

Supporting Information:

Study of Low Temperature Chlorine Atom Initiated Oxidation of Methyl and Ethyl Butyrate Using Synchrotron Photoionization TOF-Mass Spectrometry

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Complete Reference List

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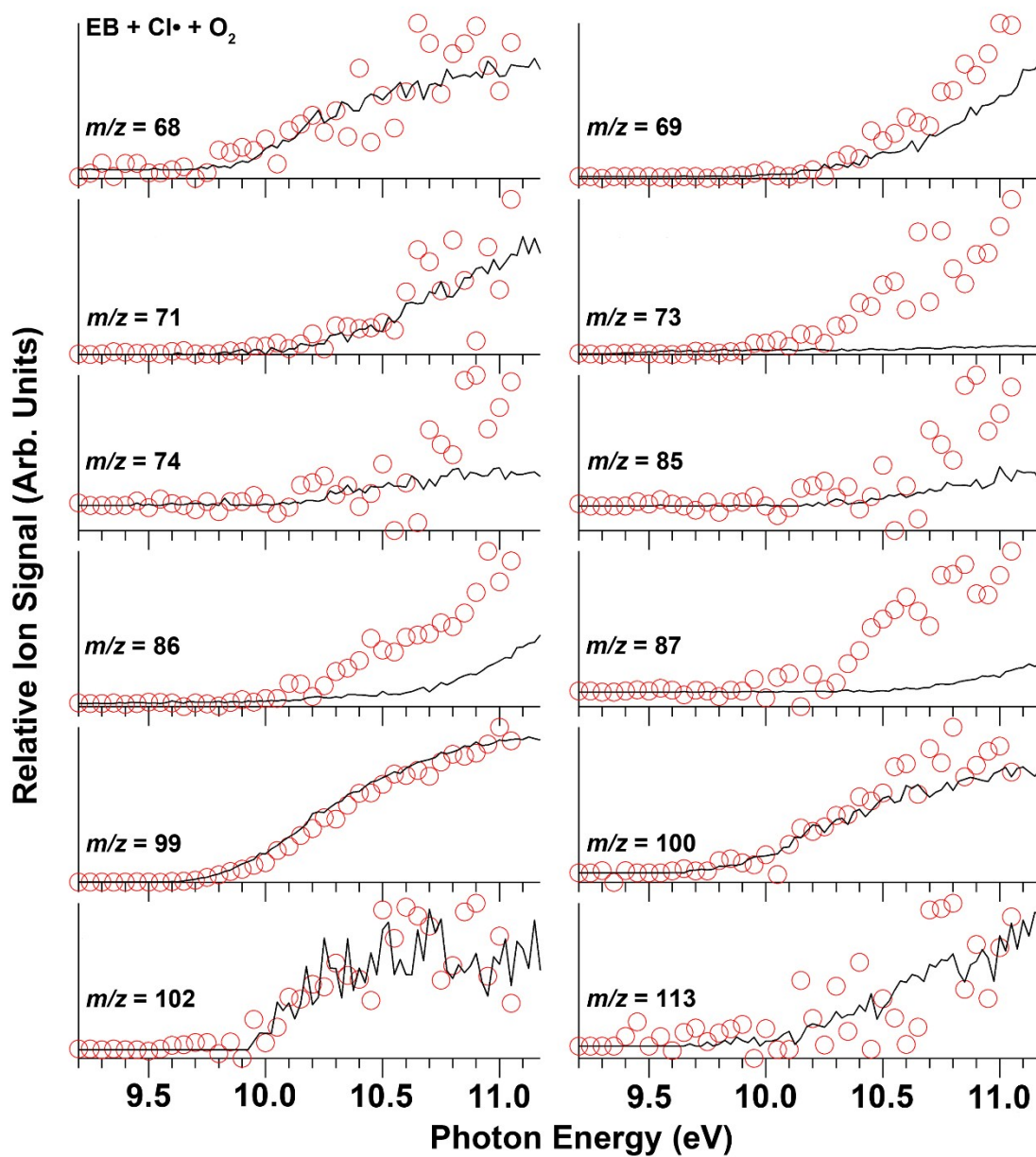


Figure S1. PI spectra of all dissociative fragments of ethyl crotonate. The red circles show the experimental data from the EB + Cl• + O₂ reaction and the black lines show the measured ion signal for ethyl crotonate.

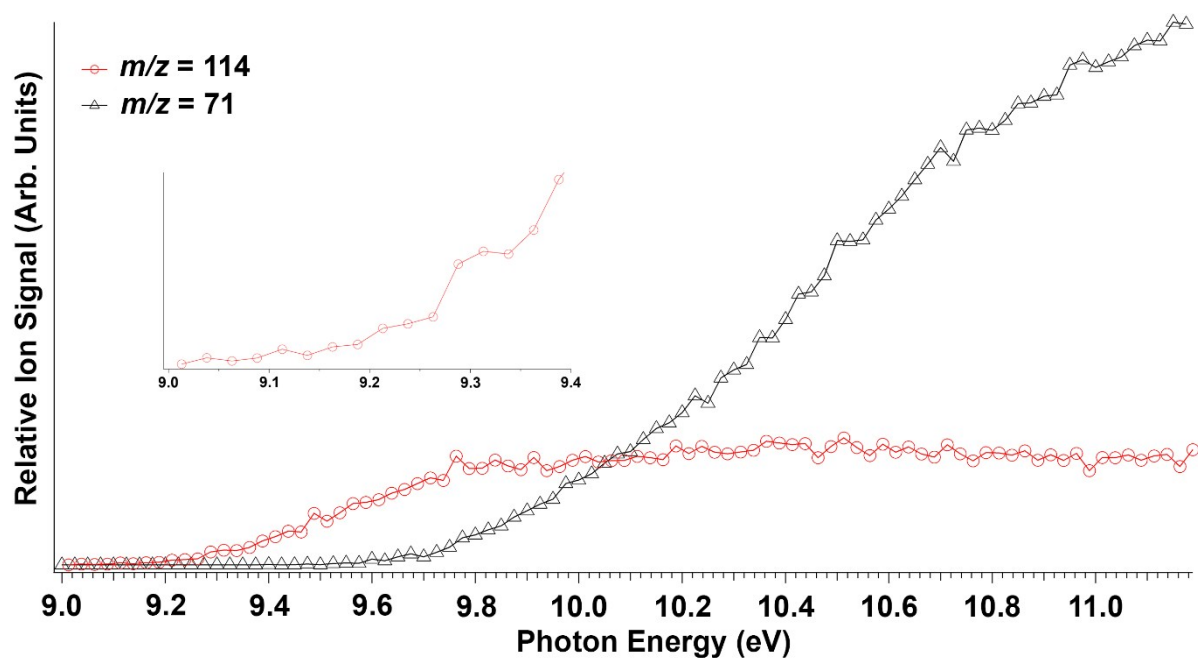


Figure S2. Measured PI spectra of vinyl butyrate ($m/z = 114$) and the only dissociative fragment ($m/z = 71$).

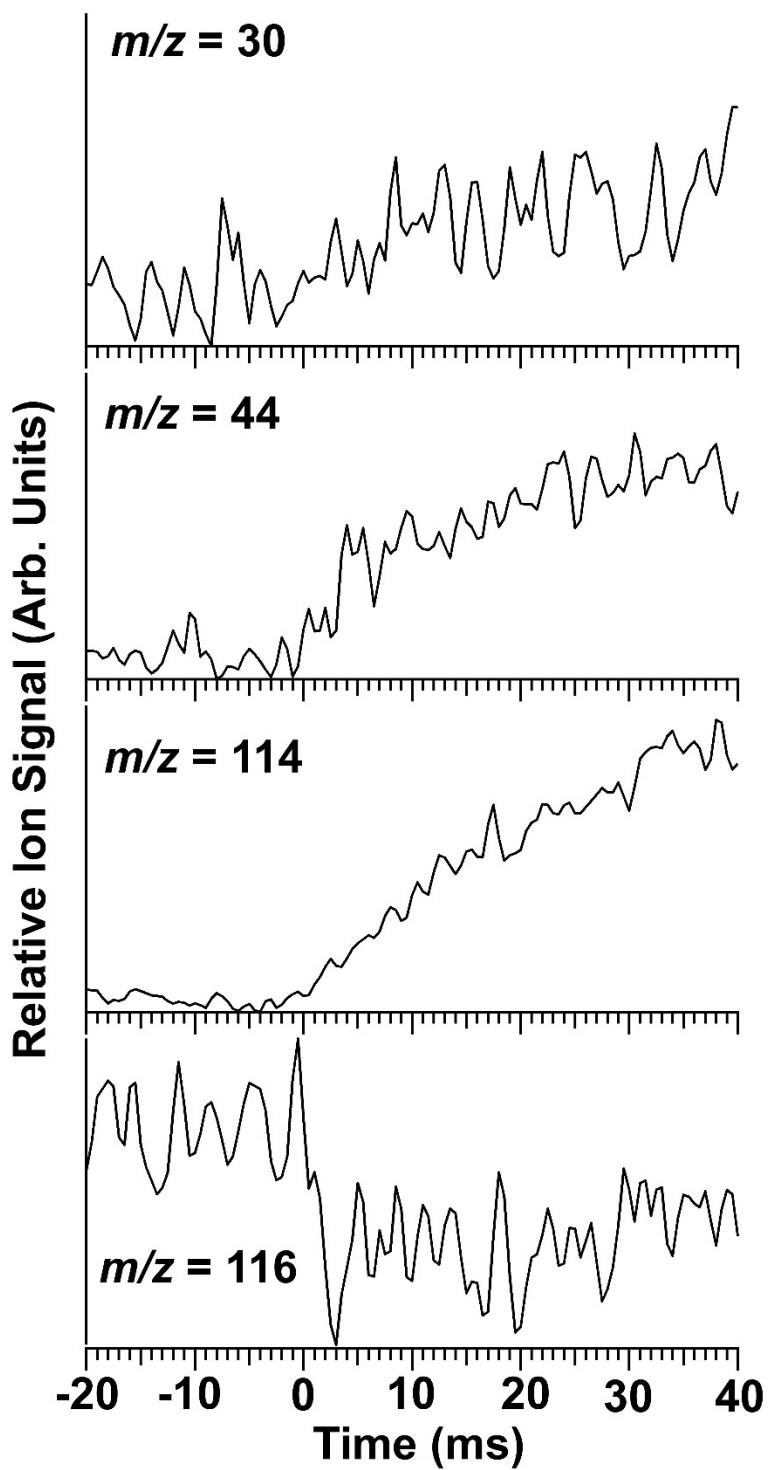


Figure S3. Time traces for the three identified products from the EB $\text{EB} + \text{Cl}\cdot + \text{O}_2$ reaction in comparison with the depletion of EB.

