Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information

Competition between Electron Transfer and Base-Induced Elimination Mechanisms in the Gas-Phase Reactions of Superoxide with Alkyl Hydroperoxides

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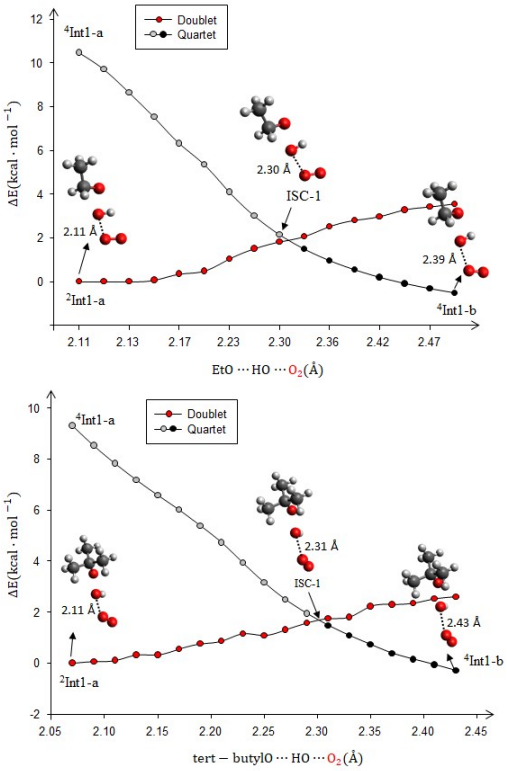

Figure S1: Relaxed scan (at the ROB2PLYP-D3//UB2PLYP-D3/6-311+(3df,2p) level) along the O_2···OH bond coordinate (in Å) showing the intersystem crossing (ICS1) for the $O_2^{\bullet-}$/EtOOH (up) and $O_2^{\bullet-}$/t-BuOOH (bottom) reactions, respectively.

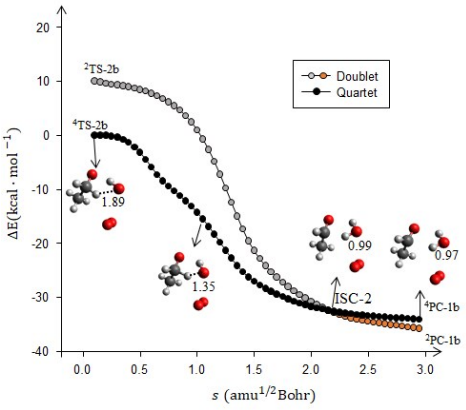

Figure S2: Relaxed scan (at the ROB2PLYP-D3//UB2PLYP-D3/6-311+(3df,2p) level) along the IRC (s, in amu1/2/a0) of the ^{4}TS-1b transition state showing the intersystem crossing (ICS2) for the $O_2^{\bullet-}$/EtOOH reaction.

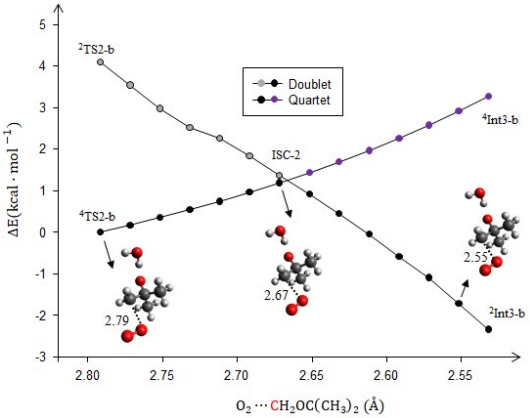

Figure S3: Relaxed scan (at the ROB2PLYP-D3//UB2PLYP-D3/6-311+(3df,2p) level) along the O–C bond coordinate between the O atom of O_2 and the C atom of the methylidene group (CH_2CMe_2O), showing the intersystem crossing (ICS2) for the $O_2^{\bullet-}$/t-BuOOH reaction.

Table S1. The optimized geometry of all stationary points for the $CH_3OOH + O^{\bullet}{}_2^-$ gas-phase reaction, calculated with the UB2PLYP-D3/6-311+G(3df,2p) method and energies with the ROB2PLYP-D3//UB2PLYP-D3/6–311+G(3df,2p).

R – CH_3OOH				R – $^2O^{\bullet}{}_2^-$			
0 1				-1 2			
C	1.12325	-0.22759	-0.02255	O	0.00000	0.00000	0.67553
O	-0.01532	0.60970	0.02209	O	0.00000	0.00000	-0.67553
O	-1.16238	-0.27322	0.09980	$<S^2>$=0.77			
H	1.16810	-0.86936	0.85672	Sum of electronic and zero-point Energies -150.2983			
H	1.13468	-0.83497	-0.92854				
H	-1.58882	-0.08063	-0.74420				
H	1.96812	0.45868	-0.02381				
Sum of electronic and zero-point Energies -190.7368							
RC – a				^{2}TS – 1a			
-1 2				-1 2			
C	-1.38872	1.00550	0.10987	O	1.65936	-0.63199	-0.29575
O	-1.45514	-0.28370	-0.46141	O	0.11014	0.11961	-0.37668
O	-0.65810	-1.14721	0.38653	H	-0.28780	-0.64077	0.05745
O	1.88831	0.79107	0.10214	O	-1.99688	0.55775	-0.20467
H	-1.85567	1.01543	1.10104	O	-2.54872	-0.41595	0.39749
H	-0.35125	1.34125	0.18479	C	2.42013	0.30848	0.35594
H	0.30906	-0.88494	0.11900	H	2.08307	0.50081	1.39038
H	-1.95384	1.65196	-0.56638	H	2.42421	1.28571	-0.15871
O	1.74793	-0.50474	-0.21447	H	3.46841	-0.03195	0.41215
$<S^2>$=0.76				$<S^2>$=0.77			
Sum of electronic and zero-point Energies -341.0781				Sum of electronic and zero-point Energies -341.0469			
^{2}Int – 1a				^{2}TS – 2a			
-1 2				-1 2			
O	-1.81456	-0.71518	0.20496	O	1.97665	-0.65918	-0.10247
O	0.01194	0.10584	0.33325	O	-0.20440	-0.25654	-0.29493
H	0.26342	-0.73447	-0.06534	O	-2.68482	0.52844	-0.15752
O	2.00455	0.54996	0.19044	H	0.30779	-0.78018	0.34881
O	2.65175	-0.39351	-0.35099	O	-1.95523	-0.34282	0.35141
C	-2.49280	0.37850	-0.28073	C	2.46079	0.60718	0.11843
H	-2.11913	0.72693	-1.25857	H	1.89368	1.17061	0.88182
H	-2.45871	1.24565	0.40084	H	3.51022	0.56846	0.47671
H	-3.55831	0.11401	-0.41378	H	2.46602	1.23888	-0.78988
$<S^2>$=0.78				$<S^2>$=0.77			
Sum of electronic and zero-point Energies -341.0489				Sum of electronic and zero-point Energies -341.0456			
^{2}PC – 1a				^{4}Int – 1a			
-1 2				-1 4			
O	-1.88740	-0.60385	0.28885	O	-1.81456	-0.71518	0.20496
O	0.70402	-0.86098	-0.32051	O	0.01194	0.10584	0.33325
O	2.54748	0.42576	-0.02320	H	0.26342	-0.73447	-0.06534
H	-0.91922	-0.75164	0.10602	O	2.00455	0.54996	0.19044
O	1.25503	0.22395	0.27222	O	2.65175	-0.39351	-0.35099
C	-2.19313	0.68817	-0.16395	C	-2.49280	0.37850	-0.28073
H	-2.04508	0.79670	-1.24534	H	-2.11913	0.72693	-1.25857
H	-3.24389	0.89137	0.05516	H	-2.45871	1.24565	0.40084
H	-1.58603	1.45551	0.32890	H	-3.55831	0.11401	-0.41378
$<S^2>$=0.76				$<S^2>$=3.79			
Sum of electronic and zero-point Energies -341.0980				Electronic Energy -341.0808			
^{4}Int – 1b				^{4}TS – 1b			
-1 4				-1 2			
O	-2.50578	-1.14748	-0.04923	O	-2.97088	-0.93567	0.10998
H	-2.99950	-0.62234	0.58808	H	-2.77111	-0.07315	0.51917
O	-1.78556	0.97298	-0.03529	O	-1.61045	0.98059	-0.19490
O	2.51059	-0.25627	-0.59998	O	2.47035	-0.76136	-0.28621
O	2.51299	-0.20988	0.61401	O	2.70949	0.26187	0.33590
C	-0.45605	0.66518	-0.00542	C	-0.35972	0.46151	-0.04184

