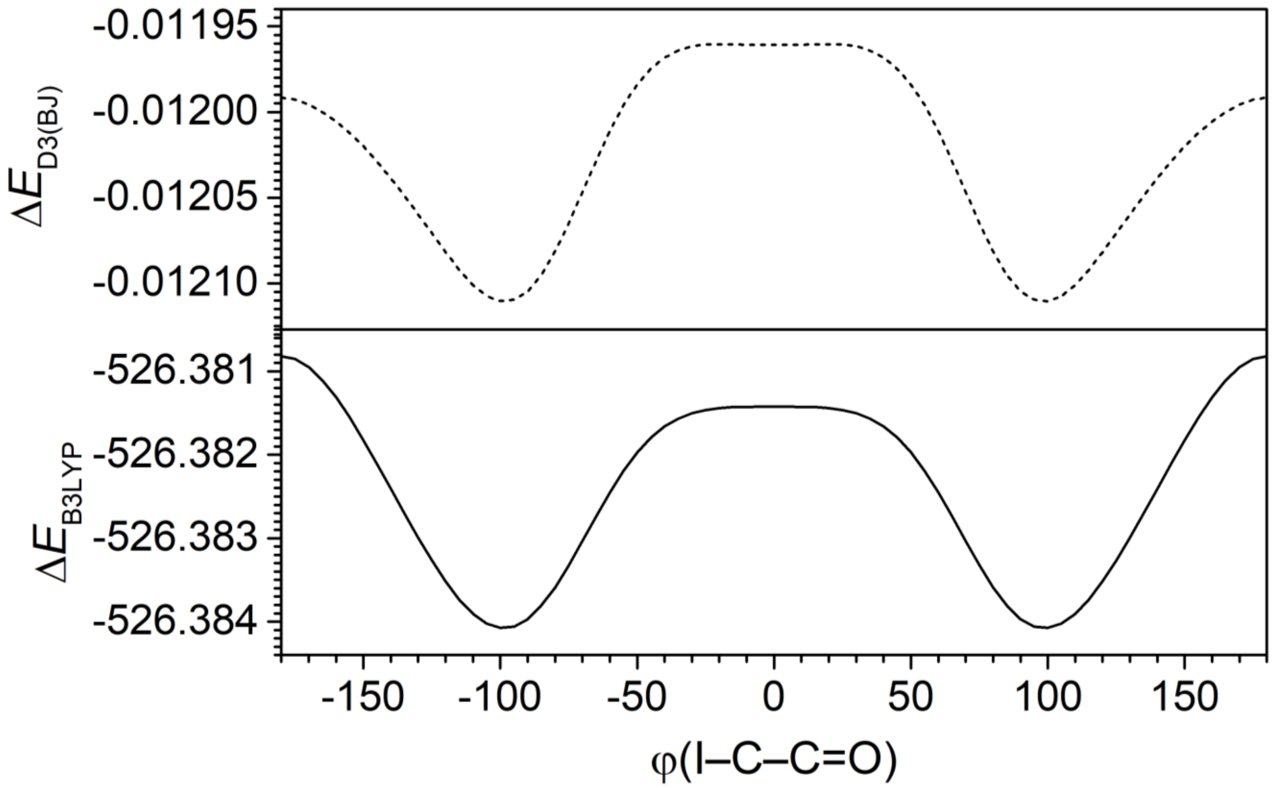

Figure S5. Absolute DFT electronic and D3(BJ)-dispersion correction energies along the relaxed B3LYP-D3(BJ)/def2-TZVPP potential energy curves of *cis*-iodoacetic acid.

