Emerging Non-Valence Anion States of [Isoprene-H·]·H_2O Accessed via Detachment of OH^-·Isoprene

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Table S1. Summary of lowest energy $C_4H_5O_2^-$ conformer computational results.

$C_4H_5O_2^-$ Isomer	Relative Energy MP2/ma-def2-TZVP(-f) (eV)	IP-EOM-CCSD/aug-cc-pVTZ VDE (eV)
C4 conjugate base of carboxylic acid	0.00	3.84
O_2-C1 (*trans*, O_2 *cis* nearest H)	4.56	2.39
O_2-C2 (toward C_4)	4.72	2.09
CHO-CH(CH_3)-CHO^-	0.02	3.04
H_2C=CH-CO-CH_2-O^-	1.97	2.58
H_2C=CH-CH(O^-)-CH=O	1.89	2.81

Table S2. CAM-B3LYP/aug-cc-pVTZ relative energies, ADEs, and VDEs for the IMC, molecular ion, alkenoxide, and peroxide species.

Form	Isomer	Relative Energy (eV)	ADE (eV)	VDE (eV)
IMC	C4/methyl pocket	0.00	2.45	2.63
Molecular Ion	C1-OH	0.14	0.71	0.87
	C2-OH	0.72	0.78	1.24
	C3-OH	0.70	0.81	1.24
	C4-OH	0.00	0.92	1.10
Alkenoxide	C1=O	1.05	1.84	2.03
	C2=O	0.86	1.94	2.05
	C3=O	0.00	1.24	1.44
	C4=O	0.92	1.89	2.04
Peroxide	O_2-C1	0.00	1.97	2.38
	O_2-C2	0.21	1.82	2.20

Tables S3 and S4. CAM-B3LYP/aug-cc-pVTZ anion OH^{-}·isoprene ion molecule complex (top) and OH·isoprene van der Waals complex (bottom) optimized geometries in which the OH^{-}/·OH is near the C4/methyl pocket.

C	2.384271820000	-0.426498070000	-0.275150140000
H	3.076160350000	0.381484780000	-0.480750960000
H	2.772682650000	-1.435398830000	-0.324304420000
C	1.102414340000	-0.185674260000	0.014022300000
C	0.616613360000	1.199536840000	0.059315490000
H	1.393136420000	1.960242430000	0.012208640000
C	-0.663179710000	1.556824290000	0.122410340000
H	-0.903924210000	2.615740410000	0.134164120000
H	-1.505613920000	0.843361690000	0.104427240000
C	0.129377890000	-1.281779840000	0.315681470000
H	-0.129628360000	-1.257937990000	1.376744490000
H	-0.833636090000	-1.158565010000	-0.199787780000
H	0.562661720000	-2.256560860000	0.088961360000
O	-2.779640590000	-0.547690770000	-0.183745500000
H	-3.611700090000	-0.485294230000	-0.659375410000

C	2.384271820000	-0.426498070000	-0.275150140000
H	3.076160350000	0.381484780000	-0.480750960000
H	2.772682650000	-1.435398830000	-0.324304420000
C	1.102414340000	-0.185674260000	0.014022300000
C	0.616613360000	1.199536840000	0.059315490000
H	1.393136420000	1.960242430000	0.012208640000
C	-0.663179710000	1.556824290000	0.122410340000
H	-0.903924210000	2.615740410000	0.134164120000
H	-1.505613920000	0.843361690000	0.104427240000
C	0.129377890000	-1.281779840000	0.315681470000
H	-0.129628360000	-1.257937990000	1.376744490000
H	-0.833636090000	-1.158565010000	-0.199787780000
H	0.562661720000	-2.256560860000	0.088961360000
O	-2.779640590000	-0.547690770000	-0.183745500000
H	-3.611700090000	-0.485294230000	-0.659375410000

Table S5. Franck-Condon simulation parameters for the OH^-·isoprene ion molecular complex at the CAM-B3LYP/aug-cc-pVTZ level of theory.

Feature	Calc'd Origin (eV)	Simulated Origin (eV)	$\omega_{neutral}$ (cm^{-1})	ω_{anion} (cm^{-1})	Mode description	ΔQ (Å)
x	2.45	2.40	1082	900	C4-C_{methyl} pocket H-atom bend	0.2
			160	177	Out-of-plane bend	0.6
			1693	1675	C=C stretch (out-of- phase)	0.05
			285	258	in-plane bend	0.5

Tables S6 and S7. CAM-B3LYP/aug-cc-pVTZ C4 OH-isoprene adduct molecular anion(top) and neutral (bottom) optimized geometries.