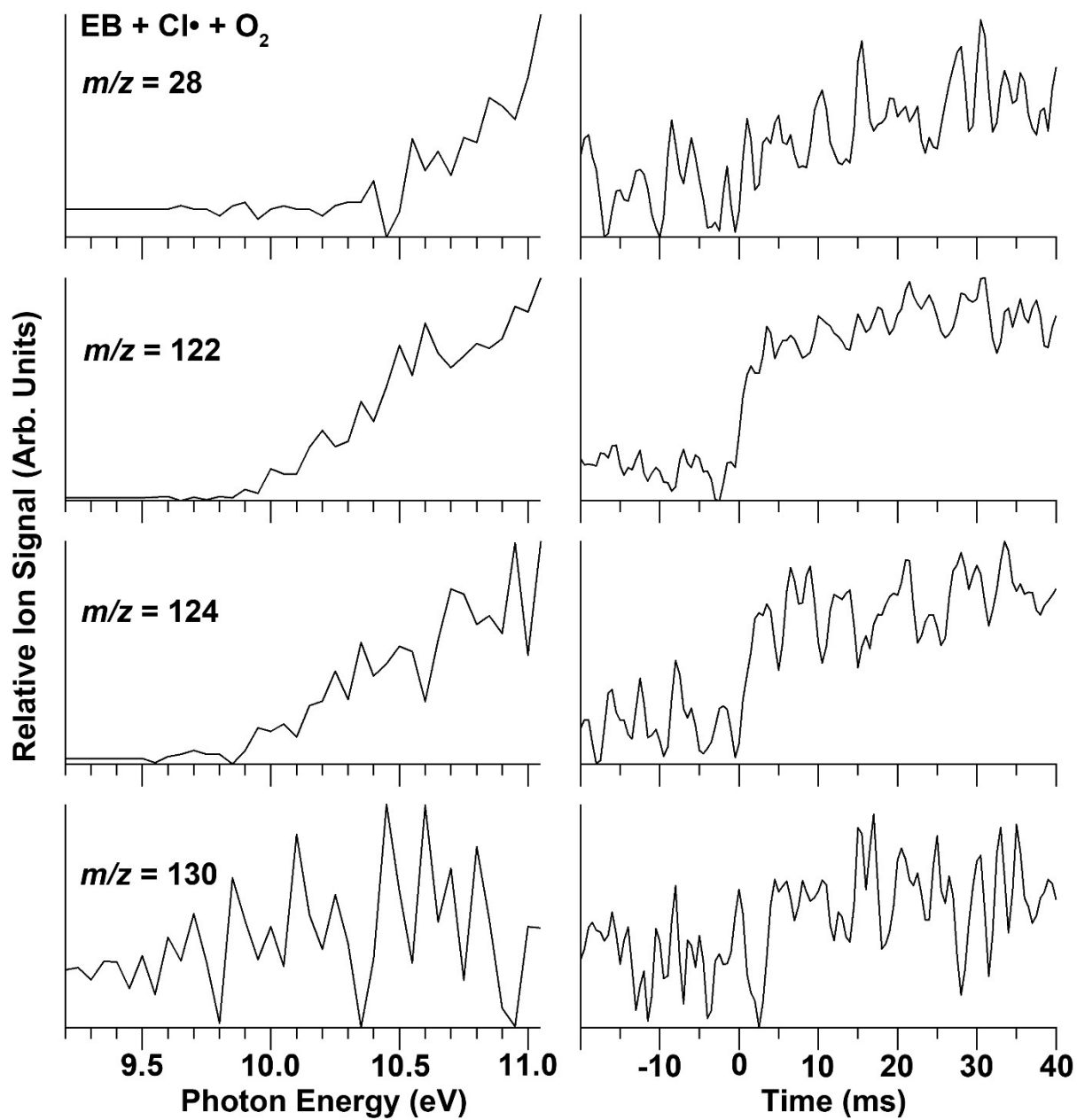


Figure S4. PI spectra (left) and time traces (right) of some other species observed in the mass spectrum of the $\text{EB} + \text{Cl}\cdot + \text{O}_2$ reaction. The excimer laser is fired at 0 ms.

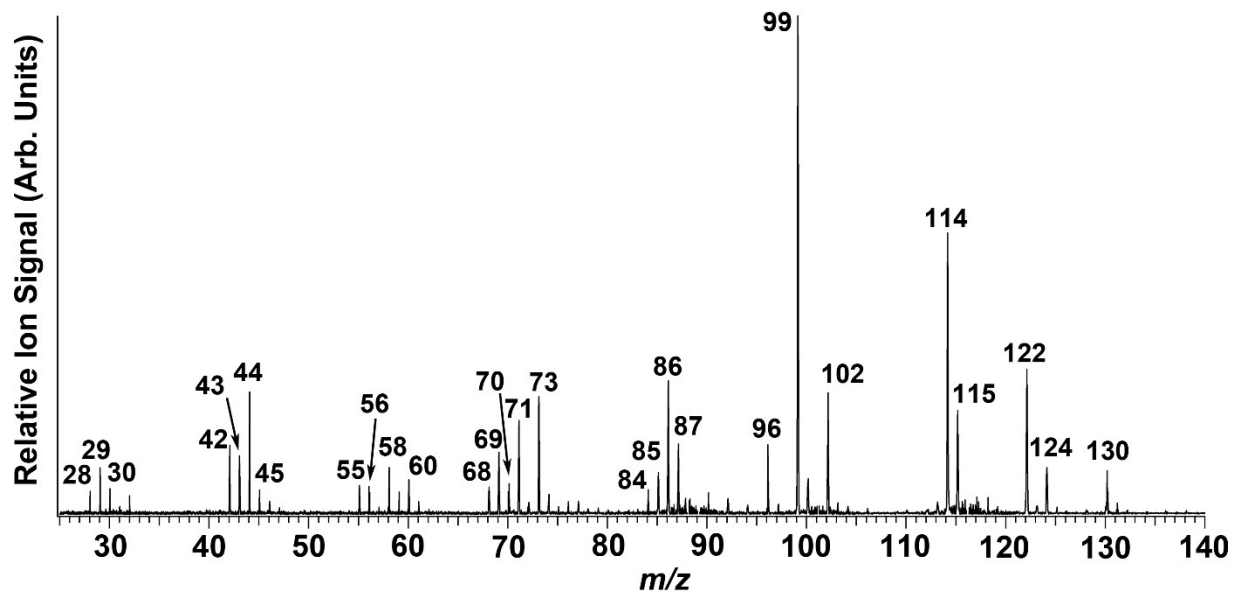


Figure S5. Mass spectrum of the $\text{EB} + \text{Cl}^\bullet + \text{O}_2$ reaction from 0 to 40 ms with 11.00 eV photon energy. Depletion of the starting material ($m/z = 116$) and dissociative fragments of EB are not shown for clarity.

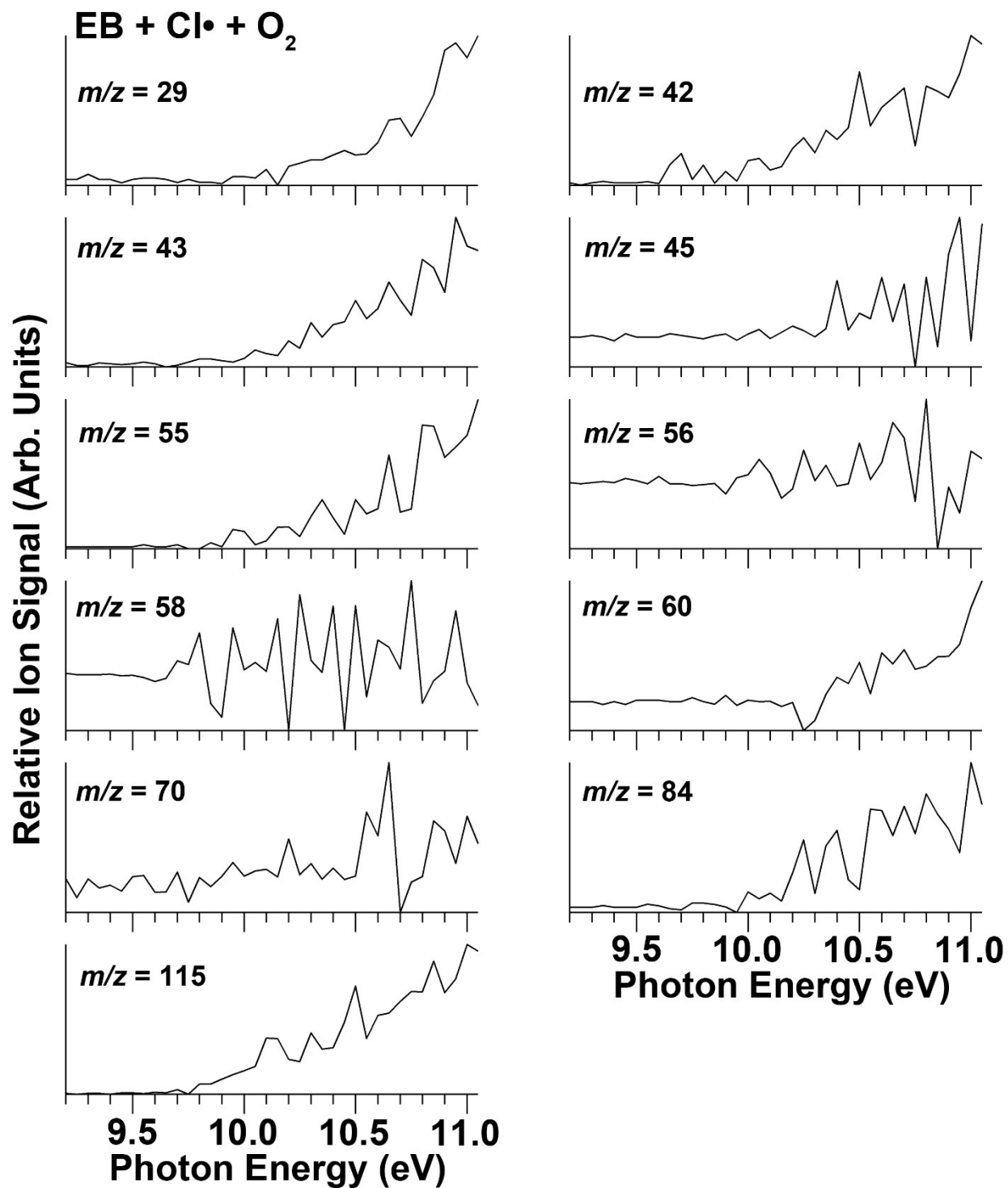


Figure S6. PI spectra of the remaining unidentified masses from the EB + Cl• + O₂ reaction products.

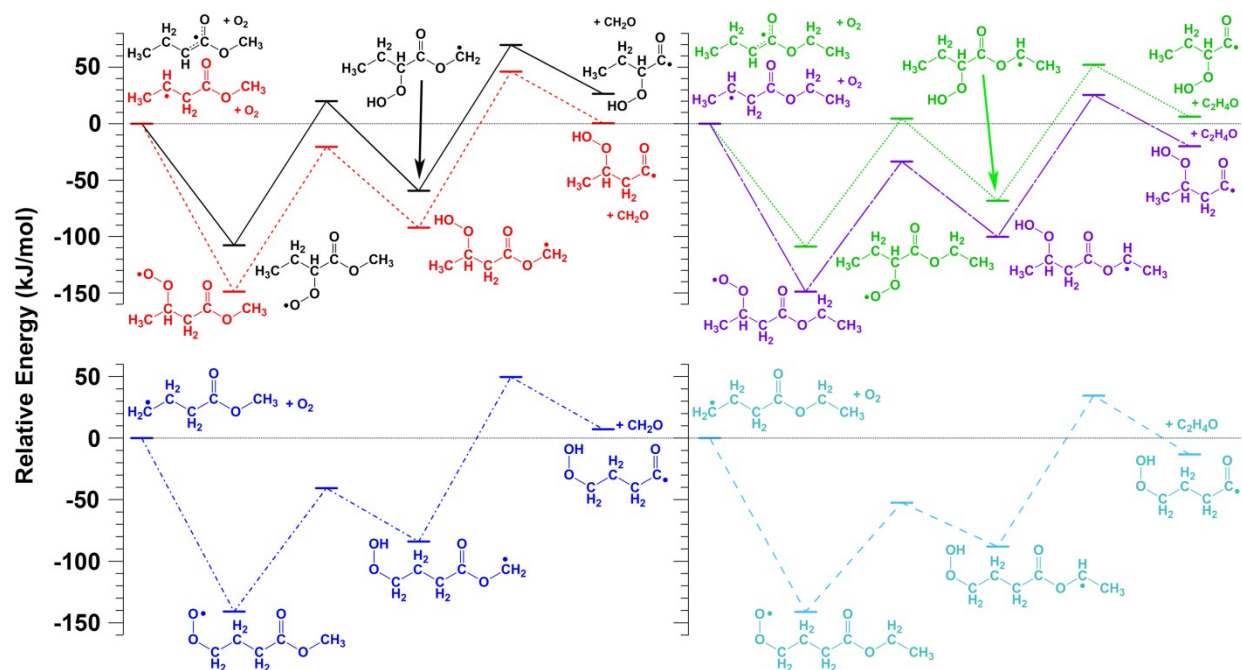


Figure S7. PES of the reaction of $R_{\beta, \gamma, \text{ or } \delta}$ with O_2 , where the peroxy radical abstracts a hydrogen atom from C_m . The QOOH radicals then decompose into a smaller radical and formaldehyde or acetaldehyde. The left side is methyl butyrate and the right side is ethyl butyrate. Relative energies are at 0 K calculated with the CBS-QB3 method.

Table S1. Calculated 0 K CBS-QB3 energies for some of the small molecules in this study.

Species	Energy (Hartrees)
O ₂	-150.164609
OH	-75.649720
HO ₂	-150.741100
H atom	-0.499818
Formaldehyde	-114.344176
Acetaldehyde	-153.582464
CH ₃ O	-114.874478
C ₂ H ₅ O	-154.105069
CHO	-113.704759
C ₂ H ₃ O	-152.942045

Table S2. Optimized CBS-QB3 geometries for the small molecules in this study.