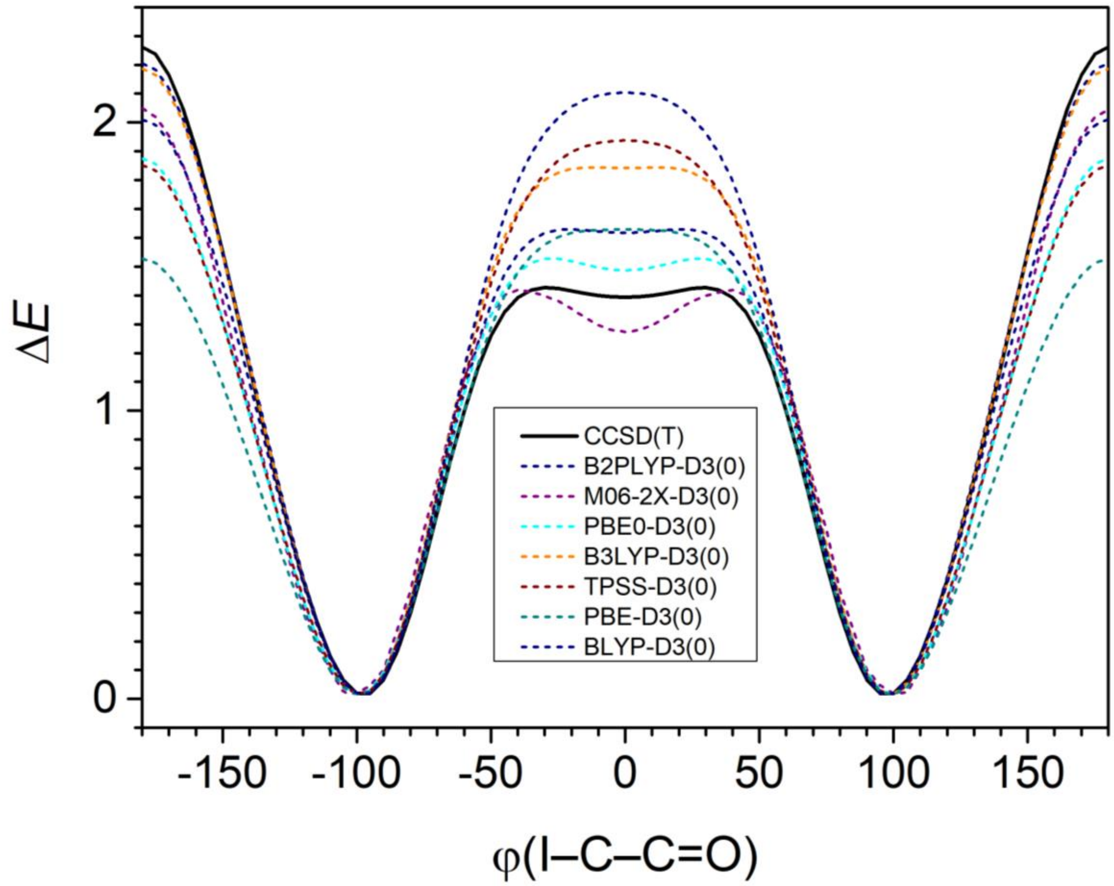

Figure S6. Plot drawn in analogy to Figure 5 in the main manuscript utilizing D3(0)-corrected DFAs.

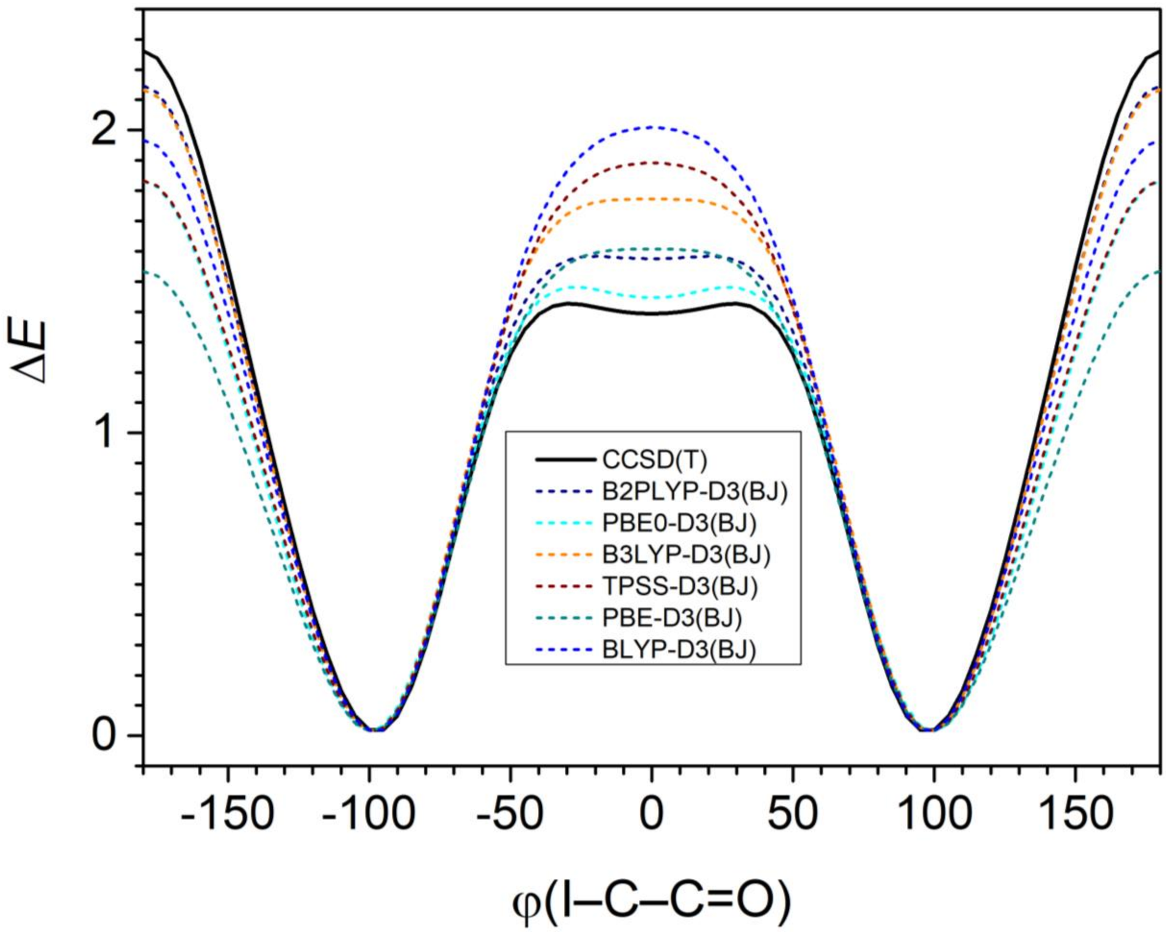

Figure S7. Plot drawn in analogy to Figure 5 in the main manuscript utilizing D3(BJ)-corrected DFAs.