C	1.468826000000	-0.137533000000	-0.571202000000
H	1.345916000000	0.843129000000	-1.038090000000
H	2.086261000000	-0.747580000000	-1.238343000000
C	0.193881000000	-0.789804000000	-0.265219000000
C	-1.021013000000	-0.127851000000	-0.021965000000
C	-1.016656000000	1.388385000000	-0.067769000000
H	-0.258885000000	1.808731000000	0.595676000000
H	-0.792386000000	1.749667000000	-1.074254000000
H	-1.989552000000	1.783632000000	0.221618000000
C	-2.232817000000	-0.720341000000	0.241328000000
H	-3.116295000000	-0.128346000000	0.436752000000
H	-2.336648000000	-1.798356000000	0.277263000000
H	0.181371000000	-1.875293000000	-0.277977000000
O	2.340365000000	0.114814000000	0.609520000000
H	1.803969000000	-0.231225000000	1.330154000000

C	1.450985000000	0.284734000000	-0.408203000000
H	1.241982000000	1.327707000000	-0.160516000000
H	1.806166000000	0.265014000000	-1.441299000000
C	0.240990000000	-0.563981000000	-0.255457000000
C	-1.054371000000	-0.121695000000	-0.019024000000
C	-1.356093000000	1.350799000000	0.111556000000
H	-0.760456000000	1.813154000000	0.898399000000
H	-1.140941000000	1.885167000000	-0.813470000000
H	-2.404816000000	1.508435000000	0.351087000000
C	-2.083957000000	-1.027769000000	0.089132000000
H	-3.099004000000	-0.709026000000	0.273389000000
H	-1.901708000000	-2.088510000000	-0.007889000000
H	0.407536000000	-1.630828000000	-0.350328000000
O	2.550102000000	-0.200120000000	0.358996000000
H	2.265098000000	-0.302679000000	1.270638000000

Table S8. Franck-Condon simulation parameters for the HO-C4 molecular ion at the CAM-B3LYP/aug-cc-pVTZ level of theory. Active vibrational modes were chosen by visually comparing differences between the anion and neutral geometries to the vibrational motions. This procedure was necessary due to the presence of the methyl rotor of the isoprene species, which made a more direct computational treatment of the anion-neutral vibrational overlap impractical.

Feature	**Calc'd Origin (eV)**	**Simulated Origin (eV)**	**$\omega_{neutral}$ (cm^{-1})**	**ω_{anion} (cm^{-1})**	**Mode description**	**ΔQ (Å)**
X′	0.92	1.18	51	85	C4 rock	0.500
			472	464	C2 bend	-0.179
			579	573	CH_2 rock	-0.100
			1035	1002	H-rock	-0.273

Tables S9 and S10. CAM-B3LYP/aug-cc-pVTZ C1=O alkenoxide (top) and alkenoxy (bottom) optimized geometries.

C	-2.455783000000	-0.480565000000	-0.224225000000
H	-3.375354000000	-0.642099000000	0.324800000000
C	-1.371173000000	0.020254000000	0.356645000000
C	-0.039064000000	0.217250000000	-0.260080000000
C	0.513373000000	1.611904000000	-0.009359000000
H	0.513541000000	1.834689000000	1.062468000000
H	1.548671000000	1.616803000000	-0.350939000000
C	1.014929000000	-0.841990000000	0.277601000000
O	2.238337000000	-0.665207000000	-0.200920000000
H	0.547431000000	-1.834432000000	0.038494000000
H	-2.453549000000	-0.756079000000	-1.272416000000
H	0.934411000000	-0.766622000000	1.403526000000
H	-1.431513000000	0.271300000000	1.414525000000
H	-0.060329000000	2.391460000000	-0.517995000000
H	-0.103700000000	0.045524000000	-1.338593000000

C	-2.429818000000	-0.503646000000	-0.248616000000
H	-3.360816000000	-0.685152000000	0.269665000000
C	-1.356648000000	-0.068035000000	0.386926000000
C	-0.027250000000	0.208577000000	-0.244799000000
C	0.427355000000	1.643556000000	0.001325000000
H	0.469417000000	1.858595000000	1.070985000000
H	1.420158000000	1.804802000000	-0.414614000000
C	1.013952000000	-0.783264000000	0.283352000000
O	2.262100000000	-0.659772000000	-0.238049000000
H	0.679057000000	-1.826159000000	0.164502000000
H	-2.417839000000	-0.689630000000	-1.315351000000
H	1.134559000000	-0.672717000000	1.378302000000
H	-1.415489000000	0.111425000000	1.457622000000
H	-0.259949000000	2.353542000000	-0.455044000000
H	-0.111447000000	0.040346000000	-1.320805000000

Table S11. Franck-Condon simulation parameters for the C1=O alkenoxide at the CAM-B3LYP/aug-cc-pVTZ level of theory.