H -0.16503 0.02828 0.84983 H 0.14694 1.59499 0.06798 H -0.10405 0.13323 -0.90949 <S^2>=3.79 Sum of electronic and zero-point Energies -341.0515	H -0.27212 -0.26215 0.78957 H 0.38812 1.26037 0.16799 H 0.02533 -0.05754 -0.94390 <S^2>=3.79 Sum of electronic and zero-point Energies -341.0493
^{4}Int – 2b	^{4}TS – 2b
-1 2 C 0.32080 0.48430 0.00006 O 1.60363 0.93962 0.00003 O 3.24935 -0.89866 -0.00005 O -2.68516 -0.26059 0.60778 H -0.27622 0.82147 -0.87941 H 2.52666 -0.08486 -0.00001 H -0.27619 0.82152 0.87953 O -2.68514 -0.26040 -0.60782 H 0.23956 -0.62362 0.00009 <S^2>=3.77 Sum of electronic and zero-point Energies -341.0585	-1 2 C 0.54857 -0.68364 -0.00006 O 1.77230 -1.20670 -0.00012 O 2.21318 1.43790 0.00011 O -2.36666 0.19899 -0.60921 H -0.08137 -0.92272 0.89191 H 2.27303 0.44474 0.00002 H -0.08138 -0.92256 -0.89207 O -2.36665 0.19890 0.60928 H 0.58090 0.46965 0.00004 <S^2>=3.78 Sum of electronic and zero-point Energies -341.0509
^{4}PC – 1b	^{2}PC – 1b
-1 2 C -0.28403 0.67844 0.00093 O -1.51103 1.10241 0.05599 O -3.21114 -0.88446 0.00627 O 2.96161 0.22180 -0.15394 H -0.01767 -0.32686 0.35934 H -2.57998 -0.09544 0.06869 H 0.54791 1.39306 -0.06316 O 2.58248 -0.89423 0.13253 H -2.82146 -1.40554 -0.69723 <S^2>=3.78 Sum of electronic and zero-point Energies -341.1125	-1 2 C -0.28747 0.78797 0.35491 O 0.76320 1.05424 -0.30410 O 2.70453 -0.70076 0.12415 O -2.36146 -0.61240 0.20253 H -1.07762 1.55409 0.43226 H 2.00386 -0.00390 -0.03657 H -0.20786 0.19676 1.28439 O -1.26546 -0.36237 -0.47641 H 2.27997 -1.50445 -0.17900 <S^2>=0.76 Sum of electronic and zero-point Energies -341.1794
^{2}TS – 3b	^{2}PC – 2b
-1 2 C -0.68820 0.86165 0.05681 O 0.40693 1.46496 -0.17908 O -1.49633 -1.06527 -0.41948 H -1.31448 0.31067 -0.89852 H -1.50605 1.44490 0.52877 O -0.66763 -0.44294 0.65832 O 2.22083 -0.69501 -0.05855 H 1.80396 0.18106 -0.16239 H 1.43547 -1.20036 0.18161 <S^2>=0.77 Sum of electronic and zero-point Energies -341.1390	-1 2 C -0.00465 0.97572 0.00037 O -1.19783 1.33251 -0.00065 O -2.26579 -1.29061 -0.00044 O 0.46131 -0.20019 0.00182 H 2.09027 -0.39723 0.00015 H 0.75705 1.79056 -0.00001 H -2.22403 -0.31710 -0.00144 H -1.31385 -1.45832 0.00078 O 3.09212 -0.52575 -0.00095 <S^2>=0.75 Sum of electronic and zero-point Energies -341.2819
^{2}TS – RC	^{2}RC – c
-1 2 C 0.43994 -0.31715 0.41538 O 1.61972 -0.54939 -0.35006 O 2.59671 0.46356 0.02664 O -2.51367 -0.53182 -0.11941 H 0.63721 -0.47666 1.47646 H 0.02149 0.67398 0.23992 H 2.25665 1.22556 -0.46053 H -0.31662 -1.01138 0.04589 O -2.35756 0.80407 -0.03142 <S^2>=0.77 Sum of electronic and zero-point Energies -341.0533	-1 2 C 0.40040 -0.23950 -0.11669 O 1.54032 0.61573 -0.02979 O 2.73319 -0.22285 -0.01830 O -2.46922 0.67617 0.05543 H 0.43282 -0.82592 -1.03334 H 0.34972 -0.90208 0.74931 H 2.78164 -0.44681 0.91956 H -0.48120 0.41383 -0.10716 O -2.48996 -0.66932 0.01414 <S^2>=0.77 Sum of electronic and zero-point Energies -341.0548
^{2}TS – 1c	^{2}PC – 1c
-1 2 O 2.84651 0.04207 -0.00104 H 3.31922 -0.79955 -0.00320 O 1.20512 -0.40139 -0.00031 O -2.83868 0.33860 -0.00246	-1 2 C 0.94266 0.12942 0.13988 O 0.11501 -0.67440 -0.29696 O 3.65318 0.26730 0.04701 O -2.81913 0.66994 -0.27744