3. Relative Energies at Different Levels

Table S1. Relative electronic energies at different levels of theory utilizing a def2-QZVPP basis set are given in kcal mol^{-1}. The energies are computed employing MP2/def2-TZVPP geometries. For wave function methods, CBS extrapolated energies are reported.

species	MP2	HF	B2PLYP	B3LYP	BLYP	M06-2X
(c,x^-)	0.00	0.00	0.00	0.00	0.00	0.00
(c,c)	1.25	1.63	1.48	1.66	1.82	1.27
$(c,\sigma)^‡$	1.32	1.70	1.45	1.57	1.64	1.38
$(c,t)^‡$	2.19	2.67	2.09	2.08	1.93	2.05
$(x,\xi^-)^‡$	11.12	10.97	11.31	11.26	11.36	10.57
$(x,x)^‡$	13.06	12.69	13.02	12.87	12.86	12.49
$(x,c^-)^‡$	13.54	13.60	13.60	13.56	13.53	13.04
(t,β^-)	3.38	5.99	3.68	3.61	3.02	3.80
$(t,t)^‡$	3.39	6.38	3.67	3.56	2.85	3.94
(t,c)	6.70	7.92	6.87	6.90	6.70	6.67
$(t,\sigma^-)^‡$	7.14	8.21	7.12	7.05	6.73	7.16

species	PBE	PBE0	TPSS	SCS-MP2	BHandHLYP	B2GP-PLYP
(c,x^-)	0.00	0.00	0.00	0.00	0.00	0.00
(c,c)	1.51	1.37	1.73	1.34	1.53	1.42
$(c,\sigma)^‡$	1.43	1.39	1.59	1.38	1.55	1.43
$(c,t)^‡$	1.54	1.80	1.79	2.33	2.27	2.13
$(x,\xi^-)^‡$	11.48	11.32	11.46	10.96	11.13	11.29
$(x,x)^‡$	13.22	13.15	13.23	12.78	12.86	13.05
$(x,c^-)^‡$	13.59	13.59	13.85	13.37	13.58	13.62
(t,β^-)	2.09	2.94	2.30	3.84	4.45	3.79
$(t,t)^‡$	1.80	2.82	2.09	3.96	4.57	3.82
(t,c)	6.28	6.59	6.56	6.77	7.25	6.91
$(t,\sigma^-)^‡$	6.50	6.91	6.68	7.14	7.53	7.22

species	DSD-PBEP86	CAM-B3LYP	B2PLYP-D3	B3LYP-D3	BLYP-D3	M06-2X-D3
(c,x^-)	0.00	0.00	0.00	0.00	0.00	0.00
(c,c)	1.30	1.24	1.61	1.88	2.10	1.26
$(c,\sigma)^‡$	1.35	1.28	1.58	1.79	1.91	1.38
$(c,t)^‡$	2.04	1.90	2.23	2.28	2.17	2.05
$(x,\xi^-)^‡$	11.26	11.30	11.13	10.96	10.95	10.58
$(x,x)^‡$	13.11	12.99	12.98	12.79	12.70	12.49
$(x,c^-)^‡$	13.57	13.38	13.68	13.67	13.62	13.04
(t,β^-)	3.51	3.86	3.77	3.74	3.17	3.80
$(t,t)^‡$	3.52	3.86	3.78	3.72	3.05	3.95
(t,c)	6.73	6.79	7.01	7.12	6.94	6.67
$(t,\sigma^-)^‡$	7.11	7.09	7.27	7.27	6.96	7.17

species	PBE-D3	PBE0-D3	TPSS-D3	B2GP-PLYP-D3	ωB97X-D3	B2PLYP-D3(BJ)
(*c*,*x*$^-$)	0.00	0.00	0.00	0.00	0.00	0.00
(*c*,*c*)	1.60	1.49	1.88	1.52	1.16	1.54
(*c*,*σ*)‡	1.52	1.51	1.74	1.53	1.24	1.51
(*c*,*t*)‡	1.60	1.91	1.91	2.23	1.80	2.13
(*x*,*ξ*$^-$)‡	11.34	11.16	11.22	11.15	11.25	11.18
(*x*,*x*)‡	13.17	13.11	13.13	13.02	12.99	12.99
(*x*,*c*$^-$)‡	13.61	13.65	13.88	13.68	13.34	13.63
(*t*,*β*$^-$)	2.13	3.02	2.37	3.86	3.75	3.54
(*t*,*t*)‡	1.85	2.91	2.19	3.90	3.74	3.54
(*t*,*c*)	6.35	6.70	6.68	7.02	6.57	6.87
(*t*,*σ*$^-$)‡	6.55	7.02	6.78	7.33	6.91	7.11