Species	Optimized coordinates (Å)			
O ₂	O	0.00000000	0.00000000	0.60278600
	O	0.00000000	0.00000000	-0.60278600
OH	O	0.00000000	0.00000000	0.10835700
	H	0.00000000	0.00000000	-0.86685200
HO ₂	O	0.71994300	0.02713000	-0.00000700
	O	-0.59913000	-0.12454300	-0.00001400
	H	-0.96649900	0.77930100	0.00016700
H atom	H	0.00000000	0.00000000	0.00000000
Formaldehyde	O	-0.00000700	-0.67401700	0.00000000
	C	-0.00000700	0.52595700	0.00000000
	H	0.93887500	1.11809600	0.00000000
	H	-0.93877600	1.11829300	0.00000000
Acetaldehyde	C	0.23559100	0.39720900	-0.00003000
	H	0.30497000	1.50868900	0.00002400
	O	1.23312200	-0.27656100	0.00000900
	C	-1.16878600	-0.14782700	0.00000300
	H	-1.70767900	0.22247500	-0.87893600
	H	-1.15549600	-1.23750400	0.00000300
	H	-1.70760100	0.22253200	0.87899400
CH ₃ O	C	0.57338800	-0.00010900	0.01408000
	H	0.87104400	0.00376300	-1.05483900
	H	1.01175900	-0.91071300	0.45144100
	H	1.01146200	0.90788600	0.45723100

	O	-0.79182400	-0.00003600	0.00771100
C ₂ H ₅ O	C	0.00000000	0.51176300	0.00000000
	H	0.12791600	1.19273700	0.86581700
	H	0.12791600	1.19273700	-0.86581700
	O	-1.30325300	0.10191600	0.00000000
	C	1.04329200	-0.60217900	0.00000000
	H	0.92621200	-1.23288300	-0.88450700
	H	2.05801800	-0.19254500	0.00000000
	H	0.92621200	-1.23288300	0.88450700
CHO	C	0.06231000	0.58418900	0.00000000
	H	-0.87234400	1.21502000	0.00000000
	O	0.06231000	-0.59001900	0.00000000
C ₂ H ₃ O	C	0.24854600	0.43388500	-0.00005000
	O	1.25929800	-0.17518700	0.00002000
	C	-1.16853700	-0.09820800	0.00003800
	H	-1.68695100	0.29021500	0.87945400
	H	-1.68695100	0.29003200	-0.87951300
	H	-1.18053600	-1.19280900	-0.00003100

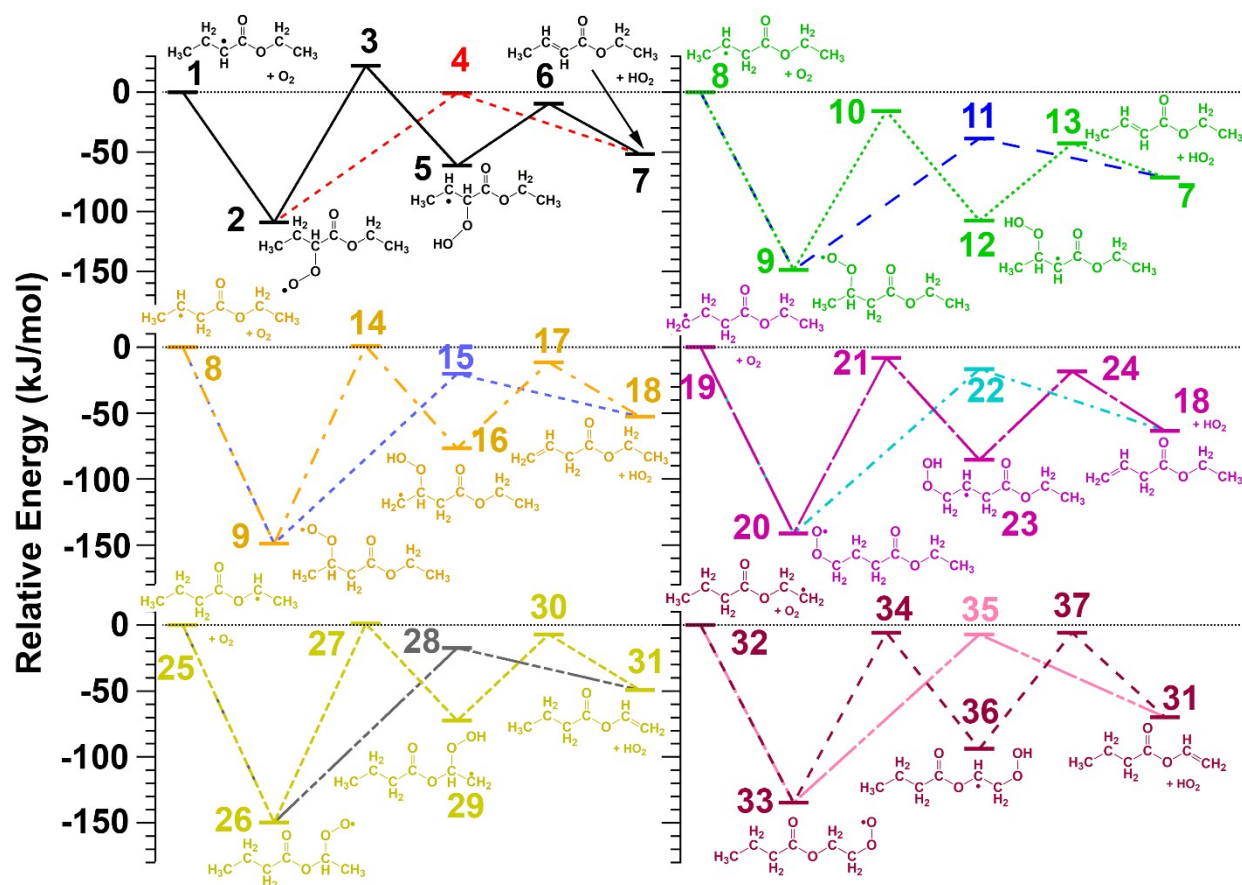


Figure S8. PES of the HO₂ elimination reactions for EB. The numbers correspond with the energies and geometries listed in the supporting information.

Table S3. Calculated 0 K CBS-QB3 energies for the structures in Figure 7.

Species	Energy (Hartrees)
1	-385.011155
2	-535.217274
3	-535.167373
4	-535.176130
5	-535.199146
6	-535.179390
7	-384.454352
8	-385.003688
9	-535.224957
10	-535.174267
11	-535.182993
12	-535.209261

13	-535.184575
14	-535.167964
15	-535.176078
16	-535.197501
17	-535.172723
18	-384.447235
19	-384.999549
20	-535.217938
21	-535.167238
22	-535.170537
23	-535.196734
24	-535.171214
25	-385.005188
26	-535.226769
27	-535.169433
28	-535.176398
29	-535.197371
30	-535.172477
31	-384.447495
32	-384.997378
33	-535.213254
34	-535.164145
35	-535.164663
36	-535.197756
37	-535.172213

Table S4. Optimized geometries for the structures in Figure S7.

Species	Optimized coordinates (Å)			
1	C	-3.51679900	-0.56591700	0.52143900
	H	-3.19794300	-0.47373800	1.56237100
	H	-3.60655700	-1.63068100	0.28872800
	H	-4.50870700	-0.11656100	0.42969000
	C	-2.52027400	0.13399700	-0.42393600
	H	-2.90816800	0.05950000	-1.45119600
	H	-2.44915200	1.19775800	-0.18826900
	C	-1.15940000	-0.45838000	-0.38177000
	H	-1.01468300	-1.51792600	-0.56320700
	C	0.01377400	0.34379000	-0.09915200
	O	0.00763900	1.53997800	0.13359400
	O	1.15026500	-0.40368500	-0.12183700
	C	2.37743200	0.30577100	0.15051500
	H	2.49436700	1.10678800	-0.58429900
	H	2.30511300	0.77380900	1.13589300
	C	3.50953500	-0.69900000	0.08045900
	H	4.46223000	-0.20215800	0.28187900

	H	3.37197500	-1.49200100	0.81889600
	H	3.56267800	-1.15669400	-0.90986200
2	C	3.46825400	-0.31295900	0.52988100
	H	3.54029600	0.74216900	0.80106600
	H	3.87906100	-0.43295200	-0.47681300
	H	4.09791800	-0.88184400	1.21765600
	C	2.02108600	-0.80512200	0.59632600
	H	1.95586400	-1.85761700	0.31056200
	H	1.63560000	-0.72587800	1.61831400
	C	1.08206200	-0.03406800	-0.33024300
	H	1.47531600	0.01526800	-1.34814500
	C	-0.29569600	-0.69462400	-0.40698300
	O	-0.43664000	-1.79108800	-0.88815000
	O	-1.26843500	0.05020900	0.11652300
	C	-2.60873300	-0.51193200	0.06566900
	H	-2.85263700	-0.72434300	-0.97723400
	H	-2.60622700	-1.45911100	0.60945200
	O	1.01266100	1.33361800	0.16294300
	O	0.63116500	2.17860000	-0.77541100
	C	-3.54605500	0.50502200	0.68078500
	H	-3.51552700	1.44543400	0.12711200
	H	-4.57002800	0.12318500	0.65910200
	H	-3.27514600	0.70706900	1.71906800
3	C	3.48674700	-0.37036500	-0.46368500
	H	3.58882200	0.63016000	-0.89083800
	H	3.59689200	-1.09625300	-1.28211100
	H	4.31051900	-0.54263400	0.23257200
	C	2.15460300	-0.54321300	0.20866800
	H	1.99972100	-1.47251700	0.75059800
	H	1.96383100	0.48421800	1.06680100
	C	0.92299500	-0.01900900	-0.53793000
	H	0.96805100	-0.17166800	-1.62316400
	C	-0.37216100	-0.66417900	-0.01853200
	O	-0.41504700	-1.74312400	0.51974900
	O	-1.43297600	0.09655300	-0.29153100
	C	-2.72103100	-0.41324400	0.14454500
	H	-2.88542100	-1.38730000	-0.32199900
	H	-2.68405700	-0.56177900	1.22583300
	O	0.96797300	1.39456000	-0.34356900
	O	1.25885900	1.50062300	1.04971300
	C	-3.76796800	0.60306100	-0.25906700
	H	-4.75664700	0.26142100	0.05823100
	H	-3.56946800	1.56981800	0.20766300
	H	-3.78182300	0.73934100	-1.34248300

4	C	3.19955900	-1.25844700	-0.66110500
	H	3.21230700	-0.80691800	-1.65624900
	H	3.13886000	-2.34370400	-0.78470000
	H	4.15418900	-1.03562100	-0.17934300
	C	2.03041900	-0.74387700	0.16600100
	H	1.96976300	-1.10063300	1.19492900
	H	2.31725400	0.51034200	0.39704100
	C	0.79846900	-0.46899600	-0.42081900
	H	0.67454800	-0.39817500	-1.49407200
	C	-0.43816300	-0.41629800	0.39431800
	O	-0.47875400	-0.53392100	1.59735100
	O	-1.51914300	-0.22335100	-0.38616900
	C	-2.79093400	-0.12166700	0.29957400
	H	-2.94719400	-1.03130100	0.88428500
	H	-2.74266600	0.71775400	0.99715900
	O	1.00539800	1.78881500	-0.30372600
	O	2.11666900	1.81129900	0.28725100
	C	-3.86047700	0.07259800	-0.75508300
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	H	-4.84049800	0.15655200	-0.27835100
	H	-3.67818400	0.98262600	-1.33045800
5	C	-3.62532800	-0.23449900	-0.23468600
	H	-3.63612400	0.84892300	-0.37693700
	H	-4.10011300	-0.43604700	0.73994400
	H	-4.25916800	-0.69478300	-0.99620500
	C	-2.24026800	-0.77332700	-0.28319100
	H	-2.04658300	-1.78801400	-0.60410500
	C	-1.10461600	-0.00076300	0.29003300
	H	-1.27271400	0.22327200	1.35752500
	C	0.21170000	-0.78742700	0.21254400
	O	0.29532900	-1.97787400	0.36463700
	O	1.27112900	0.01748500	-0.01426200
	C	2.56940400	-0.63380400	-0.08856800
	H	2.73332500	-1.18425200	0.83989100
	H	2.54374500	-1.35576300	-0.90710200
	O	-1.04154800	1.25971100	-0.39347400
	O	-0.35970900	2.21837300	0.45419600
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6	C	-3.61083400	-0.30141900	0.59574500