Feature	**Calc'd Origin (eV)**	**Simulated Origin (eV)**	**$\omega_{neutral}$ (cm^{-1})**	**ω_{anion} (cm^{-1})**	**Mode description**	**ΔQ (Å)**
X″	1.85	1.74	126	137	C1 rock	-0.152
			247	245	Methyl rotor	-0.205
			315	355	C=C-C distortion	0.2620
			1078	1210	C-O stretch	-0.200

Tables S12–S51. Geometries of the species described in this study, as optimized by MP2/ma-def2-TZVP (-f).

OH^-·isoprene ion molecule complex: OH in C1/C3 pocket

C	0.211685	0.334200	0.004425
C	0.171343	-1.169410	-0.012560
C	-0.938555	1.037420	0.040524
C	1.494170	1.029870	-0.022149
C	2.705354	0.445816	-0.063529
H	3.612714	1.037842	-0.081352
H	2.808867	-0.631965	-0.080701
H	1.444410	2.118290	-0.007131
H	-0.895730	2.125917	0.048851
H	-1.901483	0.509766	0.063119
H	-0.876112	-1.498394	0.020964
H	0.653253	-1.556342	-0.917249
H	0.717497	-1.578945	0.844779
O	-2.954107	-1.133561	0.016646
H	-3.794551	-1.525075	0.295279

OH^-·isoprene ion molecule complex: OH in C1/C3 pocket

C	-0.404226	-0.666100	0.007588
C	-0.358471	-2.170755	-0.017891
C	-1.560987	0.023568	0.038321
C	0.845848	0.097144	-0.004320
C	2.066354	-0.466761	-0.042076
H	2.957430	0.150227	-0.052260
H	2.214208	-1.541995	-0.064232
H	0.707888	1.186966	0.017808
H	-1.529495	1.119755	0.056108
H	-2.510444	-0.508433	0.043645
H	-1.368100	-2.586384	-0.004711
H	0.152919	-2.536023	-0.913972
H	0.188367	-2.564888	0.844424
O	-0.481712	2.829035	-0.014113
H	-0.490179	3.745927	0.296356

OH^-·isoprene ion molecule complex: C4 hydrogen bond

C	-1.391420	-0.260924	0.025147
C	-1.387782	-1.761534	-0.046041
C	-2.555705	0.416459	0.068429
C	-0.108926	0.437415	0.044940
C	1.103619	-0.143429	0.004655
H	2.044629	0.441549	0.027049
H	1.166348	-1.227305	-0.045955
H	-0.159701	1.522188	0.094181
H	-2.563196	1.498248	0.118858
H	-3.508872	-0.097448	0.053385
H	-2.405450	-2.151747	-0.054212
H	-0.872221	-2.102182	-0.945381
H	-0.854368	-2.185661	0.806189
O	3.629225	1.270289	-0.105957
H	4.160314	2.012115	0.210764

OH^-·isoprene ion molecule complex: OH in C4/methyl pocket

C	-0.885539	0.675311	0.051547
C	-1.012283	-0.808882	0.203651
C	-1.947037	1.470224	-0.193992
C	0.444570	1.271251	0.196366
C	1.588827	0.565404	0.240700
H	2.523953	1.109940	0.335494
H	1.635278	-0.530524	0.123066
H	0.471920	2.358990	0.248012
H	-1.830098	2.543833	-0.290747
H	-2.941271	1.057598	-0.312530
H	-2.017366	-1.136284	-0.067302
H	-0.255974	-1.365265	-0.369289
H	-0.822674	-1.084857	1.243851
O	1.494402	-2.381639	-0.384777
H	2.149800	-2.940168	-0.821983

Hydroxyl-isoprene adduct molecular ion: C1-OH (MP2 opt)

C	-0.981823	-0.278328	-2.285518
C	-0.988757	-0.254583	-0.899884
C	0.101102	-0.233623	-0.022860
C	1.487439	-0.272441	-0.586647
C	-0.091559	-0.190425	1.414757
H	-1.910947	-0.314709	-2.841997
H	-0.062246	-0.207177	-2.855672
H	-1.972401	-0.266072	-0.420994
H	1.774574	0.661633	-1.094477
H	1.584353	-1.069851	-1.342036
H	2.227806	-0.450301	0.201701
O	0.181154	1.166277	2.005798
H	0.283557	1.013064	2.960132
H	0.593732	-0.868653	1.956474
H	-1.126061	-0.451747	1.671391