species	B3LYP-D3(BJ)	BLYP-D3(BJ)	PBE-D3(BJ)	PBE0-D3(BJ)	TPSS-D3(BJ)	B2GP-PLYP-D3(BJ)
(*c*,*x*$^-$)	0.00	0.00	0.00	0.00	0.00	0.00
(*c*,*c*)	1.76	1.95	1.57	1.44	1.82	1.45
(*c*,*σ*)‡	1.68	1.76	1.49	1.46	1.68	1.47
(*c*,*t*)‡	2.15	2.02	1.58	1.84	1.85	2.17
(*x*,*ξ*$^-$)‡	10.99	11.03	11.34	11.20	11.28	11.18
(*x*,*x*)‡	12.80	12.77	13.18	13.12	13.18	13.03
(*x*,*c*$^-$)‡	13.61	13.60	13.62	13.64	13.90	13.65
(*t*,*β*$^-$)	3.29	2.63	1.92	2.81	2.10	3.68
(*t*,*t*)‡	3.26	2.48	1.64	2.70	1.91	3.71
(*t*,*c*)	6.87	6.66	6.25	6.59	6.55	6.91
(*t*,*σ*$^-$)‡	7.01	6.68	6.47	6.90	6.65	7.21

species	BHandHLYP-D3(BJ)	DSD-PBEP86-D3(BJ)
(*c*,*x*$^-$)	0.00	0.00
(*c*,*c*)	1.60	1.34
(*c*,*σ*)‡	1.63	1.38
(*c*,*t*)‡	2.33	2.09
(*x*,*ξ*$^-$)‡	10.92	11.14
(*x*,*x*)‡	12.81	13.02
(*x*,*c*$^-$)‡	13.63	13.54
(*t*,*β*$^-$)	4.19	3.45
(*t*,*t*)‡	4.33	3.48
(*t*,*c*)	7.23	6.71
(*t*,*σ*$^-$)‡	7.50	7.06

4. Electronic Energies at Different Levels

Table S2. Electronic energies at different levels of theory utilizing a def2-QZVPP basis set are given in E_h. The energies are computed employing MP2/def2-TZVPP geometries. For wave function methods, CBS extrapolated energies are reported.

species	MP2/CBS	HF/CBS	B2PLYP	B3LYP	BLYP	M06-2X
(c,x^-)	-525.682361	-523.993973	-526.040844	-526.3984011	-526.198359	-526.1359463
(c,c)	-525.680376	-523.991375	-526.038489	-526.3957594	-526.195457	-526.133926
$(c,\sigma)^‡$	-525.680251	-523.991268	-526.038527	-526.395893	-526.195749	-526.1337459
$(c,t)^‡$	-525.678876	-523.98972	-526.037515	-526.3950894	-526.195286	-526.1326828
$(x,\xi^-)^‡$	-525.664638	-523.976488	-526.022825	-526.3804551	-526.18025	-526.1190979
$(x,x)^‡$	-525.661549	-523.973745	-526.020096	-526.3778873	-526.177872	-526.1160422
$(x,c^-)^‡$	-525.660777	-523.972304	-526.019179	-526.3767995	-526.1768	-526.1151674
(t,β^-)	-525.67698	-523.984421	-526.034986	-526.3926546	-526.193541	-526.1298966
$(t,t)^‡$	-525.676957	-523.983803	-526.034996	-526.3927267	-526.193813	-526.1296715
(t,c)	-525.671686	-523.981355	-526.029902	-526.387398	-526.187683	-526.1253156
$(t,\sigma^-)^‡$	-525.670982	-523.980883	-526.029499	-526.3871633	-526.187633	-526.1245343

species	PBE	PBE0	TPSS	B2PLYP-D3	B2LYP-D3	BLYP-D3
(c,x^-)	-526.039558	-526.0629767	-526.21849	-526.043728	-526.4035266	-526.204459
(c,c)	-526.037156	-526.0607896	-526.21574	-526.041165	-526.4005374	-526.201108
$(c,\sigma)^‡$	-526.037275	-526.0607584	-526.215956	-526.041203	-526.4006707	-526.201418
$(c,t)^‡$	-526.037099	-526.0601069	-526.215635	-526.040181	-526.3998919	-526.201009
$(x,\xi^-)^‡$	-526.021265	-526.0449446	-526.200228	-526.025996	-526.3860645	-526.187012
$(x,x)^‡$	-526.01849	-526.0420231	-526.197411	-526.023038	-526.383139	-526.184225
$(x,c^-)^‡$	-526.0179	-526.0413123	-526.196424	-526.021935	-526.381749	-526.182757
(t,β^-)	-526.036232	-526.0582973	-526.214824	-526.037715	-526.3975596	-526.199402
$(t,t)^‡$	-526.036694	-526.0584849	-526.215155	-526.037698	-526.3975935	-526.199603
(t,c)	-526.029554	-526.0524726	-526.208035	-526.032558	-526.3921853	-526.193392
$(t,\sigma^-)^‡$	-526.029202	-526.0519664	-526.207845	-526.03214	-526.3919484	-526.193365