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	H	-4.19114500	-1.13767300	1.00192500
	C	-2.30124800	-0.76462300	0.06466400
	H	-2.28733600	-1.58136900	-0.65009400
	C	-1.09331700	-0.12131100	0.32594900
	H	-1.01939300	0.51503400	1.20028600
	C	0.17543000	-0.79049800	-0.10087500
	O	0.25591200	-1.80695600	-0.74220200
	O	1.25468900	-0.07609100	0.31135600
	C	2.54999900	-0.61097900	-0.06769000
	H	2.62661900	-1.63117900	0.31389200
	H	2.60230500	-0.65816800	-1.15764300
	O	-0.97175900	1.29308300	-0.84461700
	O	-0.32129700	2.34397700	-0.18778000
	H	0.60358500	2.04535500	-0.18068500
	C	3.61032200	0.29756200	0.51899900
	H	3.52096400	0.35007600	1.60610800
	H	4.60324300	-0.08785900	0.27391400
	H	3.53210800	1.31017700	0.11577000
7	C	-3.74013900	-0.58056700	0.00000000
	H	-3.60702200	-1.66410900	-0.00000300
	H	-4.33571600	-0.30374500	-0.87699500
	H	-4.33571300	-0.30374900	0.87699800
	C	-2.43492500	0.14580500	0.00000000
	H	-2.46745100	1.23315100	0.00000000
	C	-1.23027400	-0.42837400	0.00000000
	H	-1.10364900	-1.50541400	0.00000000
	C	0.00152200	0.39162200	0.00000100
	O	0.05189000	1.60038800	0.00000000
	O	1.10005100	-0.39952500	0.00000000
	C	2.37430500	0.28253300	0.00000000
	H	2.42866500	0.92648700	-0.88126000
	H	2.42866600	0.92648600	0.88126100
	C	3.45784000	-0.77639300	-0.00000100
	H	3.38216200	-1.41113700	-0.88560400
	H	4.44239700	-0.30148800	-0.00000100
	H	3.38216300	-1.41113800	0.88560200
8	C	3.78259100	-0.49177400	-0.00012800
	H	3.89210800	-1.14836300	-0.87701400
	H	3.89294600	-1.14673100	0.87789300
	H	4.62545800	0.20174000	-0.00114300
	C	2.47847500	0.22544800	-0.00018600
	H	2.43088700	1.30596500	-0.00013900

	C	1.19746500	-0.53050000	0.00035600
	H	1.11758400	-1.20590200	0.86755500
	H	1.11738800	-1.20683500	-0.86607700
	C	-0.03746400	0.35162900	0.00009200
	O	-0.04595100	1.55640300	-0.00002700
	O	-1.15711100	-0.40306400	0.00005300
	C	-2.41420200	0.31654300	-0.00010300
	H	-2.44964800	0.96080400	0.88162800
	H	-2.44949700	0.96068600	-0.88192600
	C	-3.52651800	-0.71171600	-0.00012700
	H	-4.49738900	-0.20934000	-0.00024000
	H	-3.46864300	-1.34831500	-0.88575900
	H	-3.46878800	-1.34820000	0.88559600
9	C	3.06835400	-1.19912500	-0.20168900
	H	3.02190900	-1.50414600	-1.25040000
	H	3.11376600	-2.09569300	0.42167400
	H	3.97950200	-0.62155300	-0.04195700
	C	0.52059000	-0.99646200	-0.15527300
	H	0.50865000	-2.02098800	0.23145200
	H	0.37833300	-1.05677000	-1.23583700
	C	-0.64522000	-0.26134900	0.48379200
	O	-0.60187300	0.29050500	1.55445900
	O	-1.74479500	-0.33521300	-0.28502900
	C	-2.93959000	0.30060400	0.24070000
	H	-3.18368000	-0.15796300	1.20165900
	H	-2.71918900	1.35488800	0.42056200
	C	1.86088200	-0.36029300	0.17776100
	H	1.88900700	-0.05820700	1.22523000
	O	1.87555300	0.89721200	-0.59919400
	O	2.85043500	1.69716000	-0.22596200
	C	-4.04071000	0.11088000	-0.78134700
	H	-4.23634900	-0.94999700	-0.95193100
	H	-4.96216500	0.57756300	-0.42380800
	H	-3.77018800	0.57001700	-1.73450300
10	C	-2.57647600	1.59275000	-0.61239200
	H	-2.66942400	1.40431000	-1.68405900
	H	-1.93737400	2.46540100	-0.46024500
	H	-3.56540400	1.82126000	-0.20833300
	C	-0.63826900	-0.11039000	-0.43198500
	H	-0.52279800	-0.15676800	-1.51301900
	H	-1.08844300	-1.38640300	-0.04144800
	C	0.58465400	0.22847500	0.31938900
	O	0.60483700	0.71655700	1.42978000
	O	1.69470000	-0.09954600	-0.37623200

	C	2.95910300	0.13514300	0.29135000
	H	3.03421700	1.19795400	0.53367900
	H	2.96624100	-0.41998000	1.23247600
	C	-1.98179200	0.39211000	0.09775600
	H	-1.88300400	0.56157300	1.17271300
	O	-2.88167900	-0.73481100	-0.12497000
	O	-2.14158400	-1.84811700	0.26012100
	C	4.05852300	-0.31662800	-0.64715900
	H	4.02841700	0.24636400	-1.58251500
	H	5.03366900	-0.15629700	-0.18015100
	H	3.95924900	-1.37884700	-0.88045000
11	C	2.90377200	-1.55808600	-0.38168900
	H	2.93033300	-1.42385800	-1.46500500
	H	2.73327100	-2.62283800	-0.17799200
	H	3.87978700	-1.29893900	0.03321900
	C	0.64078500	-0.38264000	-0.41231400
	H	0.46770900	-0.75139700	-1.42034100
	H	1.05985300	0.90674600	-0.65058700
	C	-0.58270300	-0.15299900	0.40923200
	O	-0.60017400	0.04435400	1.60102900
	O	-1.68831500	-0.17179100	-0.36547000
	C	-2.94599800	0.06721700	0.31260900
	H	-3.06909500	-0.68212200	1.09795700
	H	-2.90383900	1.04731000	0.79353300
	C	1.81399500	-0.75915400	0.25164200
	H	1.80167500	-0.70009700	1.33495900
	O	2.78561300	1.12713200	0.12853400
	O	1.92317100	1.79969200	-0.52559300
	C	-4.04404800	-0.01104700	-0.72789800
	H	-4.06549800	-0.99644600	-1.19850200
	H	-5.01466100	0.16687000	-0.25761000
	H	-3.89671000	0.73992400	-1.50712500
12	C	2.16033000	1.21576300	0.96403600
	H	2.12638400	0.82749500	1.98435200
	H	1.48609200	2.06989400	0.87867000
	H	3.17735800	1.54077300	0.74142100
	C	0.40138600	-0.43377200	0.25630300
	H	0.31210200	-1.33126700	0.85539700
	C	-0.79133300	0.24342100	-0.20878400
	O	-0.79457400	1.26741300	-0.86971300
	O	-1.91913500	-0.39852700	0.18412000
	C	1.74734200	0.12681500	-0.03687300
	H	1.75895300	0.54732200	-1.04976700
	O	2.62944200	-1.00883500	0.01724400

	O	3.94412100	-0.56533900	-0.40405200
	H	4.00772000	-1.00992400	-1.26069100
	C	-3.16672800	0.20425300	-0.22843300
	H	-3.21373300	1.22209600	0.16735600
	H	-3.18047500	0.27478500	-1.31907400
	C	-4.28864000	-0.66520800	0.30088700
	H	-4.25163300	-0.72742300	1.39062900
	H	-5.25437100	-0.24199900	0.01259900
	H	-4.22137800	-1.67708000	-0.10450000
13	C	-2.95168200	-1.69199200	-0.12674900
	H	-2.81415600	-2.23005000	0.81333200
	H	-2.97650000	-2.42628900	-0.93965900
	H	-3.91574600	-1.18315500	-0.10337900
	C	-0.54725400	-0.94776900	0.06025000
	H	-0.32309900	-1.76312800	0.73788600
	C	0.53080200	-0.00431100	-0.22553400
	O	0.38722000	1.12018200	-0.68160300
	O	1.73573400	-0.50971800	0.10588000
	C	-1.84781300	-0.70571100	-0.36348800
	H	-1.97544200	-0.03394700	-1.20431600
	O	-2.24585400	0.73805700	0.83656100
	O	-2.21795600	1.89603400	0.08636200
	H	-1.26614800	2.11636400	0.05862600
	C	2.87859100	0.35514300	-0.10022700
	H	2.90643800	0.65603100	-1.15004300
	H	2.74634400	1.25849300	0.50025900
	C	4.11369700	-0.42275600	0.30456100
	H	4.22231500	-1.32356300	-0.30315600
	H	5.00389800	0.19608200	0.16557200
	H	4.06089000	-0.71890000	1.35440200
14	C	0.71719600	-0.50363300	0.32377200
	O	0.72337800	-0.61712300	1.52329400
	O	1.77890600	-0.12355700	-0.40689400
	C	2.99571100	0.16370700	0.33178000
	H	3.29223200	-0.73557400	0.87663900
	H	2.77855400	0.94227700	1.06590800
	C	-1.79171100	-0.37335400	0.06992900
	H	-1.81844500	-0.66369500	1.12422500
	C	-3.06056600	-0.84344200	-0.63895900
	H	-3.57420100	-1.71586600	-0.24384800
	H	-3.64056400	0.33301700	-0.18731500
	H	-3.06168700	-0.76749200	-1.72587700
	O	-3.21508300	1.34036900	0.29170700
	O	-1.86344600	1.06469600	-0.03161000

	C	-0.47861400	-0.80739800	-0.56506700
	H	-0.49936200	-1.89279400	-0.71257600
	H	-0.35567100	-0.34016600	-1.54306100
	C	4.04335800	0.59751300	-0.67174700
	H	4.97939000	0.82435900	-0.15484200
	H	4.23629300	-0.19199200	-1.40137500
	H	3.72117300	1.49248400	-1.20810500
15	C	0.63000800	-0.68577700	0.22818200
	O	0.66613800	-0.97485700	1.39696200
	O	1.64930400	-0.12859500	-0.44723500
	C	2.85477700	0.13743800	0.31660700
	H	3.21854500	-0.80485900	0.73278600
	H	2.59715300	0.79366800	1.15047500
	C	-1.86745500	-0.86975500	0.02320500
	H	-1.84063100	-1.13441600	1.07347000
	C	-3.07964400	-0.69154000	-0.62816500
	H	-3.14329000	0.64449500	-0.41770500
	H	-3.10233400	-0.75224200	-1.71470200
	H	-3.98362100	-1.02978400	-0.12831300
	O	-2.69712700	1.73659000	0.04338900
	O	-1.64201800	1.29196200	0.60121400
	C	-0.55346800	-0.94358100	-0.68906500
	H	-0.42309500	-1.96382700	-1.08092100
	H	-0.51803300	-0.27513900	-1.55086200
	C	3.85646600	0.77293400	-0.62464000
	H	4.78310300	0.99061400	-0.08729000
	H	4.09006900	0.10403600	-1.45585500
	H	3.46765900	1.70834200	-1.03246500
16	C	0.64150200	-0.52022600	0.42190700
	O	0.63826000	-0.37704700	1.61838400
	O	1.69688200	-0.25137300	-0.36768100
	C	2.88201000	0.25241900	0.29996700
	H	3.20480100	-0.48277300	1.04084000
	H	2.61647400	1.16786500	0.83298000
	C	-1.85666700	-0.42913100	0.06233600
	H	-1.89646600	-0.42849500	1.15448800
	C	-3.05143700	-1.09114800	-0.52738600
	H	-3.70653500	-1.71198300	0.06960300
	H	-3.42555300	1.77344400	-0.44714900
	H	-3.24635800	-0.99256100	-1.58964800
	O	-2.76905600	1.71512100	0.26104100
	O	-1.73286100	0.93774500	-0.38558400
	C	-0.52789500	-1.06259500	-0.38179700
	H	-0.57762700	-2.14093300	-0.20452900