O -1.96122 -0.65032 0.00171 C 0.47257 0.64850 0.00204 H 0.41370 1.23386 0.92680 H -0.99425 -0.19389 0.00164 H 0.41204 1.23687 -0.92069 Sum of electronic and zero-point Energies -341.0436	H -1.37057 -0.47586 0.07715 H 0.54963 0.96778 0.75518 H 4.28650 -0.33178 -0.35782 H 2.07922 0.06406 -0.02239 O -2.34916 -0.38793 0.36597 $<S^2>$=0.76 Sum of electronic and zero-point Energies -341.1201
^{2}TS – 2c	^{2}PC – 2c
-1 2 C 0.96601 0.10915 -0.27157 O 0.08747 -0.75283 -0.35012 O 3.56201 0.29636 0.18392 O -2.84094 0.56621 -0.27379 H -1.31723 -0.42433 0.20287 H 0.71100 1.07927 0.18921 H 4.25590 -0.27197 0.53041 H 2.03649 -0.03505 -0.53377 O -2.24382 -0.23510 0.59508 $<S^2>$=0.76 Sum of electronic and zero-point Energies -341.1190	-1 2 C 1.40439 0.00054 -0.34650 O 0.93588 -1.17078 0.25889 O 0.93485 1.17076 0.25963 O -1.68118 0.67088 -0.04884 H -0.05807 -1.11903 0.18955 H 1.12565 0.00063 -1.41227 H -0.05904 1.11884 0.18931 H 2.49291 0.00079 -0.26099 O -1.68052 -0.67141 -0.04800 $<S^2>$=0.76 Sum of electronic and zero-point Energies -341.1901
P – $CH_2(OH)OH^-$	P – HO^-
-1 2 C -0.00001 0.50367 0.09342 O -1.17701 -0.22707 -0.14021 O 1.17698 -0.22709 -0.14025 H -1.35221 -0.80612 0.60486 H 0.00003 0.91466 1.10702 H 1.35245 -0.80581 0.60501 H -0.00003 1.30856 -0.63372 Sum of electronic and zero-point Energies -190.8338	-1 1 O 0.00000 0.00000 0.10709 H 0.00000 0.00000 -0.85671 Sum of electronic and zero-point Energies -75.7693
P – CH_2O	P – $HO_2^\bullet$
0 1 C 0.52886 0.00000 -0.00002 O -0.67442 0.00000 0.00002 H 1.11111 0.93644 0.00016 H 1.11106 -0.93647 -0.00016 Sum of electronic and zero-point Energies -114.4374	0 2 O 0.05527 0.71566 0.00000 O 0.05527 -0.60808 0.00000 H -0.88432 -0.86065 0.00000 $<S^2>$=0.75 Sum of electronic and zero-point Energies -150.8534
P – CH_3OH	P – $O_3^{\bullet-}$
O 0.74721 0.12185 0.00000 H 1.14623 -0.74970 0.00006 C -0.66591 -0.02032 0.00000 H -1.02401 -0.54175 0.89010 H -1.08070 0.98342 -0.00181 H -1.02373 -0.54486 -0.88836 Sum of electronic and zero-point Energies -115.6263	-1 2 O 1.14064 -0.24111 0.00000 O -1.14064 -0.24112 0.00000 O 0.00000 0.48224 0.00000 $<S^2>$=0.76 Sum of electronic and zero-point Energies -225.4453
P – HCO_2^-	P – H_2O
-1 1 O 1.13639 -0.20932 0.00001 O -1.13648 -0.20925 0.00001 C 0.00008 0.31684 -0.00003 H 0.00023 1.44745 0.00005 Sum of electronic and zero-point Energies -189.1367	0 1 O 0.00000 0.11688 0.00000 H 0.76066 -0.46751 0.00000 H -0.76066 -0.46750 0.00000 Sum of electronic and zero-point Energies -76.3882
P – $HO^\bullet$	P – $^4O_2^{\bullet-}$
0 2 O 0.00000 0.00000 0.10709 H 0.00000 0.00000 -0.85672 $<S^2>$=0.75 Sum of electronic and zero-point Energies -75.7042	-1 4 O 0.00000 0.00000 0.93379 O 0.00000 0.00000 -0.93379 $<S^2>$=3.87 Sum of electronic and zero-point Energies -150.222

Table S2. The optimized geometry of all stationary points for the $CH_3CH_2OOH + O^{\bullet}{}_2^-$ gas-phase reaction, calculated with the UB2PLYP-D3/6-311+G(3df,2p) and energies with the ROB2PLYP-D3//UB2PLYP-D3/6–311+G(3df,2p) method.

R – CH_3CH_2OOH			
0 1			
O	-1.38592	-0.61334	0.08659
H	-2.12816	-0.19783	0.54128
O	-0.69328	0.56717	-0.39720
C	0.55388	0.62344	0.28450
H	0.37720	0.65654	1.36204
H	0.95201	1.58883	-0.03128
C	1.48868	-0.50842	-0.09114
H	1.66355	-0.51816	-1.16506
H	2.44559	-0.38364	0.41523
H	1.06808	-1.46649	0.20252
Sum of electronic and zero-point Energies -230.001			

^{2}RC – a			
-1 2			
O	0.82158	0.92961	-0.36045
O	-0.33888	1.55664	0.23953
H	-1.09632	0.89901	-0.02137
O	-1.91431	-1.24918	0.20257
O	-2.22790	-0.07083	-0.35618
C	1.16670	-0.16929	0.46408
H	0.29378	-0.81675	0.58491
H	1.47765	0.19822	1.45011
C	2.30517	-0.89273	-0.23129
H	3.15734	-0.22994	-0.38803
H	2.63353	-1.73906	0.37369
H	1.97890	-1.26931	-1.19981
$<S^2>$=0.77			
Sum of electronic and zero-point Energies -380.343			

^{2}TS – 1a			
-1 2			
O	1.12317	-1.00255	0.46763
O	-0.35696	-0.50126	-0.25371
H	-0.75513	-0.37695	0.61326
O	-2.37028	0.16100	-0.60232
O	-2.91770	0.32906	0.53444
C	2.07126	-0.31997	-0.25768
H	1.87676	-0.40050	-1.34265
H	3.05546	-0.79143	-0.08421
C	2.16851	1.16653	0.10144
H	2.42379	1.28232	1.15652
H	2.92957	1.67527	-0.49974
H	1.20503	1.64192	-0.07408
$<S^2>$=1.07			
Sum of electronic and zero-point Energies -380.312			

^{2}Int – 1a			
-1 2			
O	1.13443	-0.70172	-0.34026
O	-0.70633	0.11914	-0.36911
H	-0.92522	-0.73391	0.02197
O	-2.67699	0.54988	-0.13369
O	-3.29988	-0.40164	0.41812
C	1.84015	0.38519	0.11861
H	1.48792	0.72371	1.10919
H	1.74025	1.25506	-0.55491
C	3.32635	0.02227	0.22603
H	3.71402	-0.27714	-0.74857
H	3.91095	0.87427	0.58860
H	3.46331	-0.81204	0.91537
$<S^2>$=0.78			
Sum of electronic and zero-point Energies -380.314			