species	M06-2X-D3	PBE-D3	PBE0-D3	TPSS-D3	B2PLYP-D3(BJ)	B3LYP-D3(BJ)
(c,x^-)	-526.1359844	-526.042175	-526.0659171	-526.222414	-526.046698	-526.4106158
(c,c)	-526.1339711	-526.039627	-526.0635447	-526.219416	-526.044251	-526.4078055
$(c,\sigma)^‡$	-526.1337909	-526.039751	-526.0635115	-526.219646	-526.044292	-526.4079426
$(c,t)^‡$	-526.1327224	-526.039618	-526.0628809	-526.219377	-526.043302	-526.4071846
$(x,\xi^-)^‡$	-526.1191266	-526.024096	-526.0481284	-526.204531	-526.02888	-526.3930974
$(x,x)^‡$	-526.1160751	-526.021194	-526.0450313	-526.201485	-526.025999	-526.3902114
$(x,c^-)^‡$	-526.1152049	-526.020486	-526.0441632	-526.200287	-526.024971	-526.38892
(t,β^-)	-526.1299221	-526.038781	-526.0611087	-526.218639	-526.04106	-526.4053789
$(t,t)^‡$	-526.1296974	-526.039228	-526.0612815	-526.218932	-526.041056	-526.4054224
(t,c)	-526.1253476	-526.032061	-526.0552354	-526.211761	-526.035755	-526.3996626
$(t,\sigma^-)^‡$	-526.1245645	-526.031733	-526.0547316	-526.211603	-526.035367	-526.3994429

species	BLYP-D3(BJ)	PBE-D3(BJ)	PBE0-D3(BJ)	TPSS-D3(BJ)	CCSD(T)/CBS	SCS-MP2/CBS
(c,x^-)	-526.213249	-526.046275	-526.0689264	-526.22715	-525.6738776	-525.579841
(c,c)	-526.21014	-526.043778	-526.0666307	-526.22425	-525.6719561	-525.577708
$(c,\sigma)^‡$	-526.210437	-526.043901	-526.0666077	-526.224475	-525.6718470	-525.577637
$(c,t)^‡$	-526.210031	-526.043757	-526.0659938	-526.224204	-525.6705199	-525.576136
$(x,\xi^-)^‡$	-526.195667	-526.028199	-526.0510819	-526.209176	-525.6566853	-525.562368
$(x,x)^‡$	-526.192897	-526.025268	-526.0480262	-526.206151	-525.6536287	-525.559472
$(x,c^-)^‡$	-526.191578	-526.024572	-526.0471959	-526.204998	-525.6529728	-525.558542
(t,β^-)	-526.209063	-526.043211	-526.0644452	-526.223799	-525.6684041	-525.573716
$(t,t)^‡$	-526.209299	-526.043658	-526.0646186	-526.224109	-525.668301	-525.573527
(t,c)	-526.202642	-526.036308	-526.0584195	-526.216708	-525.6634118	-525.569055
$(t,\sigma^-)^‡$	-526.202608	-526.035966	-526.0579373	-526.216545	-525.6627418	-525.568466

species	BHandHLYP	B2GP-PLYP	DSD-PBEP86	CAM-B3LYP	B2GP-PLYP-D3	ωB97X-D3
(c,x^-)	-526.1254845	-525.973115	-525.7614505	-526.2164726	-525.9752108	-526.298022
(c,c)	-526.1230495	-525.970853	-525.759385	-526.2144995	-525.9727942	-526.296173
$(c,\sigma)^‡$	-526.1230149	-525.970833	-525.7593009	-526.2144393	-525.9727745	-526.296042
$(c,t)^‡$	-526.1218665	-525.969718	-525.7582023	-526.213446	-525.9716514	-526.295147
$(x,\xi^-)^‡$	-526.1077409	-525.955126	-525.7435051	-526.1984711	-525.9574435	-526.28009
$(x,x)^‡$	-526.1049884	-525.952316	-525.7405589	-526.1957751	-525.9544566	-526.277315
$(x,c^-)^‡$	-526.1038392	-525.951413	-525.7398206	-526.1951484	-525.9534126	-526.27677
(t,β^-)	-526.1183962	-525.967068	-525.7558571	-526.2103232	-525.969054	-526.292043
$(t,t)^‡$	-526.1181986	-525.967025	-525.7558475	-526.2103198	-525.9689889	-526.292058
(t,c)	-526.1139265	-525.962102	-525.7507261	-526.2056575	-525.9640274	-526.287546
$(t,\sigma^-)^‡$	-526.1134926	-525.961617	-525.7501256	-526.2051733	-525.9635302	-526.287014

species	B2GP-PLYP-D3(BJ)	BHandHLYP-D3(BJ)	DSD-PBEP86-D3(BJ)
(c,x^-)	-525.97819	-526.135293	-525.7122628
(c,c)	-525.9758756	-526.13274	-525.7101228
$(c,\sigma)^‡$	-525.9758517	-526.132703	-525.7100571
$(c,t)^‡$	-525.9747294	-526.13158	-525.7089336
$(x,\xi^-)^‡$	-525.9603725	-526.117889	-525.6945111
$(x,x)^‡$	-525.9574304	-526.11488	-525.6915184
$(x,c^-)^‡$	-525.9564414	-526.113574	-525.6906922
(t,β^-)	-525.9723284	-526.128612	-525.706762
$(t,t)^‡$	-525.9722724	-526.128392	-525.7067225
(t,c)	-525.9671793	-526.123771	-525.7015734
$(t,\sigma^-)^‡$	-525.9666967	-526.123343	-525.7010058