	H	-0.36649500	-0.90210800	-1.44846900
	C	3.93321500	0.49309400	-0.76348000
	H	4.84731000	0.87548600	-0.30179100
	H	4.17510300	-0.43305800	-1.28953400
	H	3.58517000	1.22507200	-1.49536000
17	C	0.58103400	-0.50782400	0.45958000
	O	0.54028600	-0.18830700	1.62052300
	O	1.65657800	-0.33863900	-0.33155600
	C	2.81149400	0.28243500	0.28645500
	H	3.12651300	-0.32971900	1.13489900
	H	2.51419600	1.25950900	0.67322700
	C	-1.90045000	-0.71450400	0.15662700
	H	-1.94150100	-0.35122900	1.17688800
	C	-3.06058000	-1.18048200	-0.43392100
	H	-4.02905200	-0.94419300	-0.01118400
	H	-3.17677500	2.18310500	-0.39038900
	H	-3.04185300	-1.69349600	-1.38883900
	O	-2.42527000	1.95014100	0.17395900
	O	-1.73852600	1.01873500	-0.60043700
	C	-0.54433700	-1.19913100	-0.28694700
	H	-0.45340600	-2.27188000	-0.07580300
	H	-0.41525100	-1.07003400	-1.36278700
	C	3.88917400	0.39005600	-0.77250800
	H	4.78146800	0.85777800	-0.34820800
	H	4.16488500	-0.59694700	-1.15048900
	H	3.54822100	0.99836400	-1.61294800
18	C	-3.52371700	-0.60035800	-0.49750200
	H	-3.41612100	-1.66536600	-0.68099300
	H	-4.45109700	-0.14117700	-0.82000100
	C	-2.56906400	0.10943900	0.09346700
	H	-2.69859400	1.17605600	0.25031600
	C	-1.26706600	-0.46100800	0.57910300
	H	-1.12431400	-1.49217400	0.25103400
	H	-1.25168600	-0.47929400	1.67838700
	C	-0.06627800	0.37350100	0.16483000
	O	-0.08787400	1.55318400	-0.08008500
	O	1.05269300	-0.37852400	0.13808100
	C	2.28239900	0.31486100	-0.19244300
	H	2.43490200	1.12067300	0.52938200
	H	2.17162400	0.77021600	-1.17915800
	C	3.40204900	-0.70455800	-0.15575000
	H	4.35196300	-0.22211400	-0.40036100
	H	3.48912200	-1.15210400	0.83672600
	H	3.22571700	-1.50325500	-0.87953100

19	C	-3.74124800	-0.61706800	0.00156900
	H	-4.69827800	-0.24551100	0.34581100
	H	-3.72744500	-1.57026200	-0.51471700
	C	-2.53052400	0.24779900	0.04971800
	H	-2.54384800	0.87472200	0.94823400
	H	-2.53329900	0.96731800	-0.78510900
	C	-1.22128400	-0.54446800	-0.00342200
	H	-1.18411400	-1.17675800	-0.89784800
	H	-1.13958000	-1.23030000	0.84559400
	C	0.00944100	0.33781300	-0.01616600
	O	0.01022700	1.54328700	-0.05104800
	O	1.13447400	-0.40859600	0.01306600
	C	2.38695000	0.31895100	-0.00451200
	H	2.41685000	0.98650700	0.85995600
	H	2.41980700	0.93997200	-0.90287000
	C	3.50582400	-0.70180100	0.02444400
	H	3.45347300	-1.36186700	-0.84419300
	H	4.47356400	-0.19353700	0.01276300
	H	3.45030500	-1.31517200	0.92644300
20	C	1.41595800	0.33879300	0.00011100
	H	1.43273700	0.99201800	-0.87545600
	H	1.43259200	0.99168000	0.87593600
	C	0.13544100	-0.49636300	-0.00015400
	H	0.08725000	-1.15655600	0.87259700
	H	0.08744400	-1.15627400	-0.87313100
	C	-1.11775100	0.35783800	-0.00017700
	O	-1.14118000	1.56266500	-0.00013100
	O	-2.21988800	-0.41692600	-0.00010300
	C	-3.49333500	0.27849000	-0.00006000
	H	-3.53969700	0.92116600	-0.88215000
	H	-3.53954400	0.92134000	0.88191000
	C	2.64918300	-0.54538600	0.00005000
	H	2.71877700	-1.17458100	-0.89076800
	H	2.71851100	-1.17502300	0.89058200
	O	3.81697500	0.33122100	0.00044100
	O	4.93982900	-0.35619100	-0.00014700
	C	-4.58443600	-0.77157500	0.00013500
	H	-4.51479000	-1.40643700	0.88603200
	H	-5.56460200	-0.28765900	0.00016100
	H	-4.51492900	-1.40662300	-0.88563900
21	C	0.82842300	0.52485600	-0.08687900
	O	0.89564200	1.57664100	0.49800100
	O	1.86911700	-0.30759700	-0.26700500

	C	3.14028800	0.12066900	0.28761400
	H	3.01521000	0.27923300	1.36092300
	H	3.41129600	1.07892100	-0.16155700
	C	-1.67348300	0.69564900	-0.33657200
	H	-2.03826900	0.28789100	0.91855400
	C	-3.00387500	0.09202700	-0.79085100
	H	-3.81128600	0.82185600	-0.67391300
	H	-3.00432600	-0.31315000	-1.80746000
	H	-1.59014800	1.77955700	-0.32051100
	O	-3.19947100	-1.02308100	0.08719300
	O	-2.88951900	-0.47051200	1.35734500
	C	-0.42299800	-0.03383100	-0.73912200
	H	-0.50109300	-1.10315100	-0.52329000
	H	-0.27446600	0.03549200	-1.82852000
	C	4.15496300	-0.96150300	-0.01674100
	H	4.25709500	-1.10878100	-1.09406300
	H	5.13077400	-0.67798000	0.38591900
	H	3.85915900	-1.91070000	0.43495400
22	C	0.75564600	0.04276300	0.32139100
	O	0.57868300	-0.94371000	0.99152500
	O	1.94862400	0.39690800	-0.19470600
	C	3.05881600	-0.49498200	0.08030900
	H	2.81396600	-1.48680600	-0.30647800
	H	3.17794600	-0.58056800	1.16278300
	C	-1.65571200	0.77025400	0.59765800
	H	-1.91111900	-0.51465000	0.30901400
	C	-2.83167700	1.24152100	0.02767800
	H	-3.73251200	1.36457000	0.61398700
	H	-2.85622400	1.66199700	-0.97055200
	H	-1.62904200	0.70058700	1.68419600
	O	-3.54552500	-0.67769000	-0.72388900
	O	-2.62255200	-1.41925400	-0.27179800
	C	-0.31329500	1.05071300	-0.05809800
	H	-0.40204700	1.04375600	-1.14982500
	H	0.06284600	2.04559100	0.20282200
	C	4.28653500	0.09118800	-0.58535700
	H	5.15079300	-0.55266400	-0.40291700
	H	4.14191700	0.17488700	-1.66462700
	H	4.50775300	1.08451800	-0.18894600
23	C	0.92260000	0.31917100	-0.28172200
	O	0.91953200	1.51581800	-0.42522700
	O	2.02237300	-0.39786200	0.02116500
	C	3.25352800	0.35081000	0.18501100
	H	3.11141200	1.08764700	0.97902600

	H	3.45697500	0.89486300	-0.74014400
	C	-1.51689900	0.10544400	-0.87411200
	H	-2.93149900	0.94024800	1.55404700
	C	-2.84202600	-0.55632800	-0.75179300
	H	-3.61283500	-0.04440200	-1.33209200
	H	-2.80451400	-1.60914900	-1.05845500
	H	-1.43919600	1.13886000	-1.18541400
	O	-3.29484900	-0.66871500	0.61966500
	O	-3.70633400	0.65361600	1.05058700
	C	-0.28692300	-0.58905000	-0.40445600
	H	-0.44991500	-1.06190200	0.57519300
	H	-0.01099600	-1.42721300	-1.06281400
	C	4.34788600	-0.64218300	0.51675300
	H	4.46925500	-1.37169500	-0.28690700
	H	5.29707200	-0.11693300	0.65074900
	H	4.11946400	-1.18035600	1.43921700
24	C	-1.04470100	0.39346300	0.04649900
	O	-1.08147300	1.59801200	0.06771400
	O	-2.13559400	-0.39102900	-0.04192800
	C	-3.41258400	0.29118900	-0.13337400
	H	-3.39376200	0.95286700	-1.00237600
	H	-3.53950800	0.91332500	0.75543100
	C	1.40841600	0.29206700	0.60074100
	H	4.00932100	0.72448300	-1.48602900
	C	2.53242000	-0.34012200	1.08949900
	H	3.30812500	0.24418700	1.56678300
	H	2.47543700	-1.37909000	1.39582500
	H	1.40586500	1.36727100	0.45866400
	O	3.57292300	-0.76500800	-0.44443600
	O	4.43146700	0.29753900	-0.72638700
	C	0.21878600	-0.44810500	0.07947600
	H	0.40046400	-0.76736800	-0.95924400
	H	0.02660200	-1.36995900	0.63475700
	C	-4.48650900	-0.77083500	-0.24603300
	H	-4.48147700	-1.42456400	0.62881500
	H	-5.46959700	-0.29827000	-0.31686000
	H	-4.33501500	-1.38492800	-1.13631200
25	C	3.66431600	-0.61572300	0.02316200
	H	3.71742600	-1.17207800	-0.91796500
	H	3.65078300	-1.34583400	0.83848200
	H	4.58450200	-0.03355600	0.11561200
	C	2.43279900	0.29212700	0.06600500
	H	2.41949700	0.86270600	0.99928900
	H	2.48324300	1.03341000	-0.73636100

	C	1.12650900	-0.49191400	-0.05971300
	H	1.02904300	-1.23447600	0.74029100
	H	1.10066800	-1.06617800	-0.99368200
	C	-0.10341300	0.38425900	-0.03172300
	O	-0.12779300	1.58526800	0.01474000
	O	-1.23608300	-0.38850900	-0.07302500
	C	-2.46571800	0.23332700	-0.10721000
	H	-2.46315000	1.29971500	0.06610600
	C	-3.62284500	-0.66736300	0.09422000
	H	-3.68088300	-1.05002200	1.12585600
	H	-4.55388300	-0.13638500	-0.11432600
	H	-3.56612000	-1.53965100	-0.56546400
26	C	-4.36362600	0.16507500	-0.42421400
	H	-4.34413700	0.11449300	-1.51726100
	H	-4.53399200	1.20927400	-0.14393200
	H	-5.22435700	-0.41414300	-0.08150800
	C	-3.06523300	-0.37170100	0.18280000
	H	-3.12078200	-0.34146600	1.27482900
	H	-2.93328000	-1.42455100	-0.08157600
	C	-1.83930800	0.41661800	-0.27855500
	H	-1.92499100	1.47860700	-0.02193000
	H	-1.73578000	0.38930100	-1.36956400
	C	-0.54439300	-0.09107100	0.30336400
	O	-0.40109300	-1.03408300	1.02829100
	O	0.50299900	0.70689500	-0.11182500
	C	2.71038800	1.52027500	0.26024000
	H	2.41217900	2.21964800	1.04356300
	H	3.73431900	1.19370800	0.44426700
	H	2.65475600	2.02182400	-0.70742800
	C	1.79716500	0.32173800	0.27292500
	H	1.78629400	-0.23323300	1.20939900
	O	2.21686500	-0.64575600	-0.76230800
	O	3.31370600	-1.27443900	-0.39768600
27	C	-2.68805000	1.22104900	-0.62576900
	H	-3.68568700	0.44557300	-0.03683200
	C	-1.74691400	0.07238600	-0.31406300
	H	-1.66794000	-0.65237400	-1.12533400
	H	-2.90844900	1.42880800	-1.66846300
	O	-2.29185200	-0.55111500	0.86339900
	O	-3.68621600	-0.54486600	0.61040000
	H	-2.56518500	2.09522700	0.00949100
	O	-0.47347000	0.54817700	0.05194400
	C	0.62523300	-0.21497400	-0.29008100
	O	0.55229800	-1.22711900	-0.92704100