^{2}TS – 2a			
-1 2			
O	-1.56799	0.87600	-0.11749
O	0.71308	0.43487	-0.26238
H	0.04804	0.76415	0.37341
O	3.19283	0.07816	0.56588
O	3.81933	-0.50138	-0.29925
C	-2.11000	-0.37379	-0.25564
H	-1.52267	-1.14941	0.27160
H	-2.15324	-0.70279	-1.31451
C	-3.54468	-0.41768	0.29885
H	-4.17156	0.30669	-0.22438
H	-3.98739	-1.41396	0.18180
H	-3.54308	-0.15707	1.35875
$<S^2>$=1.08			
Sum of electronic and zero-point Energies -380.309			

^{2}PC – 1a			
-1 2			
O	-1.46256	-1.18646	0.01453
O	1.18756	-0.99921	0.58190
H	-0.49992	-1.22824	0.23431
O	2.06662	0.97816	-0.10279
O	1.59231	-0.23216	-0.45413
C	-1.69584	0.09515	-0.52884
H	-2.74431	0.11488	-0.84111
H	-1.08258	0.25175	-1.42410
C	-1.41964	1.21877	0.46186
H	-0.36545	1.22350	0.73595
H	-1.66456	2.18809	0.01901
H	-2.02185	1.08379	1.36170
$<S^2>$=0.76			
Sum of electronic and zero-point Energies -380.364			

P – CH_3CH_2OH			
0 1			
O	1.23713	-0.25702	-0.10774
H	1.25618	-0.90108	0.60369
C	0.07888	0.55666	0.04682
H	0.13066	1.11950	0.98367
H	0.12528	1.27564	-0.76881
C	-1.21096	-0.24147	-0.02150
H	-2.07515	0.41849	0.05820
H	-1.27439	-0.78526	-0.96223

^{4}Int – 1b			
-1 4			
O	-2.72946	-0.91576	-0.55039
H	-2.85304	-1.25078	0.34335
O	-1.63495	0.23577	1.08832
O	2.61131	-0.86721	-0.32172
O	2.92126	0.13124	0.29634
C	-0.43477	0.27274	0.43132
H	-0.08945	-0.73539	0.13836
H	0.33530	0.66709	1.12987

H -1.26714 -0.96226 0.79556 Sum of electronic and zero-point Energies -154.890	C -0.45281 1.15263 -0.82118 H -0.72300 2.17719 -0.55687 H 0.52123 1.16495 -1.32387 H -1.21085 0.75242 -1.49207 $<S^2>$=3.80 Sum of electronic and zero-point Energies -380.319
^{4}TS – 1b	^{4}Int – 2b
-1 4 O -2.86064 -0.98919 -0.52050 H -2.51653 -1.00198 0.39616 O -1.58214 0.24309 1.06265 O 2.57665 -0.89426 -0.36759 O 2.87009 0.06275 0.32456 C -0.38401 0.29874 0.41335 H -0.04334 -0.69650 0.05840 H 0.41641 0.64192 1.10874 C -0.39284 1.24354 -0.79491 H -0.66389 2.25206 -0.47624 H 0.58322 1.28163 -1.29234 H -1.14642 0.89005 -1.49825 $<S^2>$=3.78 Sum of electronic and zero-point Energies -380.317	-1 4 C -0.42240 0.55901 0.00042 O -1.77761 0.61789 0.00131 O -2.90495 -1.61404 -0.00068 O 2.49799 -0.83760 0.60782 H -0.00338 0.00968 -0.87873 H -2.41843 -0.64958 0.00025 H -0.00225 0.01105 0.87986 O 2.49768 -0.83858 -0.60760 C 0.22359 1.95492 -0.00107 H -0.10282 2.50978 0.88071 H 1.31862 1.90583 -0.00156 H -0.10368 2.50832 -0.88344 $<S^2>$=3.78 Sum of electronic and zero-point Energies -380.327
^{4}TS – 2b	^{4}PC – 1b
-1 4 C -1.46312 -0.28026 0.43168 O -2.11678 0.43641 -0.48411 O -0.02176 1.98000 0.10619 O 2.46771 -0.21337 -0.61449 H -0.85992 1.57328 -0.25029 H -2.04307 -0.47729 1.36709 O 2.16560 -0.21712 0.55911 H -0.54680 0.30595 0.82211 C -0.90309 -1.62433 -0.07323 H -0.25389 -1.44965 -0.93210 H -0.33174 -2.14467 0.70422 H -1.72554 -2.26740 -0.39534 $<S^2>$=3.78 Sum of electronic and zero-point Energies -380.318	-1 4 C 1.31703 -0.45121 0.34236 O 0.49159 -0.65107 -0.64916 O -1.44833 -2.27132 0.00377 O -1.01223 1.95746 -0.25926 H -0.68335 -1.67334 -0.28815 H 1.48506 -1.26892 1.06403 O -1.82909 1.29363 0.33891 H -1.72800 -1.86238 0.82417 C 2.49638 0.46069 0.11971 H 2.16781 1.45029 -0.21201 H 3.08419 0.58285 1.03472 H 3.17829 0.08502 -0.66912 $<S^2>$=3.78 Sum of electronic and zero-point Energies -380.378
^{2}PC – 1b	^{2}TS – 3b
-1 2 C 0.46323 -0.70440 0.33840 O -0.39451 -1.49932 -0.10737 O 0.80647 1.95696 0.20484 H 0.33363 -0.25597 1.33805 O 0.13947 1.01307 -0.42461 O -2.70018 0.03108 0.05146 H -2.01755 -0.67177 0.03378 H -2.15970 0.79880 -0.16222 C 1.91178 -0.83540 -0.08199 H 2.46114 0.07694 0.14160 H 2.36377 -1.66890 0.46358 H 1.95866 -1.05461 -1.14778 $<S^2>$=0.76 Sum of electronic and zero-point Energies -380.449	-1 2 C -0.34017 0.04757 0.12010 O 0.61740 -0.50262 0.77181 O -2.14100 -0.75237 -0.72315 H -0.55108 -0.38837 -0.98114 O -1.67506 -0.20707 0.54305 O 3.08773 -0.25681 -0.28802 H 2.19366 -0.30605 0.13713 H 3.09243 -1.01168 -0.87776 C -0.21139 1.56846 -0.14214 H -1.03485 1.90142 -0.76939 H -0.24603 2.08491 0.81804 H 0.74264 1.77445 -0.62420 $<S^2>$=0.75 Sum of electronic and zero-point Energies -380.399
^{2}PC – 2b	P – CO_2CH_3
-1 2 C -0.06252 0.69590 -0.00914 O -1.19841 1.21033 -0.08102 O -2.65405 -1.19972 0.01789 O 0.19549 -0.54702 0.05685 H 1.69321 -1.15489 -0.00055 H -1.74413 -1.52309 0.05994 H -2.44653 -0.24812 -0.03411	-1 1 C 0.20839 0.00149 -0.00003 O 0.69681 1.15821 0.00001 O 0.80294 -1.10388 0.00001 C -1.34637 -0.05191 -0.00002 H -1.72793 0.47126 0.87899 H -1.72818 0.47405 -0.87726 H -1.71410 -1.07743 -0.00151