C1=O alkenoxide

C	-2.366262	-0.266300	-0.301464
H	-3.220828	-0.923523	-0.421314
C	-1.251862	-0.682929	0.319460
C	0.022145	0.060326	0.484077
C	-0.019232	1.508457	0.037445
H	-0.274966	1.566462	-1.026161
H	-0.744138	2.107750	0.599564
C	1.197952	-0.678400	-0.294619
O	2.396781	-0.113638	-0.124079
H	0.823856	-0.696590	-1.359819
H	-2.450540	0.735151	-0.705689
H	1.121206	-1.750017	0.046487
H	-1.242046	-1.707034	0.694429
H	0.983633	1.919632	0.160185
H	0.333130	0.010361	1.535566

C2=O alkenoxide

C	-2.155412	-0.043905	-0.141863
H	-3.092479	-0.583765	-0.042769
C	-0.978148	-0.635609	0.107259
C	0.416044	-0.027170	0.143552
C	1.223228	-0.697693	-1.004308
H	0.799987	-0.506813	-1.999840
H	2.248286	-0.317610	-0.960726
C	0.355596	1.487317	-0.166465
O	0.966949	-0.276206	1.359621
H	-0.082466	1.719845	-1.146432
H	1.378430	1.870137	-0.133580
H	-2.219512	0.999289	-0.428971
H	-0.219746	1.987759	0.615593
H	1.254148	-1.775763	-0.825529
H	-0.970106	-1.681063	0.416234

C3=O alkenoxide (*cis*)

C	-1.770621	0.890496	-0.000017
H	-1.374853	1.907789	0.000012
H	-2.408788	0.762195	-0.879257
C	-0.724047	-0.231199	-0.000017
C	0.629789	0.067686	0.000007
C	1.257955	1.430390	0.000051
H	0.532783	2.244871	0.000041
H	1.910576	1.582031	0.877517
H	1.910633	1.582059	-0.877367
C	1.615940	-1.062475	0.000008
O	-1.231353	-1.415626	-0.000044
H	1.077309	-2.011524	-0.000047
H	2.278900	-1.037016	0.880821
H	-2.408825	0.762159	0.879190
H	2.278971	-1.036951	-0.880750

C3=O alkenoxide (*trans*)

C	-1.778883	0.817695	-0.000051
H	-1.713590	1.461676	-0.883606
H	-2.751292	0.324776	-0.000137
C	-0.705834	-0.293721	-0.000116
C	0.626968	0.081280	0.000004
C	1.113492	1.498860	0.000216
H	0.297379	2.224143	0.000046
H	1.743689	1.724727	0.878775
H	1.744126	1.724809	-0.878004
C	1.696134	-0.967285	0.000040
O	-1.157780	-1.499611	-0.000180
H	1.231408	-1.955141	-0.000126
H	2.356337	-0.895393	0.880918
H	-1.713659	1.461506	0.883634
H	2.356579	-0.895203	-0.880639

C4=O alkenoxide

C	1.515117	-0.600395	0.222608
H	2.255677	-1.304423	-0.252337
C	0.237858	-0.762872	-0.698908
C	-0.951685	-0.057145	-0.140433
C	-1.970918	-0.707859	0.446598
H	-1.991734	-1.791469	0.493599
H	-2.792578	-0.169888	0.908924
C	-0.888005	1.441165	-0.191542
O	1.958008	0.657004	0.374031
H	0.099945	1.725967	0.193963
H	-1.699547	1.904298	0.377312
H	1.215985	-1.113395	1.178598
H	-0.941064	1.785544	-1.229843
H	0.508602	-0.335775	-1.671843
H	0.026431	-1.834272	-0.820556

Hydroxyl-isoprene adduct molecular ion: C1-OH (MP2 from CAM-B3LYP opt)

C	-0.854875	-0.602133	0.651085
H	-0.265396	-1.238261	1.326997
H	-1.795626	-0.335748	1.145614
C	-0.081405	0.581771	0.253666
C	-0.818505	1.849638	-0.081160
H	-0.114601	2.681883	-0.198861
H	-1.530369	2.138004	0.706154
H	-1.403040	1.797723	-1.016394
C	1.263964	0.423234	-0.091436
H	1.775322	1.347048	-0.384054
C	2.052131	-0.725319	-0.147602
H	1.656874	-1.708210	0.091152
H	3.124373	-0.644351	-0.284181
O	-1.285562	-1.473988	-0.476512
H	-0.530891	-1.409341	-1.081635