	C	1.87920900	0.42463200	0.25124400
	H	1.90059500	1.46253900	-0.09973300
	H	1.76470100	0.48873500	1.33960100
	C	3.15743000	-0.32248700	-0.12972700
	H	3.22819600	-0.37965500	-1.21984400
	H	3.08483900	-1.35584500	0.22051400
	C	4.41153100	0.34110700	0.44405200
	H	4.37789300	0.37966700	1.53722900
	H	5.31078400	-0.21070800	0.16001200
	H	4.52353300	1.36713700	0.07980400
28	C	2.81298800	-1.08741200	-0.68163600
	H	3.28230600	0.18095100	-0.64811400
	C	1.70256700	-0.86906900	0.11771300
	H	1.67090400	-1.00742400	1.18877800
	H	2.63659000	-1.26641700	-1.73832100
	O	2.23281600	1.31630300	0.50713900
	O	3.25138600	1.38533400	-0.25982600
	H	3.62848100	-1.64601600	-0.23233100
	O	0.50587900	-0.63098200	-0.47644500
	C	-0.60193100	-0.41531000	0.34139400
	O	-0.56079700	-0.54001500	1.52946600
	C	-1.78559600	-0.02852900	-0.50309400
	H	-1.52460300	0.90851900	-1.00972800
	H	-1.88384900	-0.77260700	-1.30141900
	C	-3.08166600	0.11562500	0.29504900
	H	-2.93166500	0.85165900	1.08959100
	H	-3.29998200	-0.83072400	0.79872200
	C	-4.26332800	0.52516000	-0.58718400
	H	-4.45202700	-0.21481200	-1.37113100
	H	-5.17711000	0.62173500	0.00383300
	H	-4.08152100	1.48722700	-1.07600000
29	C	2.61099200	1.59522200	0.37229200
	H	4.06241100	-0.85547400	-0.86023200
	C	1.78365000	0.37475500	0.27333400
	H	1.77314800	-0.23209900	1.17831000
	H	3.51171700	1.59052100	0.97030600
	O	2.21708200	-0.48726800	-0.81652800
	O	3.35438800	-1.23398500	-0.32124100
	H	2.40017200	2.43264500	-0.27965800
	O	0.47092700	0.73747700	-0.11377500
	C	-0.55784900	-0.06876100	0.31166900
	O	-0.41351800	-0.98170100	1.07530700
	C	-1.85593700	0.38375900	-0.31217300
	H	-1.94614600	1.46378600	-0.15283900

	H	-1.75118900	0.25648300	-1.39626300
	C	-3.07921600	-0.36614800	0.21517900
	H	-3.14399700	-0.22930300	1.29873000
	H	-2.93568100	-1.43849300	0.05714700
	C	-4.37771500	0.09618500	-0.45012500
	H	-4.35052900	-0.06434100	-1.53243800
	H	-5.23688400	-0.45208600	-0.05594700
	H	-4.55760800	1.16211700	-0.27829000
30	C	2.69803200	1.63170700	0.02673600
	H	3.89300500	-1.47798000	-0.72137200
	C	1.75030000	0.68134300	0.35018300
	H	1.82597700	0.05591700	1.22931000
	H	3.69325500	1.55234900	0.44037300
	O	2.19401300	-0.71974200	-0.82917200
	O	3.08491500	-1.58894300	-0.20013400
	H	2.49672700	2.37210500	-0.73537000
	O	0.47173700	0.91008000	-0.09982200
	C	-0.53624400	0.11115300	0.40737600
	O	-0.37622800	-0.64627000	1.32046800
	C	-1.81560000	0.36366000	-0.34844000
	H	-1.97235500	1.44700000	-0.39201000
	H	-1.63921700	0.05213200	-1.38506900
	C	-3.02568700	-0.35726300	0.24559900
	H	-3.16333600	-0.03313200	1.28151800
	H	-2.81419300	-1.42892800	0.29244600
	C	-4.30483000	-0.10628100	-0.55636300
	H	-4.20325800	-0.45522000	-1.58874000
	H	-5.15468500	-0.63031200	-0.11229500
	H	-4.55324700	0.95915100	-0.59005100
31	C	3.61518600	-0.55328500	-0.00001700
	H	3.65011400	-1.19916000	-0.88294000
	H	3.65027200	-1.19850900	0.88337500
	H	4.52164100	0.05696400	-0.00032200
	C	2.36176700	0.32517400	-0.00022000
	H	2.36474700	0.98475900	0.87223800
	H	2.36459300	0.98414000	-0.87314700
	C	1.07440700	-0.49917400	0.00017500
	H	1.02638800	-1.16184600	0.87195700
	H	1.02619700	-1.16244100	-0.87113800
	C	-0.17884100	0.34265600	0.00007700
	O	-0.23362600	1.54222900	0.00011600
	O	-1.28605800	-0.46783900	0.00000100
	C	-2.53551300	0.12781400	-0.00006300
	H	-2.51575500	1.20935900	-0.00011900

	C	-3.62907300	-0.61983300	-0.00007000
	H	-3.57672200	-1.70122800	0.00001100
	H	-4.60159700	-0.14726800	-0.00014200
32	C	3.65819200	-0.56627800	0.00131700
	H	3.70254100	-1.18015000	0.90648500
	H	4.56521500	0.04259200	-0.03029700
	H	3.68351400	-1.24336600	-0.85836800
	C	2.40475800	0.31202100	-0.01678800
	H	2.41703200	1.00216300	0.83168000
	H	2.39868700	0.94074700	-0.91172800
	C	1.11639400	-0.50956200	0.02560900
	H	1.07681800	-1.13930500	0.92158700
	H	1.06195300	-1.20386700	-0.82073200
	C	-0.13933400	0.33625600	0.00425900
	O	-0.17881900	1.53993900	-0.05254000
	O	-1.24262100	-0.44377900	0.05868900
	C	-2.51371400	0.24938300	0.03713200
	H	-2.51442200	0.93676400	-0.82224700
	H	-2.59795000	0.87889700	0.92998500
	C	-3.59394800	-0.75623300	-0.03950500
	H	-3.41613200	-1.70628700	-0.52483500
	H	-4.59981400	-0.49099800	0.25713700
33	C	4.68849500	-0.74913100	-0.00011400
	H	4.68041200	-1.39569900	0.88300200
	H	5.63372800	-0.20098700	-0.00003500
	H	4.68053400	-1.39565000	-0.88326700
	C	3.49719700	0.21150800	-0.00016800
	H	3.54427700	0.86935200	0.87233200
	H	3.54437800	0.86938900	-0.87263300
	C	2.15636900	-0.52317600	-0.00026600
	H	2.06422800	-1.18092700	0.87157100
	H	2.06435600	-1.18091200	-0.87212900
	C	0.96319500	0.40561000	-0.00039400
	O	0.99390900	1.60791300	-0.00029900
	O	-0.19825600	-0.30290100	0.00032800
	C	-1.40574300	0.47751800	0.00067100
	H	-1.44063700	1.11785700	-0.88316500
	H	-1.44090400	1.11662400	0.88540200
	C	-2.53745500	-0.53187300	-0.00017300
	H	-2.52517200	-1.15974800	0.89205800
	H	-2.52450700	-1.15883200	-0.89305400
	O	-3.77173300	0.23667200	-0.00022400
	O	-4.83055100	-0.54708500	0.00051800

34	C	0.78046700	1.02523300	0.07943400
	O	0.61656200	2.16405400	-0.25621200
	C	2.66766400	-0.60799000	-0.38571700
	H	2.85976400	-0.10640700	-1.34014200
	H	1.94072800	-1.40010400	-0.58420900
	C	-1.47535500	0.47642500	-0.43439900
	H	-2.38493400	0.60673700	0.57986100
	C	-2.32815800	-0.69444700	-0.91699800
	H	-3.06543700	-0.31242500	-1.63166300
	H	-1.75412700	-1.51590200	-1.34978400
	H	-1.44900500	1.39593600	-1.01450600
	O	-2.97075100	-1.20531400	0.25190000
	O	-3.36897600	-0.03790200	0.93810000
	C	2.05034500	0.40500700	0.59900200
	H	2.74687200	1.22094000	0.79856200
	H	1.82464200	-0.09879300	1.54422900
	O	-0.22590400	0.07629400	0.01410900
	C	3.96666000	-1.21345300	0.15050300
	H	3.79559200	-1.74928800	1.08882700
	H	4.39148500	-1.92197700	-0.56475700
	H	4.71723800	-0.44041700	0.33946500
35	C	-0.64891300	-0.11694800	0.41405200
	O	-0.52739900	0.65375100	1.33009000
	C	-3.11948100	0.40769700	0.13261500
	H	-2.88205000	1.47330300	0.06788900
	H	-3.28233600	0.20194200	1.19440800
	C	1.63582300	-0.70739700	0.58130700
	H	1.99664500	0.56671600	0.37515600
	C	2.71766800	-1.24961200	-0.08846400
	H	3.64127800	-1.44393400	0.43743900
	H	2.61829800	-1.64135300	-1.09106900
	H	1.57807900	-0.73287200	1.66639900
	O	3.51110900	0.64942300	-0.83190700
	O	2.71956600	1.43953200	-0.24013000
	O	0.37926700	-0.86907900	-0.06612700
	C	-1.91836100	-0.40244600	-0.35528900
	H	-2.11206100	-1.47911500	-0.28841900
	H	-1.71263700	-0.20874600	-1.41426900
	C	-4.39057800	0.10248600	-0.66340200
	H	-4.66698700	-0.95374400	-0.58555400
	H	-5.23381900	0.69291600	-0.29676800
	H	-4.26170600	0.33317900	-1.72553500
36	C	-0.80799000	-0.47498800	-0.20234200
	O	-0.80488300	-1.64960700	0.04397000

	C	-3.27607500	-0.20838200	0.32600200
	H	-3.10853200	-0.60523500	1.33159600
	H	-3.49563100	-1.07441300	-0.30461900
	C	1.50377700	-0.47420800	-0.71511600
	H	3.14544400	-0.22364500	1.86298200
	C	2.71249900	0.35886400	-0.86596800
	H	3.51857300	-0.21472400	-1.33061800
	H	2.50073900	1.24878500	-1.46609400
	H	1.48759700	-1.52386100	-0.46275800
	O	3.20400400	0.93088500	0.36910800
	O	3.78396000	-0.15481300	1.14014400
	C	-1.99245400	0.45805600	-0.16943200
	H	-1.72286500	1.32003700	0.45116500
	H	-2.12196100	0.85944100	-1.18187700
	O	0.32768000	0.21512800	-0.57120500
	C	-4.46661100	0.75332200	0.33320600
	H	-4.67480100	1.13820200	-0.66994400
	H	-5.37067500	0.25417500	0.69015500
	H	-4.28284400	1.61250200	0.98578500
37	C	-0.85835000	0.47055300	0.14722200
	O	-0.81750700	1.58542500	-0.29390200
	C	-3.32457600	0.18500000	-0.38055600
	H	-3.13225200	0.48122900	-1.41570200
	H	-3.54927400	1.10960000	0.15884500
	C	1.42995900	0.51525400	0.73911500
	H	3.63903400	0.30186000	-1.82625200
	C	2.56154200	-0.16723900	1.10933000
	H	3.44971600	0.40564600	1.33476900
	H	2.45727300	-1.12610000	1.60059700
	H	1.40505900	1.53034900	0.36879800
	O	3.28408300	-0.94134900	-0.47628900
	O	4.15285100	-0.02640400	-1.07404800
	C	-2.05802700	-0.44067100	0.20390600
	H	-1.79284600	-1.36675300	-0.31925000
	H	-2.20327100	-0.73133100	1.25084300
	O	0.23968800	-0.16409000	0.69008000
	C	-4.52385300	-0.76395800	-0.31985300
	H	-4.75659300	-1.04867800	0.71093300
	H	-5.41549200	-0.29486900	-0.74268700
	H	-4.33445000	-1.68323900	-0.88261500

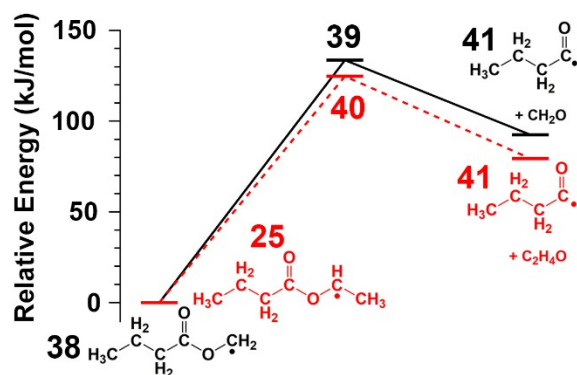


Figure S9. PES of the dissociation of R_m . The numbers correspond with the energies and geometries listed in the supporting information.