O 2.62105 -1.55581 -0.04702 C 1.14172 1.64490 0.03905 H 1.99396 1.22481 -0.49171 H 0.87809 2.61827 -0.36812 H 1.43754 1.77598 1.08154 <S^2>=0.75 Sum of electronic and zero-point Energies -380.549	Sum of electronic and zero-point Energies -228.402
P – $OCHCH_3$	^{2}TS – RC
0 1 C -0.23088 0.39836 0.00010 O -1.23171 -0.27633 -0.00007 H -0.30681 1.50295 -0.00002 C 1.16512 -0.14881 0.00000 H 1.70000 0.22262 -0.87575 H 1.69996 0.22231 0.87592 H 1.15509 -1.23453 -0.00017 Sum of electronic and zero-point Energies -153.711	-1 2 O 2.58690 -0.32931 0.48291 H 2.38865 -1.17732 0.90069 O 1.71361 -0.39886 -0.68094 O -2.45316 -0.43212 0.74911 O -2.60693 -0.19795 -0.56981 C 0.37929 -0.06591 -0.26294 H 0.05825 -0.72739 0.54250 H -0.23833 -0.31088 -1.12596 C 0.19636 1.38142 0.12547 H 0.46618 2.04097 -0.70065 H -0.85703 1.50922 0.36626 H 0.80509 1.63836 0.99185 <S^2>=0.77 Sum of electronic and zero-point Energies -380.320
^{2}RC – c	^{2}TS – 1c
-1 2 O 2.68784 -0.23126 0.26597 H 2.70849 -0.81300 1.03563 O 1.49064 -0.73787 -0.40152 O -2.56151 0.13132 0.62205 O -2.55123 -0.68544 -0.44943 C 0.35073 -0.03266 0.10988 H 0.31268 -0.15465 1.19502 H -0.51365 -0.56015 -0.31394 C 0.32565 1.42713 -0.28508 H 0.36581 1.52272 -1.37039 H -0.61781 1.84353 0.06248 H 1.16025 1.98069 0.14592 <S^2>=0.77 Sum of electronic and zero-point Energies -380.320	-1 2 O 2.84387 -0.26097 0.23272 H 2.92709 -1.10410 0.69316 O 1.26229 -0.73159 -0.37083 O -2.81669 0.00135 0.51689 O -2.20055 -0.65357 -0.45431 C 0.32209 0.03499 0.18402 H 0.22586 -0.09270 1.27259 H -0.71342 -0.43015 -0.22032 C 0.32394 1.49969 -0.21582 H 0.33030 1.59305 -1.30196 H -0.56956 1.98820 0.17200 H 1.21215 1.99584 0.17965 <S^2>=0.77 Sum of electronic and zero-point Energies -380.314
^{2}PC – 1c	^{2}TS – 2c
-1 2 C -0.85770 -0.33068 0.00015 O 0.11594 -1.09157 0.00010 O -3.55716 -0.04831 -0.00035 O 2.85581 0.73368 -0.00031 H 1.62064 -0.68850 0.00005 H -4.48159 -0.31044 0.00025 H -1.91536 -0.67836 0.00016 O 2.63635 -0.57145 0.00005 C -0.71417 1.15518 0.00028 H -1.26241 1.53615 0.86233 H 0.32504 1.47897 0.00023 H -1.26257 1.53637 -0.86157 <S^2>=0.76 Sum of electronic and zero-point Energies -380.394	-1 2 C 0.85801 -0.33012 0.00050 O -0.11574 -1.09082 0.00026 O 3.55717 -0.04914 -0.00047 O -2.85688 0.73305 -0.00083 H -1.62067 -0.68827 0.00006 H 4.48153 -0.31147 -0.00086 H 1.91578 -0.67771 0.00057 O -2.63642 -0.57188 -0.00001 C 0.71474 1.15583 0.00059 H 1.26395 1.53693 -0.86078 H -0.32440 1.47989 -0.00025 H 1.26225 1.53666 0.86318 <S^2>=0.76 Sum of electronic and zero-point Energies -380.394
^{2}PC – 2c	P – $CH_3CH(OH)_2$
-1 2 O -0.41689 -1.16603 0.28825 H 0.57487 -1.09790 0.18950 O -0.41754 1.16644 0.28847 O 2.18410 -0.67120 -0.07783 O 2.18358 0.67121 -0.07856 C -0.93977 0.00001 -0.28763	0 1 O 0.63578 1.17271 -0.18715 H 1.50719 1.30012 0.19489 O 0.63569 -1.17277 -0.18713 C 0.05194 -0.00001 0.34086 H 0.16376 0.00001 1.43090 H 1.50718 -1.30012 0.19475

H	-0.70239	0.00033	-1.36528
H	0.57407	1.09868	0.19033
C	-2.44204	-0.00043	-0.09107
H	-2.65645	-0.00010	0.97722
H	-2.88306	0.88813	-0.54158
H	-2.88221	-0.88992	-0.54066
$<S^2>$=0.77			
Sum of electronic and zero-point Energies -380.460			

C	-1.40071	0.00004	-0.06175
H	-1.46613	0.00014	-1.14785
H	-1.89553	-0.88762	0.32336
H	-1.89552	0.88764	0.32352
Sum of electronic and zero-point Energies -230.104			

^{2}TS – 3c			
-1 2			
O	-2.80363	1.32649	0.09017
H	-3.33367	2.07417	-0.19992
O	0.26470	-0.60790	-0.62368
O	3.16506	0.00236	0.53556
O	2.45170	0.70516	-0.33059
C	-0.65585	-0.48011	0.18918
H	-0.56424	0.25021	1.00217
H	1.56797	0.19906	-0.42987
C	-1.92919	-1.19586	0.12330
H	-1.93001	-1.97267	-0.63763
H	-2.21414	-1.57750	1.10406
H	-2.63820	-0.32630	-0.08533
$<S^2>$=0.76			
Sum of electronic and zero-point Energies -380.396			

^{2}PC – 3c			
-1 2			
O	-2.31007	1.75758	0.18712
H	-1.51947	1.23550	-0.08352
O	-0.18305	0.11552	-0.36721
O	2.79958	-0.11688	0.48121
O	2.18104	0.71229	-0.35202
C	-0.45867	-1.11794	-0.01985
H	0.39740	-1.71557	0.30816
H	1.10713	0.42336	-0.33413
C	-1.67787	-1.70743	-0.02183
H	-2.56279	-1.18176	-0.35460
H	-1.77340	-2.73524	0.29623
H	-2.72953	1.17779	0.82513
$<S^2>$=0.76			
Sum of electronic and zero-point Energies -380.448			

P – $[H_2O\cdots CH_2CHO]^-$			
0 -1			
C	-1.14682	-0.37875	0.09214
O	-0.10209	-1.09045	-0.10871
O	2.17331	0.28040	0.02262
H	1.34062	-0.26894	-0.07811
H	-2.04668	-0.92336	0.44954
C	-1.33025	0.97294	-0.06446
H	1.83500	1.07931	0.43060
H	-0.54302	1.61601	-0.43917
H	-2.29324	1.41227	0.15977
Sum of electronic and zero-point Energies -380.400			

P – CH_2CHO^-			
0 -1			
O	-1.22176	-0.22986	0.00002
C	-0.09767	0.35519	-0.00004
H	-0.10944	1.47560	0.00007
C	1.18041	-0.17039	0.00000
H	2.03461	0.49559	0.00005
H	1.35244	-1.24110	0.00001
Sum of electronic and zero-point Energies -153.132			

Table S3. The optimized geometry of all stationary points for the $(CH_3)COOH + O^{\bullet}{}_2^-$ gas-phase reaction, calculated with the UB2PLYPD3/6-311+G(3df,2p) and energies with the ROB2PLYP-D3//UB2PLYP-D3/6–311+G(3df,2p) method.