5. Optimized Geometries

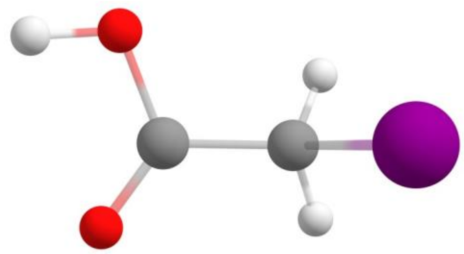

Figure S3. Optimized geometry of (c,x^-) (in Å) at the MP2/def2-TZVPP level of theory.

H	0.721085000	0.368172000	1.816017000
O	2.216274000	1.180006000	-0.012890000
O	2.463037000	-1.006079000	-0.516095000
C	1.882668000	-0.126238000	0.072351000
C	0.714499000	-0.331240000	0.988889000
H	0.683988000	-1.360208000	1.321743000
H	2.952641000	1.227295000	-0.639629000
I	-1.082551000	0.021098000	-0.087428000

Electronic MP2 energy (in E_h)

-525.2695839

Zero-point vibrational energy (in kcal mol^{-1})

33.22916

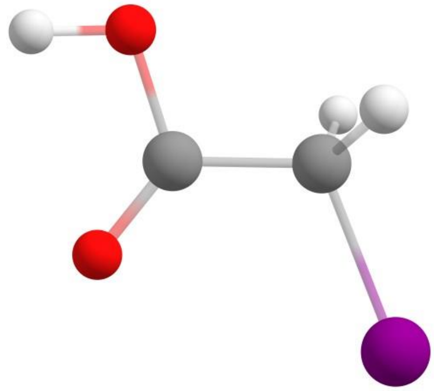

Figure S4. Optimized geometry of (c,c) (in Å) at the MP2/def2-TZVPP level of theory.

H	-1.488679000	-0.869487000	0.880198000
O	-0.489989000	-3.076502000	0.000000000
O	1.360610000	-1.786273000	0.000000000
C	0.162058000	-1.887934000	0.000000000
C	-0.859820000	-0.778803000	0.000000000
H	-1.488679000	-0.869487000	-0.880198000
H	0.198965000	-3.757026000	0.000000000
I	0.000000000	1.139597000	0.000000000

Electronic MP2 energy (in E_h)

-525.267412

Zero-point vibrational energy (in kcal mol^{-1})

32.84198

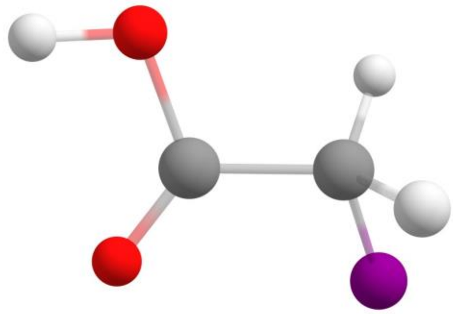

Figure S5. Optimized geometry of $(c,\sigma)^{\ddagger}$ (in Å) at the MP2/def2-TZVPP level of theory.

H	0.767767000	-1.044784000	1.442475000
O	2.979534000	-0.592323000	-0.294521000
O	1.874658000	1.320681000	0.159964000
C	1.886546000	0.120544000	0.068984000
C	0.752458000	-0.822609000	0.378883000
H	0.850813000	-1.743721000	-0.182123000
H	3.685379000	0.057247000	-0.430034000
I	-1.131538000	0.021071000	-0.046058000

Electronic MP2 energy (in E_h)

-525.2673125

Zero-point vibrational energy (in kcal mol^{-1})

32.94115

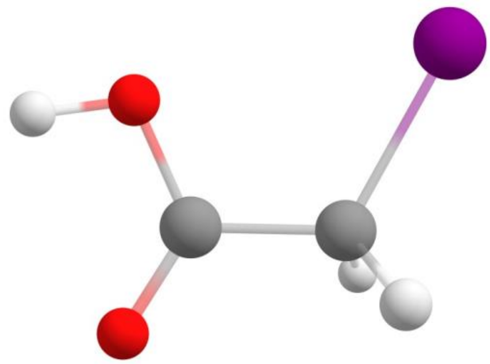

Figure S6. Optimized geometry of (c,t)‡ (in Å) at the MP2/def2-TZVPP level of theory.