Hydroxyl-isoprene adduct molecular ion: C2-OH

C	-2.152471	-0.086840	-0.008181
H	-2.214465	0.777381	-0.656075
H	-3.071475	-0.539720	0.349544
C	-0.954263	-0.572573	0.352225
H	-0.906434	-1.448465	0.997860
C	0.380591	0.030510	0.036086
C	0.924387	0.748741	1.223428
H	0.185510	1.040119	1.970177
H	1.823194	0.311238	1.660956
O	0.202244	0.963307	-1.102497
H	0.628033	1.740044	-0.693554
C	1.335886	-1.059236	-0.451941
H	2.338744	-0.630771	-0.530932
H	1.362021	-1.897408	0.249766
H	1.032157	-1.422509	-1.437454

Hydroxyl-isoprene adduct molecular ion: C3-OH

C	-1.720519	-1.024793	-0.236719
H	-1.481415	-2.039474	-0.536254
H	-2.768137	-0.777223	-0.095272
C	-0.748938	-0.124411	-0.012610
C	0.710758	-0.466381	-0.125465
H	0.797366	-1.485596	-0.524124
C	-1.081730	1.293820	0.359655
H	-0.798389	1.960806	-0.456079
H	-2.149668	1.408153	0.565631
H	-0.514535	1.603249	1.239635
C	1.478153	-0.324955	1.129564
H	1.027063	0.272114	1.920734
H	1.943771	-1.237949	1.496123
O	1.258945	0.430042	-1.198873
H	2.046033	0.735901	-0.705954

C1=O alkenoxide (MP2 from CAM-B3LYP opt)

C	-1.855912	-0.620808	0.784306
C	-0.675819	-0.001985	0.643948
C	-0.589177	1.496592	0.597728
H	-0.225418	1.781044	-0.392954
H	0.123703	1.872886	1.337984
H	-1.563275	1.957990	0.779407
C	0.618070	-0.744902	0.482546
C	1.480378	-0.189128	-0.697661
H	0.405283	-1.803691	0.299329
H	1.204920	-0.661003	1.413312
O	0.827955	-0.121921	-1.867307
H	2.396213	-0.846382	-0.695445
H	1.875046	0.799544	-0.319762
H	-2.780657	-0.061080	0.885912
H	-1.924685	-1.702561	0.765472

$C_4H_5O_2^-$: conjugate base of a carboxylic acid

C	-2.456177	-1.121460	-0.014525
C	-1.290504	-0.181445	-0.120615
H	-2.974131	-1.228309	-0.973495
H	-3.198446	-0.760785	0.705361
H	-2.129605	-2.113580	0.305341
C	-0.019877	-0.508425	0.138068
C	1.152169	0.467639	0.022992
H	-1.479291	0.843728	-0.429699
H	0.227620	-1.521811	0.451783
O	2.274212	-0.037584	0.313183
O	0.880812	1.642945	-0.340034

$C_4H_5O_2^-$: $CHO=C(CH_3)=CHO^-$

C	-1.152715	0.763937	-0.004262
C	0.000231	-0.044993	0.016156
C	1.203168	0.508523	-0.469572
O	2.334594	-0.030652	-0.542744
O	-2.307725	0.455913	0.380441
H	1.096770	1.558907	-0.824277
H	-0.984785	1.785952	-0.413819
C	-0.063709	-1.447156	0.541590
H	-0.441156	-1.469691	1.568775
H	0.933658	-1.890474	0.517366
H	-0.741309	-2.068653	-0.053074

$C_4H_5O_2^-$: H_2C=CH-CO-CH_2-O^- (*trans*)

C	-2.224033	-0.442097	-0.111278
C	-1.101962	0.272769	0.043824
C	0.238186	-0.376958	0.193134
C	1.340810	0.613253	0.476851
H	-3.198662	0.029353	-0.165981
H	-2.166048	-1.520601	-0.208338
H	-1.115657	1.352758	0.122924
O	0.396293	-1.579511	-0.039398
O	1.297055	1.398359	-0.640463
H	2.280195	0.040971	0.631548
H	1.135395	1.144934	1.443568

$C_4H_5O_2^-$: H_2C=CH-CO-CH_2-O^- (*cis*)

C	0.132010	-0.381000	-1.904263
C	-0.764047	0.166550	-1.070212
C	-0.543923	0.329396	0.393892
C	0.857138	0.091716	0.986498
H	-0.084518	-0.462545	-2.966588
H	1.060042	-0.752021	-1.470238
H	-1.731529	0.520932	-1.423059
O	-1.499656	0.714694	1.077993
O	1.586123	-0.929094	0.484930
H	0.660123	0.052496	2.084746
H	1.317100	1.116348	0.836263