R – $(CH_3)_3COOH$			
0 1			
O	0.72523	0.08662	-0.88835
O	1.97248	-0.09028	-0.13184
H	2.40486	0.75095	-0.34426
C	-0.39108	-0.00094	0.03648
C	-1.58090	0.15035	-0.90925
H	-1.57726	-0.64269	-1.65861
H	-2.50967	0.08727	-0.33859
H	-1.55013	1.11538	-1.41830
C	-0.39096	-1.36602	0.71904
H	0.50107	-1.48759	1.33347
H	-1.27069	-1.46498	1.35943
H	-0.41091	-2.16083	-0.02873
C	-0.33521	1.14214	1.04677
H	-1.22348	1.12485	1.68244
H	0.54310	1.04956	1.68635
H	-0.29976	2.10410	0.53015
Sum of electronic and zero-point Energies -308.532			

^{2}TS – 1a			
-1 2			
O	0.48893	-0.36196	-0.94150
O	-1.00335	0.26806	-0.32816
H	-1.44068	-0.55119	-0.59935
O	-3.05669	0.51305	0.22767
O	-3.67612	-0.57208	-0.09148
C	1.46604	-0.04108	0.00422
C	2.80420	-0.54406	-0.56655
H	2.99965	-0.06232	-1.52807
H	3.63708	-0.32590	0.11477
H	2.75512	-1.62418	-0.72801
C	1.54226	1.48316	0.21477
H	0.57849	1.84725	0.57257
H	2.32262	1.75457	0.93666
H	1.75913	1.97104	-0.73982
C	1.19108	-0.73802	1.35047
H	0.21913	-0.41705	1.72720
H	1.16182	-1.82150	1.20010
H	1.96396	-0.50734	2.09421
$<S^2>$=1.08			

	Sum of electronic and zero-point Energies -458.845
^{2}Int – 1a	^{2}TS – 2a
-1 2	-1 2
O 0.62391 -0.55854 -0.91156	O -0.52317 -0.29809 -0.98773
O -1.16040 0.18457 -0.23054	O 1.33143 0.44678 -0.20976
H -1.44270 -0.63789 -0.65830	O 3.57573 -0.64556 -0.12411
O -3.12340 0.46754 0.25315	H 1.26488 -0.44219 -0.60951
O -3.86046 -0.50119 -0.14136	O 2.97667 0.45139 0.21215
C 1.54791 -0.03776 -0.00579	C -1.48824 -0.05184 -0.02042
C 1.27582 -0.54828 1.42140	C -2.83457 -0.59314 -0.55141
H 2.00380 -0.15537 2.14324	H -3.65307 -0.42334 0.16075
H 0.26877 -0.24685 1.71132	H -3.07873 -0.09899 -1.49561
H 1.32498 -1.64134 1.43254	H -2.74813 -1.66686 -0.73955
C 2.93302 -0.53339 -0.47219	C -1.62027 1.46334 0.23527
H 3.12918 -0.18257 -1.48874	H -2.38346 1.69397 0.99065
H 3.72752 -0.16544 0.18931	H -0.65389 1.84813 0.56596
H 2.95438 -1.62644 -0.47387	H -1.88547 1.96521 -0.69974
C 1.52262 1.50122 -0.02506	C -1.15204 -0.76440 1.30729
H 1.73762 1.85519 -1.03737	H -1.06257 -1.84023 1.12811
H 0.52297 1.83963 0.24885	H -0.19295 -0.39718 1.67687
H 2.25997 1.93123 0.66543	H -1.92120 -0.59842 2.07325
$<S^2>$=0.78	$<S^2>$=1.08
Sum of electronic and zero-point Energies -458.848	Sum of electronic and zero-point Energies -458.843
^{2}PC – 1a	^{4}Int – 1b
-1 2	-1 4
O -0.66137 1.25636 -0.00211	O 2.06553 0.82758 0.00040
O 2.10203 1.17552 -0.00039	O 3.08093 -1.24337 -0.00104
O 2.14020 -1.12205 0.00036	H 3.68655 -0.48882 -0.00250
H 0.31738 1.09812 -0.00153	O -3.20102 -1.02600 0.00198
O 2.85494 0.03782 -0.00011	O -3.62788 0.12600 -0.00256
C -1.34628 0.00640 -0.00002	C 0.73286 0.43669 0.00035
C -2.83418 0.35862 -0.00015	C -0.11044 1.73234 0.00136
H -3.45039 -0.54601 0.00140	H 0.12555 2.32787 -0.88522
H -3.07737 0.95258 0.88496	H -1.18506 1.51109 0.00136
H -3.07786 0.94988 -0.88693	H 0.12582 2.32665 0.88869
C -0.98075 -0.79110 1.25925	C 0.40700 -0.38776 -1.25905
H -1.53706 -1.73485 1.30111	H 1.08793 -1.24008 -1.27654
H 0.08892 -1.01073 1.25177	H -0.63735 -0.72838 -1.27296
H -1.22181 -0.20234 2.14913	H 0.59118 0.22050 -2.15058
C -0.98143 -0.79489 -1.25708	C 0.40748 -0.38937 1.25881
H -1.22301 -0.20882 -2.14859	H -0.63689 -0.72993 1.27273
H 0.08826 -1.01445 -1.24953	H 1.08835 -1.24176 1.27492
H -1.53770 -1.73880 -1.29581	H 0.59210 0.21772 2.15105
$<S^2>$=0.76	$<S^2>$=3.79
Sum of electronic and zero-point Energies -458.897	Sum of electronic and zero-point Energies -458.852
^{4}TS – 1b	^{4}Int – 2b
-1 4	-1 4
O 3.28992 -1.20924 -0.00472	O 2.03906 0.77216 -0.00084
H 3.24651 -0.30858 -0.39480	O 3.61726 -1.14265 -0.00217
O 2.04767 0.82213 0.05571	O -3.28785 -1.06152 0.00359
O -3.21731 -1.04031 0.05028	H 2.91743 -0.30330 -0.00160
O -3.63853 0.10693 -0.07718	O -3.71294 0.09047 -0.00465
C 0.71763 0.44081 0.01526	C 0.69891 0.44112 0.00054
C 0.39620 -0.34469 -1.27527	C 0.33167 -0.38838 -1.25600
H 1.03860 -1.22647 -1.31110	H -0.73225 -0.66095 -1.29042
H -0.65629 -0.65545 -1.32400	H 0.57609 0.19294 -2.15018
H 0.61721 0.28165 -2.14572	H 0.93049 -1.30282 -1.27168
C -0.14881 1.72223 0.05423	C -0.14764 1.73324 0.00113
H -1.22314 1.49647 0.02968	H -1.22833 1.53493 0.00291
H 0.07422 2.28353 0.96591	H 0.10467 2.32608 0.88520
H 0.09712 2.35368 -0.80443	H 0.10193 2.32527 -0.88426
C 0.37279 -0.43769 1.23595	C 0.33411 -0.38783 1.25817
H 1.02648 -1.31196 1.21713	H 0.93315 -1.30214 1.27320