H	-1.539169000	-0.841277000	0.878987000
O	1.310651000	-1.726095000	0.000000000
O	-0.462452000	-3.111791000	0.000000000
C	-0.004388000	-1.993378000	0.000000000
C	-0.905569000	-0.783013000	0.000000000
H	-1.539169000	-0.841277000	-0.878987000
H	1.752483000	-2.588539000	0.000000000
I	0.000000000	1.125142000	0.000000000

Electronic MP2 energy (in E_{h})

-525.2659252

Zero-point vibrational energy (in kcal mol^{-1})

32.94459

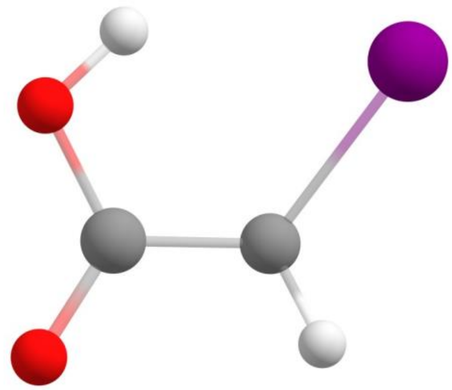

Figure S7. Optimized geometry of (t,β^{-}) (in Å) at the MP2/def2-TZVPP level of theory.

H	0.837021000	1.785161000	0.286426000
O	1.876148000	-1.306661000	-0.114086000
O	3.049647000	0.545304000	0.267515000
C	1.998147000	0.025611000	-0.002836000
C	0.784257000	0.884932000	-0.312558000
H	0.803328000	1.147132000	-1.366820000
H	0.943059000	-1.526950000	-0.253007000
I	-1.107249000	-0.014675000	0.037704000

Electronic MP2 energy (in E_h)

-525.2635142

Zero-point vibrational energy (in kcal mol^{-1})

32.91336

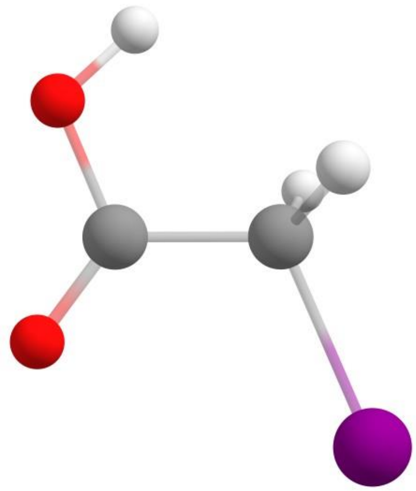

Figure S8. Optimized geometry of (*t*,*c*) (in Å) at the MP2/def2-TZVPP level of theory.

H	-1.469404000	-0.873995000	0.884141000
O	-0.364410000	-3.140632000	0.000000000
O	1.383391000	-1.764388000	0.000000000
C	0.194030000	-1.899184000	0.000000000
C	-0.842023000	-0.790420000	0.000000000
H	-1.469404000	-0.873995000	-0.884141000
H	-1.325079000	-3.067796000	0.000000000
I	0.000000000	1.135728000	0.000000000

Electronic MP2 energy (in E_h)

-525.2584894

Zero-point vibrational energy (in kcal mol^{-1})

32.68043

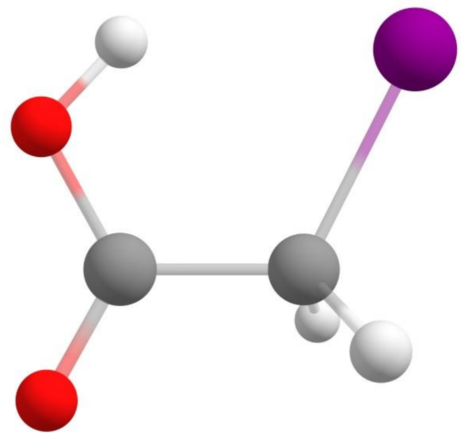

Figure S9. Optimized geometry of (t,t)‡ (in Å) at the MP2/def2-TZVPP level of theory.

H	0.837056000	-1.547197000	0.882941000
O	1.846138000	1.316213000	0.000060000
O	3.109556000	-0.515961000	-0.000058000
C	2.016268000	-0.011891000	0.000012000
C	0.792613000	-0.918932000	0.000074000
H	0.837076000	-1.547343000	-0.882687000
H	0.896227000	1.511182000	0.000095000
I	-1.114513000	0.014458000	-0.000016000

Electronic MP2 energy (in E_h)

-525.263416

Zero-point vibrational energy (in kcal mol^{-1})

32.82862

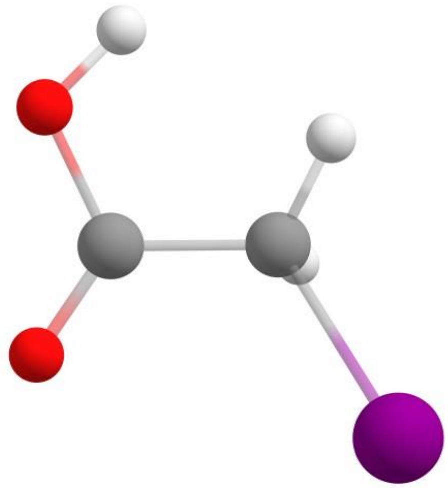

Figure S10. Optimized geometry of $(t,\sigma^{-})^{\ddagger}$ (in Å) at the MP2/def2-TZVPP level of theory.