$C_4H_5O_2^-$: H_2C=CH-CH(O^-)-CH=O

C	-1.795029	-0.298570	-1.366105
C	-1.034439	0.550786	-0.667952
C	-0.196019	0.076824	0.507105
C	1.265763	0.154996	0.105989
H	-2.390064	0.018316	-2.216229
H	-1.813918	-1.334447	-1.044625
H	-0.980855	1.606913	-0.939515
O	-0.338402	-1.222537	0.860505
O	2.161873	0.793554	0.650756
H	-0.342494	0.821048	1.325603
H	1.497889	-0.584200	-0.689545

$C_4H_5O_2^-$: H_2C=CH-CH(O^-)-CH=O (higher energy)

C	0.481940	1.953890	0.460104
C	-0.598116	1.271336	0.056180
C	-0.705360	-0.238449	-0.192466
C	0.349974	-0.918018	0.681974
H	0.498255	3.039401	0.471310
H	1.393917	1.447305	0.757562
H	-1.475861	1.821767	-0.276900
O	-0.763382	-0.509653	-1.489382
O	1.242577	-1.674779	0.342166
H	-1.622402	-0.551475	0.418834
H	0.201881	-0.694103	1.772156

$C_4H_5O_2^-$:C_1 peroxide (*trans*, O_2 *trans* nearest H)

C	-0.662029	0.735576	0.000235
C	0.366168	-0.161492	-0.000004
C	1.719072	0.310000	0.000147
H	1.844047	1.394730	0.000447
C	2.847107	-0.439026	-0.000042
H	3.827295	0.021381	0.000097
O	-1.953685	0.509361	0.000148
O	-2.266306	-0.904025	-0.000458
H	-0.458963	1.808657	0.000541
H	2.799660	-1.522275	-0.000337
H	0.125960	-1.215522	-0.000297

$C_4H_5O_2^-$: C_1 peroxide (*trans*, O_2 *cis* nearest H)

C	-0.576928	0.325453	0.002954
C	0.447679	-0.582353	-0.003250
C	1.808971	-0.142759	-0.006821
H	1.950145	0.938392	-0.004026
C	2.920524	-0.916806	-0.013179
H	3.909690	-0.477261	-0.015360
O	-1.840733	0.002028	0.006117
O	-2.677663	1.208416	0.013560
H	-0.391303	1.398389	0.005657
H	2.852284	-1.999254	-0.016268
H	0.224892	-1.645050	-0.005636

$C_4H_5O_2^-$: C_1 peroxide (*trans*, O_2 *cis* nearest H)
(forced symmetry)

C	-0.000	0.142395	0.646915
C	0.000	-0.425870	-0.598495
H	-0.000	1.222688	0.783376
H	0.000	-1.507246	-0.696423
C	-0.000	0.392812	-1.771581
O	-0.000	-0.536678	1.760772
H	-0.000	1.467954	-1.590211
O	0.000	0.372019	2.914093
C	0.000	-0.022107	-3.060993
H	0.000	-1.077148	-3.312485
H	-0.000	0.687641	-3.878252

$C_4H_5O_2^-$: C_1 peroxide (*cis*, O_2 *cis* nearest H)

C	-0.963829	-0.142313	-0.008953
C	0.116594	-0.986281	-0.013169
C	1.480744	-0.541827	0.003016
H	1.623308	0.536638	0.019410
C	2.580175	-1.328786	-0.000246
H	3.575969	-0.903921	0.013031
O	-0.883461	1.162481	0.010228
O	-2.228954	1.755204	0.008695
H	-1.984088	-0.518281	-0.021649
H	2.497811	-2.410849	-0.016263
H	-0.095793	-2.049807	-0.029788

$C_4H_5O_2^-$: C_1 peroxide (*cis*, O_2 *cis* nearest H)
(forced symmetry)

C	0.000	-0.641944	0.732944
C	-0.000	-0.765863	-0.632434
O	0.000	0.498393	1.372433
C	-0.000	0.346997	-1.538110
H	0.000	1.330791	-1.073537
H	0.000	-1.510873	1.386705
H	0.000	-1.774938	-1.030228
O	-0.000	0.267470	2.824449
C	-0.000	0.281299	-2.888572
H	-0.000	-0.672897	-3.405691
H	-0.000	1.178073	-3.495274

$C_4H_5O_2^-$: C_1 peroxide (*cis*, O_2 *trans* nearest H)

C	-1.339927	-0.148680	-0.008743
C	-0.227476	-0.943810	-0.016682
C	1.164100	-0.569506	-0.003882
H	1.343269	0.499290	0.014773
C	2.183454	-1.457835	-0.013926
H	3.215054	-1.127246	-0.003513
O	-1.520843	1.152554	0.011928
O	-0.288592	1.913131	0.030262
H	-2.314456	-0.640391	-0.021488
H	2.004611	-2.529581	-0.032669
H	-0.453902	-2.008567	-0.035222