H 0.57761 0.12270 2.15312 H -0.67919 -0.75561 1.24055 $<S^2>$=3.78 Sum of electronic and zero-point Energies -458.850	H 0.58005 0.19399 2.15162 H -0.72969 -0.66061 1.29469 $<S^2>$=3.77 Sum of electronic and zero-point Energies -458.864
^{4}TS – 2b	^{4}Int – 3b
-1 4 O -2.14497 0.87718 0.00556 O -2.68945 -1.64748 -0.12441 O 3.11725 -0.97549 0.29768 H -2.75587 -0.62418 -0.00279 O 3.50495 0.00414 -0.33368 C -0.81201 0.55878 0.03194 C -0.32512 0.30329 1.48431 H 0.74774 0.07017 1.54648 H -0.52907 1.19693 2.08131 H -0.89309 -0.52880 1.90813 C 0.03918 1.70655 -0.57306 H 1.11457 1.48112 -0.59880 H -0.30799 1.90681 -1.59044 H -0.11806 2.61061 0.02373 C -0.53634 -0.71782 -0.80368 H -1.47073 -1.47679 -0.49717 H -0.68164 -0.55491 -1.87435 H 0.39772 -1.25254 -0.59433 $<S^2>$=3.79 Sum of electronic and zero-point Energies -458.842	-1 4 O -1.95375 0.68916 -0.26706 O -3.44550 -1.39663 0.14684 O 3.57737 -1.20070 -0.19123 H -2.85208 -0.56696 0.04437 O 3.32568 -0.06930 0.21301 C -0.58649 0.57636 -0.04357 C -0.29580 -0.02399 1.34729 H 0.78060 -0.12449 1.53743 H -0.73571 0.62011 2.11586 H -0.76431 -1.00846 1.42450 C 0.08064 1.96158 -0.14700 H 1.16542 1.91352 0.01371 H -0.11329 2.37992 -1.13881 H -0.36429 2.63159 0.59594 C -0.07933 -0.33653 -1.13434 H -3.45189 -1.75975 -0.74475 H -0.08413 0.06325 -2.14677 H -0.32477 -1.39346 -1.04818 $<S^2>$=3.78 Sum of electronic and zero-point Energies -458.881
^{4}TS – 3b	^{4}PC – 1b
-1 4 O -2.22580 0.28313 -0.63125 O -3.68939 -1.93470 0.11264 O 4.79712 0.06809 -0.03102 H -3.22302 -1.09358 -0.10626 O 5.16716 -1.10258 -0.00289 C -1.04477 0.73727 0.05884 C -0.92559 0.26243 1.49099 H 0.09112 0.41648 1.85670 H -1.62169 0.81612 2.13054 H -1.15488 -0.80281 1.56479 C -0.75444 2.20970 -0.13434 H 0.25527 2.44689 0.20441 H -0.83072 2.47637 -1.19078 H -1.47116 2.80987 0.43724 C -0.68663 -0.19197 -1.00840 H -3.06417 -2.61837 -0.14829 H -0.38981 0.17137 -1.98289 H -0.51512 -1.23845 -0.78797 $<S^2>$=3.77 Sum of electronic and zero-point Energies -458.835	-1 4 O -2.20466 0.51374 -0.62806 O -4.17439 -1.42857 -0.01621 O 4.53387 -0.41925 -0.03362 H -3.54871 -0.71571 -0.25670 O 5.75272 -0.56209 -0.13215 C -0.95510 0.57516 0.13691 C -0.84969 -0.40292 1.27968 H 0.18961 -0.48327 1.60635 H -1.44940 -0.07116 2.13467 H -1.17031 -1.40617 0.98374 C -0.45289 1.97067 0.40792 H 0.60721 1.93953 0.66791 H -0.56827 2.60584 -0.47457 H -0.99535 2.41968 1.24714 C -0.94779 0.06395 -1.23459 H -3.62891 -2.04620 0.48469 H -0.58534 0.69166 -2.04368 H -0.87803 -1.00603 -1.40876 $<S^2>$=3.77 Sum of electronic and zero-point Energies -458.842
^{2}Int – 3b	^{2}TS – 3b
-1 2 O -1.36326 0.62009 -0.77010 O -3.07129 -1.13502 0.00643 O 2.78406 -0.91672 -0.26768 H -2.40177 -0.39628 -0.26806 O 1.69331 -0.97941 0.49610 C -0.19360 0.64314 -0.05541 C -0.43559 0.87488 1.45303 H 0.49191 0.85388 2.03867 H -0.91629 1.84906 1.58008 H -1.11716 0.11033 1.83501 C 0.76749 1.72287 -0.58965 H 1.73362 1.73190 -0.07222	-1 2 O -1.26203 0.29942 -0.87632 O -3.50017 -0.82529 0.16204 O 2.24950 -1.21027 -0.32788 H -2.68156 -0.44586 -0.25557 O 2.78004 -0.42051 0.62172 C -0.11640 0.55228 -0.05760 C -0.33059 0.34203 1.43023 H 0.63810 0.32722 1.93437 H -0.94922 1.15054 1.83699 H -0.83470 -0.61004 1.61001 C 0.58573 1.85830 -0.37421 H 1.57625 1.86031 0.08592