1	-0.758528000	0.776310000	-1.613729000
8	-2.989778000	0.500388000	0.388210000
8	-1.888486000	-1.353459000	-0.154499000
6	-1.895769000	-0.157600000	-0.076306000
6	-0.761468000	0.743402000	-0.527747000
1	-0.833300000	1.752861000	-0.135786000
1	-2.818439000	1.447321000	0.403969000
53	1.120374000	-0.012580000	0.058494000

Electronic MP2 energy (in E_{h})

-525.2579132

Zero-point vibrational energy (in kcal mol^{-1})

32.8189

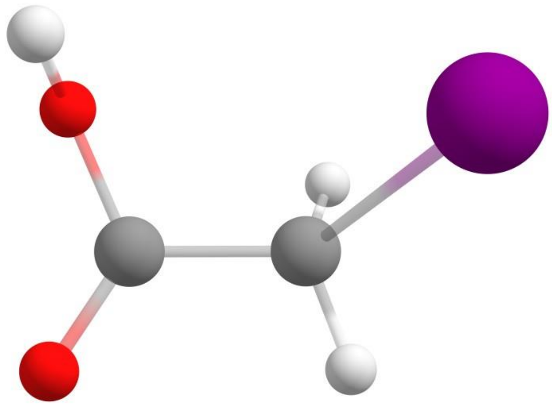

Figure S11. Optimized geometry of $(x,\xi)^{\ddagger}$ (in Å) at the MP2/def2-TZVPP level of theory.

H	0.731266000	-0.236010000	1.839643000
O	2.098224000	1.243440000	0.200368000
O	2.622107000	-0.802393000	-0.620408000
C	1.894390000	-0.110698000	0.037441000
C	0.736787000	-0.640468000	0.833903000
H	0.723496000	-1.722470000	0.822277000
H	1.597406000	1.727576000	-0.464791000
I	-1.067960000	0.022821000	-0.076696000

Electronic MP2 energy (in E_{h})

-525.2514413

Zero-point vibrational energy (in kcal mol^{-1})

32.0786

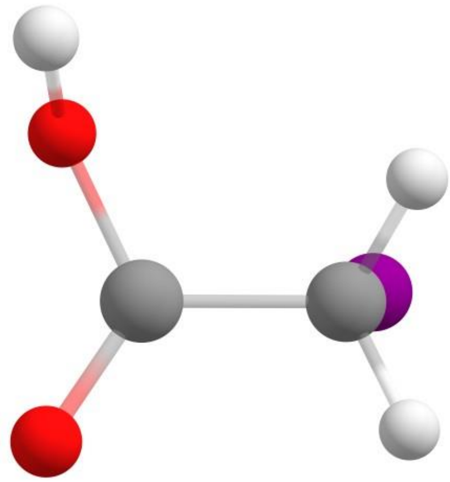

Figure S12. Optimized geometry of $(x,x)^{\ddagger}$ (in Å) at the MP2/def2-TZVPP level of theory.

H	-0.730566000	-0.183539000	-1.835500000
O	-2.135035000	-1.220772000	0.114498000
O	-2.512846000	0.968976000	0.546618000
C	-1.889592000	0.129696000	-0.042834000
C	-0.727772000	0.435008000	-0.944828000
H	-0.700367000	1.490733000	-1.182110000
H	-2.717592000	-1.527018000	-0.588081000
I	1.076146000	-0.021774000	0.080052000

Electronic MP2 energy (in E_h)

-525.2485335

Zero-point vibrational energy (in kcal mol^{-1})

32.05899

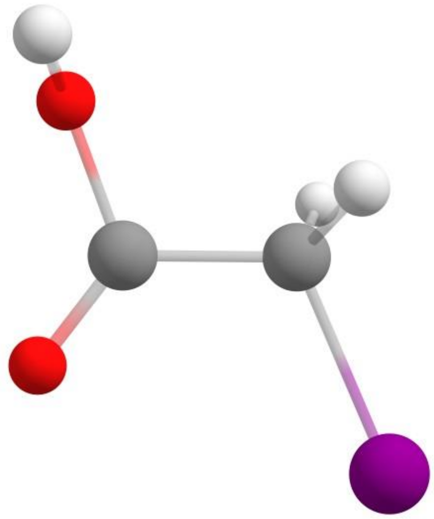

Figure S13. Optimized geometry of $(x,c^{-})^{\ddagger}$ (in Å) at the MP2/def2-TZVPP level of theory.

H	0.872669000	-1.534525000	0.768053000
O	3.129267000	-0.473524000	-0.060856000
O	1.798444000	1.359083000	-0.013995000
C	1.900043000	0.168590000	-0.011498000
C	0.779412000	-0.840312000	-0.062425000
H	0.868819000	-1.408129000	-0.984258000
H	3.405000000	-0.715928000	0.829329000
I	-1.144244000	0.011404000	0.008099000

Electronic MP2 energy (in E_{h})

-525.2476135

Zero-point vibrational energy (in kcal mol^{-1})

31.7280

6. Complete References

Gaussian reference:

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