Table S5. Calculated 0 K CBS-QB3 energies for the structures in Figure S8.

Species	Energy (Hartrees)
38	-345.771935
39	-345.721105
40	-384.957683
41	-231.392538

Table S6. Optimized geometries for the structures in Figure S8.

Species	Optimized coordinates (Å)			
38	C	3.18255100	-0.32065800	0.00136500
	H	3.28324400	-0.96655700	0.87923300
	H	4.02071800	0.38042700	0.00872800
	H	3.28617300	-0.95149800	-0.88704600
	C	1.84497000	0.42317800	0.00544600
	H	1.77867800	1.07198000	0.88353700
	H	1.78121400	1.08669500	-0.86168200
	C	0.64885300	-0.52880000	-0.00447200
	H	0.66898100	-1.20050000	0.86158600
	H	0.67265800	-1.18584500	-0.88179100
	C	-0.68142800	0.18330900	-0.00255300
	O	-0.86616300	1.36985900	-0.00346800
	O	-1.70878800	-0.73282700	0.00003000
	C	-2.99362300	-0.27002000	-0.01298900
	H	-3.16324500	0.79252600	0.04562800
	H	-3.73675600	-1.04553900	0.05853500
39	C	3.03572100	-0.53097500	-0.17304000
	H	3.57164000	0.19039400	0.45141500
	H	3.62222600	-0.68191400	-1.08327100
	H	3.00889800	-1.48288900	0.36580100
	C	1.62537900	-0.03932800	-0.50549400

	H	1.67211200	0.90148000	-1.06140000
	H	1.12065400	-0.76246600	-1.15337700
	C	0.76575900	0.17109900	0.75562800
	H	1.24246500	0.90066000	1.42141300
	H	0.64522500	-0.75788300	1.31456400
	C	-0.59718600	0.72557300	0.45216800
	O	-0.95841000	1.57497100	-0.28886800
	O	-1.68497400	-0.87678100	0.30222300
	C	-2.72028700	-0.75145100	-0.37200300
	H	-2.76047700	-0.05292900	-1.21681600
	H	-3.63198100	-1.28948100	-0.08872700
40	C	3.45888900	-0.86963900	-0.17343600
	H	3.30796500	-1.78814800	0.40190600
	H	4.09941500	-0.20825400	0.41811200
	H	4.00497900	-1.13398400	-1.08306300
	C	2.12524500	-0.19813000	-0.50775700
	H	2.29278300	0.70964900	-1.09443900
	H	1.51656800	-0.86433100	-1.12708800
	C	1.32009900	0.17006900	0.75351300
	H	1.90973900	0.83840000	1.39225000
	H	1.07484600	-0.71722900	1.33902300
	C	0.04831500	0.91072400	0.44671200
	O	-0.17254600	1.80924000	-0.29951700
	O	-1.21713900	-0.46150800	0.31381300
	C	-2.23033300	-0.19581500	-0.36831000
	H	-2.13790800	0.52799400	-1.18825300
	C	-3.58070900	-0.74045000	-0.03492400
	H	-4.25072100	0.07001000	0.28295600
	H	-4.04108900	-1.19958800	-0.91625400
	H	-3.50813100	-1.47692700	0.76570800
41	C	2.37646300	-0.18908300	-0.06190200
	H	2.53906100	-0.76761600	0.85270400
	H	3.20525300	0.51619100	-0.16091500
	H	2.42765200	-0.88253800	-0.90661700
	C	1.03391200	0.54426700	-0.02326100
	H	1.01324400	1.24934500	0.81333500
	H	0.91307700	1.14248200	-0.93230600
	C	-0.15414100	-0.41446000	0.10809500
	H	-0.06877600	-0.99724400	1.03457000
	H	-0.20457800	-1.12757100	-0.72458500
	C	-1.49536000	0.29764400	0.21180000
	O	-2.54877200	-0.07040700	-0.17307200

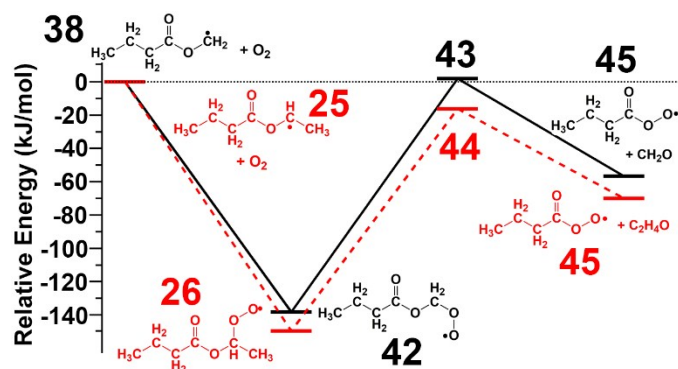


Figure S10. PES for the reaction of O₂ with R_m. The numbers correspond with the energies and geometries listed in the supporting information.

Table S7. Calculated 0 K CBS-QB3 energies for the structures in Figure S9.

Species	Energy (Hartrees)
42	-495.989219
43	-495.935839
44	-535.175962
45	-381.613955

Table S8. Optimized geometries for the structures in Figure S9.

Species	Optimized coordinates (Å)			
42	C	4.07443100	-0.26513000	0.39850900
	H	4.32640400	-0.98708700	-0.38446500
	H	4.02290900	-0.80910700	1.34672000
	H	4.89978100	0.44716400	0.47002000
	C	2.75693100	0.45198200	0.09463800
	H	2.54223500	1.19070900	0.87169000
	H	2.84290600	1.01489600	-0.83940900
	C	1.58023000	-0.51845900	-0.01102300
	H	1.45438300	-1.09204800	0.91493800
	H	1.74327400	-1.26631500	-0.79500700
	C	0.26496500	0.16001200	-0.29159500
	O	0.05837900	1.33700800	-0.36618800
	O	-0.72667400	-0.78921700	-0.46873900
	C	-2.02535300	-0.31562100	-0.65125400
	H	-2.05276000	0.66706600	-1.11815800
	H	-2.59076200	-1.07113600	-1.19183300
	O	-2.61373400	-0.18599700	0.68273900
	O	-3.85492000	0.24185100	0.58842000
43	C	-0.14912100	-0.34159200	0.47725800
	O	-0.41150300	-0.36995900	1.61958200
	O	-0.86788700	1.25977500	-0.35729500

	C	-2.06698500	1.29735000	-0.03429000
	H	-2.79731300	1.75475000	-0.70941900
	H	-2.38080900	1.11770000	1.00078700
	C	2.26883100	0.29527100	0.30867900
	H	1.99664800	1.35423000	0.33289300
	C	3.57208000	0.10524100	-0.47046100
	H	4.38272900	0.68057500	-0.01688900
	H	3.87822100	-0.94514100	-0.48598600
	H	3.46804100	0.43811400	-1.50733300
	H	2.40067400	-0.02000900	1.34750700
	O	-2.53778100	-0.65461400	-0.52000400
	O	-1.38092100	-1.20987400	-0.50605600
	C	1.10762400	-0.49454000	-0.31270900
	H	0.91170700	-0.18521700	-1.33861300
	H	1.33027100	-1.56801200	-0.32362500
44	C	0.28746600	-0.60341000	0.40469100
	O	0.11746200	-0.95939500	1.51284300
	O	-0.72586500	0.92133400	0.00347800
	C	-1.89204400	0.71074700	0.39671600
	H	-2.04482200	0.18955000	1.34897400
	C	2.55680500	0.46582100	0.34117500
	H	2.11790000	1.43198500	0.60689900
	C	3.83024200	0.67719600	-0.48072200
	H	4.55889600	1.27131100	0.07625500
	H	4.30344600	-0.27615700	-0.73471500
	H	3.61743800	1.20334400	-1.41602600
	H	2.79380400	-0.04062100	1.28103800
	O	-2.05498000	-1.17030800	-0.57532600
	O	-0.81787400	-1.46951300	-0.74055900
	C	1.50847700	-0.35765000	-0.42107300
	H	1.21066900	0.12979600	-1.34883800
	H	1.90561500	-1.34681200	-0.67622700
	C	-3.05434200	1.43679500	-0.19859700
	H	-3.94965500	0.81353000	-0.16878800
	H	-3.25014600	2.33551900	0.39792300
	H	-2.83271700	1.73461900	-1.22312400
45	C	3.16105500	-0.32832800	0.00002600
	H	3.25515600	-0.96707800	-0.88341400
	H	3.25515300	-0.96695300	0.88355800
	H	4.00643600	0.36350100	-0.00002000
	C	1.83383900	0.43333900	-0.00000100
	H	1.77608900	1.08891000	0.87352500
	H	1.77608400	1.08885300	-0.87356600
	C	0.62689800	-0.50687000	0.00001100

H	0.63548700	-1.17194400	0.87158900
H	0.63552100	-1.17202300	-0.87151200
C	-0.68581600	0.22246300	-0.00004000
O	-0.91590600	1.38201800	-0.00002200
O	-1.74370300	-0.77393500	-0.00010900
O	-2.95986300	-0.25644300	0.00011400

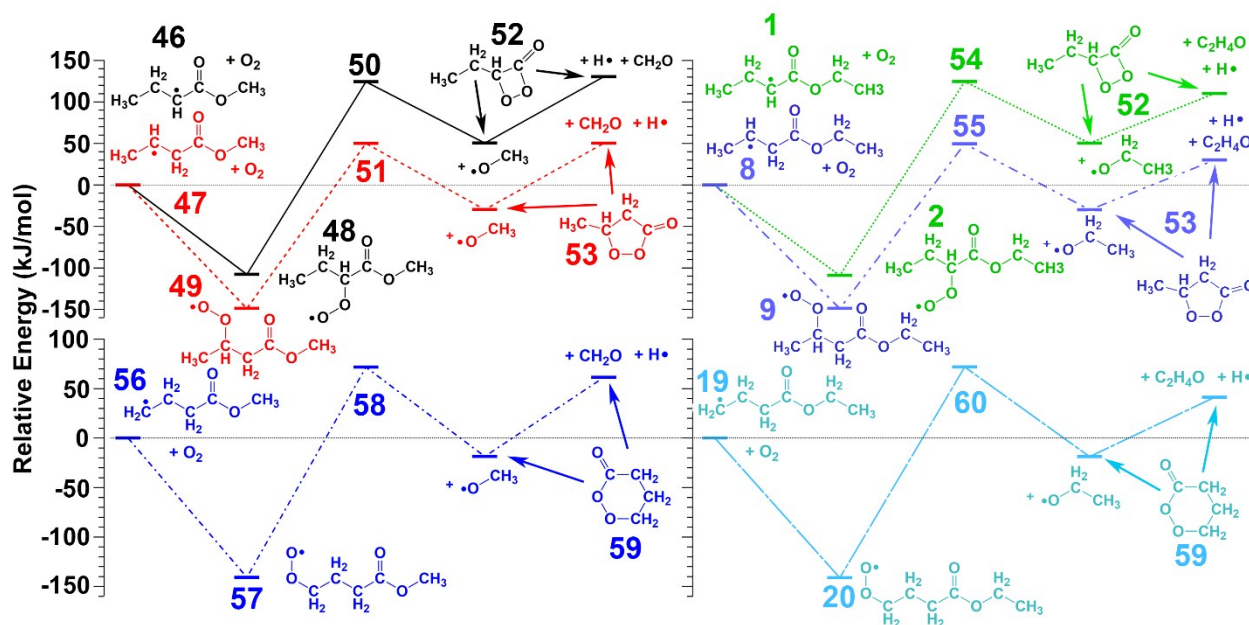


Figure S11. PES of the reaction of $R_{\beta, \gamma, \text{ or } \delta}$ with O_2 , where the peroxy radical forms a bond with C_{α} to elimination the $CH_3O\bullet$ or $C_2H_5O\bullet$. The numbers correspond with the energies and geometries listed in the supporting information.

Table S9. Calculated 0 K CBS-QB3 energies for the structures in Figure S10.