H 0.93835 1.55811 -1.65657 H 0.28767 2.69815 -0.46875 C 0.44329 -0.75944 -0.25768 H -3.28436 -1.56621 -0.82749 H 0.67773 -0.92320 -1.30794 H -0.24183 -1.51592 0.12758 $<S^2>$=0.76 Sum of electronic and zero-point Energies -458.945	H 0.69025 1.97036 -1.45531 H -0.00518 2.69981 0.00397 C 0.24899 -0.61228 -0.84683 H -3.48591 -0.46564 1.05472 H 0.63540 -0.48146 -1.84344 H -0.04843 -1.59407 -0.51768 $<S^2>$=0.76 Sum of electronic and zero-point Energies -458.915
^{2}PC – 1b	^{2}TS – 4b
-1 2 O -1.50993 0.90513 -0.11090 O -3.66936 -0.86618 -0.05463 O 2.67656 -0.31197 -0.94245 H -2.95261 -0.19705 -0.09172 O 3.08581 -0.82011 0.25433 C -0.14851 0.39186 0.21134 C -0.06826 -1.06853 0.56069 H 0.99236 -1.34633 0.53448 H -0.46559 -1.24023 1.56731 H -0.62945 -1.67581 -0.15378 C 0.67003 1.30500 1.08140 H 1.71139 0.98307 1.00416 H 0.56837 2.34320 0.75864 H 0.34233 1.22822 2.12316 C -0.48677 0.79397 -1.14548 H -3.22424 -1.65968 0.26064 H -0.13002 1.74540 -1.52760 H -0.67598 0.03041 -1.89382 $<S^2>$=0.76 Sum of electronic and zero-point Energies -458.923	-1 2 O 1.63293 0.90648 -0.53969 O 3.09250 -1.40027 0.06162 O -2.53350 -0.67934 0.77140 H 2.67878 -0.52848 -0.11626 O -2.07822 -0.84688 -0.59547 C 0.52020 1.02916 0.00807 C -0.57234 1.84409 -0.64199 H -1.55426 1.43673 -0.39837 H -0.50935 2.86733 -0.24725 H -0.42002 1.87609 -1.72045 C 0.29441 0.66404 1.45509 H -0.70527 0.23149 1.58034 H 1.07065 -0.01987 1.79912 H 0.35632 1.58886 2.04614 C -0.79213 -1.21156 -0.65573 H 2.35968 -2.01930 -0.02681 H -0.41753 -1.79915 0.18040 H -0.46951 -1.42809 -1.67233 $<S^2>$=0.76 Sum of electronic and zero-point Energies -458.922
^{2}Int – 4b	^{2}TS – 5b
-1 2 O 1.84098 0.66568 -0.86735 O -1.51009 -1.10508 1.07229 O -1.51870 0.00698 0.11677 C 1.50381 -0.31107 -0.19080 C 1.44861 -0.27017 1.31069 H 2.06373 -1.07457 1.72820 H 1.78676 0.69608 1.68318 H 0.40212 -0.47975 1.59356 C 1.07207 -1.60842 -0.82211 H 0.06469 -1.83045 -0.44637 H 1.08217 -1.52449 -1.90791 H 1.73384 -2.41970 -0.49984 C -2.33398 -0.24100 -0.92870 H -3.12716 -0.95853 -0.74781 H -2.49715 0.64248 -1.54056 O -0.24079 2.61539 0.15955 H 0.56354 2.24660 -0.23413 H -0.78680 1.82259 0.30706 $<S^2>$=0.76 Sum of electronic and zero-point Energies -458.929	-1 2 O -1.78966 0.81138 -0.49289 O 2.61285 -0.83696 0.88940 O 2.11992 -1.07573 -0.38850 C -0.79010 0.88494 0.26792 C -0.70508 0.00111 1.49993 H -0.87395 0.61189 2.39383 H -1.47174 -0.77301 1.46117 H 0.29090 -0.44360 1.57895 C 0.35567 1.71207 -0.03299 H 1.19670 0.92836 -0.68953 H 0.14477 2.52716 -0.72434 H 0.96030 1.99776 0.82635 C 2.22878 0.01587 -1.21388 H 3.16316 0.56332 -1.06741 H 2.01343 -0.29882 -2.23729 O -3.66609 -1.20471 -0.44003 H -3.05064 -0.43426 -0.41181 H -3.12461 -1.91468 -0.79966 $<S^2>$=0.76 Sum of electronic and zero-point Energies -458.914
^{2}PC – 2b	p – $[CH_3CO(CH_2)\cdots H_2O]^-$
-1 2 O 1.17070 0.56200 -1.24100 O -1.01280 -1.29740 0.88381 O -1.63477 -0.03402 0.61945 C 1.36955 -0.37000 -0.39363 C 2.19286 -0.03698 0.84313 H 2.32997 -0.90056 1.49691 H 3.16922 0.34934 0.53520 H 1.68510 0.75268 1.40228	-1 1 O -0.18138 -0.87883 -0.43444 O -2.66003 -0.15068 0.22743 H -1.77023 -0.48507 -0.09627 C 0.66864 0.04844 -0.12789 C 0.45392 1.41297 -0.14350 H 1.23884 2.10668 0.13570 H -0.48910 1.82235 -0.48956 H -2.40584 0.64633 0.70561

C 0.81199 -1.65199 -0.50175 H -1.52681 -0.26731 -1.43272 H 0.24716 -1.91769 -1.38500 H 1.04322 -2.42800 0.21416 C -2.27150 -0.12513 -0.64509 H -2.98836 -0.95364 -0.64655 H -2.78772 0.82809 -0.79285 O -0.20591 2.50028 0.29920 H 0.38238 2.05196 -0.34121 H -0.70931 1.74281 0.64217 <S²>=0.77 Sum of electronic and zero-point Energies -458.935	C 2.04570 -0.46325 0.30219 H 2.74263 0.34376 0.54900 H 1.93386 -1.11883 1.17169 H 2.47162 -1.06802 -0.50484 Sum of electronic and zero-point Energies -268.812
P _ $[CH_3CO(CH_2)]^-$	P _ $CH_3O_2^\bullet$
-1 1 O -0.18272 1.39052 0.00009 C -0.13151 0.10950 0.00009 C -1.19589 -0.78331 -0.00050 H -1.03449 -1.85625 0.00185 H -2.21744 -0.41630 0.00046 C 1.28745 -0.49242 -0.00002 H 1.29324 -1.58805 0.00069 H 1.82961 -0.13376 -0.88154 H 1.83060 -0.13250 0.88039 Sum of electronic and zero-point Energies -192.398	0 2 C 1.09682 -0.18766 -0.00000 H 1.14092 -0.80148 0.89765 H 1.87516 0.57241 -0.00052 H 1.14044 -0.80228 -0.89712 O -0.15347 0.55005 0.00000 O -1.18871 -0.28039 0.00000 <S²>=0.76 Sum of electronic and zero-point Energies -190.107
P _ $cyc-CH_2C(CH_3)_2O$	P _ $(CH_3)_3COH$
0 1 O -1.00601 0.00011 0.83645 C 0.13276 0.00002 -0.05834 C 0.93169 -1.28116 -0.04877 H 1.56340 -1.34737 -0.93857 H 1.57887 -1.31489 0.83135 H 0.26908 -2.14677 -0.02204 C 0.93227 1.28080 -0.04872 H 1.56303 1.34734 -0.93917 H 0.27003 2.14665 -0.02064 H 1.58044 1.31364 0.83070 C -1.23796 0.00028 -0.58900 H -1.66452 0.91916 -0.98202 H -1.66478 -0.91837 -0.98226 Sum of electronic and zero-point Energies -232.200	0 1 O -0.02767 -0.00001 1.44971 H -0.94605 0.00002 1.73324 C 0.00547 0.00000 0.01259 C 1.48448 -0.00006 -0.34485 H 1.61849 -0.00006 -1.42562 H 1.97039 0.88255 0.06739 H 1.97031 -0.88272 0.06737 C -0.68213 1.25715 -0.51465 H -0.63486 1.30257 -1.60262 H -1.73442 1.27040 -0.22533 H -0.20316 2.14576 -0.10734 C -0.68224 -1.25708 -0.51466 H -0.20334 -2.14574 -0.10736 H -1.73453 -1.27024 -0.22535 H -0.63497 -1.30250 -1.60264 Sum of electronic and zero-point Energies -233.422