$C_4H_5O_2^-$:C_1 peroxide (*trans*, O_2 *trans* nearest H)
(forced symmetry)

C	0.000	-0.157079	-0.368083
C	0.000	0.727564	0.670824
H	0.000	-1.213920	-0.140564
C	-0.000	0.330644	-1.715222
H	-0.000	1.803009	0.480672
O	0.000	0.485838	1.959667
H	-0.000	1.416798	-1.827147
O	-0.000	-0.931205	2.255274
C	0.000	-0.404768	-2.852180
H	0.000	-1.488509	-2.817758
H	-0.000	0.067390	-3.826762

$C_4H_5O_2^-$:C_2 peroxide (toward C_1)

C	-0.800069	1.542957	0.000000
H	-1.877397	1.504854	0.000009
C	-0.085478	0.386532	-0.000001
C	1.381709	0.428895	-0.000014
H	1.812808	1.426844	-0.000024
C	2.192064	-0.641099	-0.000016
H	3.269465	-0.523277	-0.000026
O	-0.576284	-0.844335	0.000010
O	-2.029809	-0.850001	0.000019
H	-0.265551	2.484439	-0.000010
H	1.780064	-1.641887	-0.000007

$C_4H_5O_2^-$:C_2 peroxide (toward C_4)

C	0.430001	1.173363	1.619222
H	0.311858	0.851253	2.645557
C	0.122006	0.333050	0.580192
C	0.317346	0.865653	-0.777981
H	0.691906	1.887477	-0.759999
C	0.107876	0.293993	-1.975122
H	0.318654	0.868897	-2.873571
O	-0.323526	-0.881991	0.874044
O	-0.641183	-1.749878	-0.260032
H	0.795181	2.169703	1.418734
H	-0.263320	-0.718746	-2.020704

[Isoprene-H]$^-\cdot H_2O$

C	-1.463019	0.315213	-0.731123
C	-0.312857	-0.361499	-0.300399
H	-1.576774	0.614632	-1.769162
H	-2.354199	0.312116	-0.113440
C	0.879951	-0.538349	-1.001991
H	0.927853	-0.320107	-2.064054
H	1.714109	-1.071909	-0.565554
O	0.726599	2.573911	-0.549948
H	-0.184602	2.230803	-0.471524
H	1.184378	1.712865	-0.631839
C	-0.413482	-0.858183	1.091394
C	0.364862	-1.776460	1.686410
H	-1.229923	-0.432847	1.673555
H	1.182451	-2.252636	1.159609
H	0.191178	-2.068516	2.716262

C4 alkenoxy radical

C	1.515117	-0.600395	0.222608
H	2.255677	-1.304423	-0.252337
C	0.237858	-0.762872	-0.698908
C	-0.951685	-0.057145	-0.140433
C	-1.970918	-0.707859	0.446598
H	-1.991734	-1.791469	0.493599
H	-2.792578	-0.169888	0.908924
C	-0.888005	1.441165	-0.191542
O	1.958008	0.657004	0.374031
H	0.099945	1.725967	0.193963
H	-1.699547	1.904298	0.377312
H	1.215985	-1.113395	1.178598
H	-0.941064	1.785544	-1.229843
H	0.508602	-0.335775	-1.671843
H	0.026431	-1.834272	-0.820556

$C_4H_5O_2$: C_1 peroxy radical (*trans*, O_2 *trans* nearest H)

C	-0.662029	0.735576	0.000235
C	0.366168	-0.161492	-0.000004
C	1.719072	0.310000	0.000147
H	1.844047	1.394730	0.000447
C	2.847107	-0.439026	-0.000042
H	3.827295	0.021381	0.000097
O	-1.953685	0.509361	0.000148
O	-2.266306	-0.904025	-0.000458
H	-0.458963	1.808657	0.000541
H	2.799660	-1.522275	-0.000337
H	0.125960	-1.215522	-0.000297

$C_4H_5O_2$: C_1 peroxy radical (*trans*, O_2 *cis* nearest H)

C	-0.576928	0.325453	0.002954
C	0.447679	-0.582353	-0.003250
C	1.808971	-0.142759	-0.006821
H	1.950145	0.938392	-0.004026
C	2.920524	-0.916806	-0.013179
H	3.909690	-0.477261	-0.015360
O	-1.840733	0.002028	0.006117
O	-2.677663	1.208416	0.013560
H	-0.391303	1.398389	0.005657
H	2.852284	-1.999254	-0.016268
H	0.224892	-1.645050	-0.005636

$C_4H_5O_2$: C_1 peroxy radical (*cis*, O_2 *cis* nearest H)
(forced symmetry)

C	0.000	-0.641944	0.732944
C	-0.000	-0.765863	-0.632434
O	0.000	0.498393	1.372433
C	-0.000	0.346997	-1.538110
H	0.000	1.330791	-1.073537
H	0.000	-1.510873	1.386705
H	0.000	-1.774938	-1.030228
O	-0.000	0.267470	2.824449
C	-0.000	0.281299	-2.888572
H	-0.000	-0.672897	-3.405691
H	-0.000	1.178073	-3.495274

$C_4H_5O_2$: C_2 peroxide (toward C_4)

C	0.430001	1.173363	1.619222
H	0.311858	0.851253	2.645557
C	0.122006	0.333050	0.580192
C	0.317346	0.865653	-0.777981
H	0.691906	1.887477	-0.759999
C	0.107876	0.293993	-1.975122
H	0.318654	0.868897	-2.873571
O	-0.323526	-0.881991	0.874044
O	-0.641183	-1.749878	-0.260032
H	0.795181	2.169703	1.418734
H	-0.263320	-0.718746	-2.020704

[Isoprene-H·]·H_2O : above C2, nearer C1 (type 1)

C	0.023812	0.640994	0.682831
C	-0.854705	1.641794	0.295229
C	1.352750	0.919335	0.992338
C	-0.498979	-0.739449	0.766415
C	0.239891	-1.849245	0.621245
H	-0.523005	2.669251	0.216565
H	-1.889523	1.420896	0.070613
H	-1.568909	-0.836110	0.923844
H	-0.212522	-2.829806	0.683297
H	1.304739	-1.801812	0.428367
H	2.020109	0.155673	1.364351
H	1.735777	1.926124	0.890947
O	-0.258338	-0.503256	-2.573022
H	-0.165164	-0.816326	-1.660734
H	-0.211425	0.457602	-2.481408

[Isoprene-H·]·H_2O : above C2, nearer C4 (type 1)

C	-0.720996	0.528793	0.224764
C	-1.047386	-0.483128	1.126188
C	-1.644569	0.986425	-0.703902
C	0.618483	1.151911	0.231982
C	1.730140	0.592685	0.730304
H	2.673602	1.121249	0.699792
H	1.725660	-0.392376	1.179456
H	0.685255	2.131879	-0.230791
H	-1.395015	1.777922	-1.397391
H	-2.635958	0.555628	-0.757487
H	-2.023775	-0.948774	1.090220
H	0.066988	-1.680682	-0.764640
H	-0.361316	-0.800000	1.898235
O	0.781177	-2.127069	-1.243371
H	1.401128	-1.408410	-1.426433

[Isoprene-H·]·H_2O : C1/methyl pocket (type 2)

O	3.212988	-0.083183	1.411325
H	3.794568	0.646210	1.663266
H	3.686971	-0.877086	1.692028
H	0.671538	0.093936	1.507334
H	1.742248	-0.047248	-0.665651
C	0.768410	-0.013525	-1.136539
C	-0.295996	0.146302	1.026400
C	-0.379160	0.074730	-0.365169
H	0.709660	-0.056761	-2.216359
H	-1.174901	0.281995	1.640316
C	-1.681113	0.100767	-1.060845
H	-1.643014	0.337965	-2.120153
C	-2.870304	-0.166157	-0.503815
H	-2.964272	-0.437185	0.540012
H	-3.777717	-0.129048	-1.091588

[Isoprene-H·]·H_2O : C4/methyl pocket (type 2)

H	-0.894284	-0.478233	-1.271773
H	-0.056933	1.263682	-0.372329
C	-0.670346	-1.389065	-0.731857
C	0.492359	1.067067	0.536667
C	0.055080	-1.399678	0.395576
C	0.644373	-0.220592	1.060748
H	-1.056794	-2.316029	-1.135483
H	0.242007	-2.350165	0.887217
C	1.356991	-0.432101	2.227122
H	1.478326	-1.425821	2.637389
H	1.810752	0.395271	2.757648
H	0.938913	1.906116	1.054425
O	-1.330180	1.656762	-2.462274
H	-0.908069	1.887300	-3.300410
H	-2.183234	2.109974	-2.488043

$CH_3O_2^-$: test

C	-1.047182	-0.145556	-0.118992
O	0.129646	0.593039	-0.157793
H	-0.997248	-1.018530	-0.786928
H	-1.864582	0.516583	-0.444652
H	-1.258714	-0.513518	0.896181
O	1.170810	-0.356940	0.288963