Species	Energy (Hartrees)
46	-345.780606
47	-345.773162
48	-495.986268
49	-495.994451
50	-495.897908
51	-495.918776
52	-381.051555
53	-381.074636
54	-535.128363
55	-535.149469
56	-345.769000
57	-495.987256
58	-495.906308

59	-381.066201
60	-535.136760

Table S10. Optimized geometries for the structures in Figure S10.

Species	Optimized coordinates (Å)			
46	C	-3.05726000	-0.25631300	0.50921900
	H	-2.74488700	-0.15473300	1.55123200
	H	-3.28402200	-1.31027200	0.32580400
	H	-3.97915000	0.31473400	0.37443900
	C	-1.96238800	0.25754600	-0.44666900
	H	-2.34191600	0.18509700	-1.47725200
	H	-1.75274400	1.31270500	-0.25987100
	C	-0.69421100	-0.50836300	-0.34949000
	H	-0.69098400	-1.58571400	-0.47466800
	C	0.57257100	0.14374700	-0.08826900
	O	0.72792800	1.33949100	0.08549400
	O	1.59923600	-0.74942300	-0.05635200
	C	2.89414200	-0.18733100	0.19897700
	H	3.58588500	-1.02706100	0.18381800
	H	3.15809900	0.54050400	-0.57086200
	H	2.91528100	0.30847300	1.17160200
47	C	-3.29898500	-0.19124600	-0.00003500
	H	-3.49213000	-0.82697200	0.87781200
	H	-3.49170200	-0.82823200	-0.87704600
	H	-4.04601600	0.60451800	-0.00075900
	C	-1.91366900	0.35269100	-0.00009900
	H	-1.72728900	1.41803800	-0.00001600
	C	-0.74082900	-0.56215100	0.00008300
	H	-0.74841700	-1.24274300	-0.86663100
	H	-0.74845700	-1.24245400	0.86703200
	C	0.59658600	0.15352100	0.00002700
	O	0.76386800	1.34626400	0.00004400
	O	1.60978600	-0.74027900	-0.00002400
	C	2.93523100	-0.18039300	-0.00004400
	H	3.61124200	-1.03254500	-0.00011900
	H	3.09173100	0.43403500	-0.88808000
	H	3.09180000	0.43393100	0.88805400
48	C	-3.03757400	-0.67958500	-0.23432700
	H	-3.27690700	0.32282000	-0.59448800
	H	-3.32666200	-0.73966500	0.81895300
	H	-3.65000700	-1.39311300	-0.79009100
	C	-1.55126900	-0.99388800	-0.41657500
	H	-1.31830700	-1.99429400	-0.04421900

	H	-1.28305800	-0.97596400	-1.47818800
	C	-0.63693200	-0.01910600	0.32481100
	H	-0.92578700	0.08245400	1.37326100
	C	0.81756400	-0.48833000	0.29667500
	O	1.16612600	-1.48909500	0.87046600
	O	1.61275800	0.29858200	-0.42991200
	C	2.99929100	-0.09692600	-0.48813400
	H	3.48547800	0.65316000	-1.10643600
	H	3.42926800	-0.11132500	0.51380600
	H	3.09174200	-1.08796900	-0.93391100
	O	-0.80743800	1.28888300	-0.29030500
	O	-0.44297600	2.26549300	0.51807700
49	C	2.59192100	-1.23241100	0.06670900
	H	2.66491400	-1.58891200	-0.96412200
	H	2.54427800	-2.09730400	0.73322300
	H	3.48897900	-0.66073300	0.30697000
	C	0.06215100	-0.99238700	-0.20327900
	H	-0.01614400	-1.99672600	0.22637200
	H	0.04849400	-1.10479500	-1.28901700
	C	-1.15747700	-0.21188200	0.25327800
	O	-1.22931000	0.41539200	1.27934800
	O	-2.16895400	-0.34008100	-0.62383800
	C	-3.39369600	0.33153100	-0.26730800
	H	-4.08542300	0.12280900	-1.07989100
	H	-3.77976700	-0.05477300	0.67705300
	H	-3.22291500	1.40439600	-0.17163800
	C	1.36506200	-0.35814600	0.25673800
	H	1.27450500	-0.00221000	1.28351000
	O	1.49782100	0.85673500	-0.57486400
	O	2.43485700	1.66270700	-0.12555800
50	C	-0.51189900	0.49583700	-0.20042200
	O	-0.88517800	1.56250800	-0.55854300
	O	-1.74877300	-0.42012300	0.77063100
	C	-3.05073800	-0.03302100	0.45296600
	H	-3.56431200	-0.81720500	-0.11631100
	H	-3.58550500	0.08260600	1.40755700
	H	-3.07010500	0.91930700	-0.08877000
	C	0.77419100	-0.07881300	0.38687600
	C	2.03900600	0.68061800	0.03394000
	H	2.03089900	0.89799400	-1.03769000
	C	3.31016300	-0.07966600	0.42236200
	H	4.19944900	0.49184300	0.14808100
	H	3.35026300	-0.26533200	1.49973300
	H	3.36061400	-1.04376200	-0.08913600

	H	1.99042300	1.64431800	0.55263000
	H	0.71019100	-0.33522900	1.44486300
	O	0.59395400	-1.28824300	-0.41222600
	O	-0.55828500	-0.78967700	-1.08677300
51	C	0.61874000	0.78089200	0.06552300
	O	1.44380500	1.59666000	0.34134400
	O	1.30572800	-0.70298300	-0.68082600
	C	2.65035800	-0.89693100	-0.34977600
	H	2.76843900	-1.76474300	0.30962500
	H	3.18640600	-1.11477000	-1.28482100
	H	3.07868500	-0.00095200	0.11302800
	C	-1.48201800	-0.33240300	-0.34967900
	H	-1.15300300	-1.18605400	-0.94772900
	C	-2.99005800	-0.19789300	-0.34756500
	H	-3.45346700	-1.10136000	0.05443700
	H	-3.30415700	0.65582700	0.25668900
	H	-3.34984500	-0.05810700	-1.36994300
	O	0.22406200	-0.21666300	1.21388200
	O	-1.08597500	-0.64144100	1.03081100
	C	-0.67309900	0.89833200	-0.71667100
	H	-0.44981200	0.95216900	-1.78113100
	H	-1.16774500	1.82143100	-0.40284000
52	C	2.42273800	0.41329600	-0.02413400
	H	2.04688900	1.42426300	0.14799900
	H	2.71067700	0.33490600	-1.07637700
	H	3.32383800	0.28122900	0.57772300
	C	1.37447000	-0.64212000	0.34812500
	H	1.76275400	-1.64883500	0.16482600
	H	1.12510400	-0.58413300	1.41128200
	C	0.09921900	-0.47901400	-0.46055400
	H	0.27745700	-0.52089700	-1.53938400
	C	-0.84931400	0.63343600	-0.06564800
	O	-0.88988700	1.81481400	0.01225400
	O	-1.84120700	-0.26181000	0.26640100
	O	-0.96008000	-1.40801900	-0.08775500
53	C	2.43434700	-0.32497400	0.13469000
	H	2.84684800	-1.24862100	-0.27837500
	H	2.42843400	-0.39550900	1.22434400
	H	3.08536700	0.50080100	-0.15919400
	C	1.03153700	-0.10607800	-0.39478300
	H	1.03278800	-0.03421800	-1.48990800
	C	-0.05495000	-1.06643000	0.06485700
	H	0.10868800	-1.39833800	1.09512600

	H	-0.20030200	-1.94039200	-0.56846600
	C	-1.28805600	-0.18251700	0.03227900
	O	-2.44753400	-0.46268000	0.02200200
	O	-0.87910400	1.12963900	-0.02022600
	O	0.57175100	1.15757400	0.14250000
54	C	-0.06309800	-0.22783300	0.57991300
	O	-0.39675100	-0.98447700	1.42976600
	O	-1.41851900	0.26632400	-0.53227300
	C	-2.67509300	0.20124100	0.08304300
	H	-3.06277300	1.21802300	0.22106400
	H	-2.59744400	-0.30004600	1.05492900
	C	1.12568800	-0.09768000	-0.36892900
	C	2.41161400	-0.73872200	0.11708500
	H	2.56950800	-0.46044600	1.16271900
	C	3.62266300	-0.34915500	-0.73524400
	H	4.53017200	-0.82193600	-0.35362700
	H	3.49477700	-0.66080900	-1.77608700
	H	3.77761300	0.73228400	-0.72264700
	H	2.25733800	-1.82314000	0.09816200
	H	0.89769800	-0.33030600	-1.40962800
	O	1.10705500	1.35127100	-0.18570800
	O	0.06071200	1.31326400	0.78277800
	C	-3.61274700	-0.58606100	-0.84708900
	H	-3.25388800	-1.60893000	-0.97340800
	H	-4.61180400	-0.61701100	-0.40384200
	H	-3.67533300	-0.10947700	-1.82682300
55	C	0.10182500	0.91400100	-0.28884900
	O	0.76044000	1.89198700	-0.46884900
	O	1.08474000	-0.56488200	0.00977800
	C	2.36817100	-0.28694600	0.50699600
	H	2.44897500	-0.67632400	1.52899500
	H	2.53962000	0.79553400	0.51441100
	C	-1.74327200	-0.63471000	-0.15425400
	H	-1.21228900	-1.58952300	-0.11974200
	C	-3.23186300	-0.82733300	-0.35299700
	H	-3.65042600	-1.43076700	0.45523600
	H	-3.74904100	0.13420500	-0.37620900
	H	-3.41436200	-1.34902500	-1.29573300
	O	-0.37069000	0.66263500	1.18641300
	O	-1.57103300	-0.03804200	1.17646900
	C	-1.03173200	0.31717300	-1.09782100
	H	-0.62725100	-0.18546000	-1.97496700
	H	-1.67929200	1.13836700	-1.41688900
	C	3.39598000	-0.98254400	-0.39628400

	H	3.34905600	-0.57723300	-1.40887400
	H	4.40098000	-0.81324700	0.00094100
	H	3.21172700	-2.05796200	-0.43838800
56	C	-3.27809700	-0.30635800	-0.00557500
	H	-4.17878000	0.18928500	0.33424800
	H	-3.38831300	-1.25472700	-0.51914200
	C	-1.96426400	0.39224200	0.04131300
	H	-1.90015900	1.02724200	0.93182300
	H	-1.86729100	1.09427300	-0.80281000
	C	-0.77124700	-0.56705200	0.00802200
	H	-0.81403900	-1.21256900	-0.87659100
	H	-0.78471000	-1.24449000	0.86749100
	C	0.56511800	0.14339900	-0.01023100
	O	0.73070500	1.33646900	-0.06013900
	O	1.58059900	-0.74713800	0.03307900
	C	2.90500800	-0.18505900	0.01057200
	H	3.05873500	0.46868100	0.87058300
	H	3.58273200	-1.03493700	0.04990300
	H	3.06228200	0.38955100	-0.90364100
57	C	-0.86278200	0.30198200	-0.00008500
	H	-0.83173300	0.95454900	0.87562400
	H	-0.83154700	0.95448700	-0.87583400
	C	0.35259400	-0.62518800	0.00007800
	H	0.35242300	-1.28711400	-0.87265100
	H	0.35222400	-1.28706800	0.87284200
	C	1.66468100	0.13397700	0.00021500
	O	1.78196400	1.33268200	0.00020300
	O	2.70652400	-0.72203600	0.00026500
	C	4.01357300	-0.11655200	0.00035600
	H	4.14763700	0.50225900	0.88873400
	H	4.71748600	-0.94543600	0.00038100
	H	4.14774400	0.50229700	-0.88798000
	C	-2.15775300	-0.48918200	-0.00019700
	H	-2.27295600	-1.11204800	0.89042100
	H	-2.27275300	-1.11212600	-0.89078800
	O	-3.25694800	0.47081500	-0.00036500
	O	-4.42784100	-0.13146300	-0.00047200
58	C	-0.41669700	0.66222400	-0.18946400
	O	-0.95284900	1.32238600	-1.02617900
	O	-1.54095700	-0.29748500	0.78586600
	C	-2.78122100	-0.47350800	0.16876000
	H	-2.94000100	-1.52863800	-0.07855800
	H	-3.54264500	-0.18239200	0.90760500

	H	-2.87567800	0.16075500	-0.71882600
	C	2.02046100	0.81453500	0.17072300
	H	2.08987200	1.38568200	-0.75742100
	C	2.21826100	-0.68583800	-0.11150900
	H	2.62707200	-0.86343600	-1.11031300
	H	2.86565100	-1.16368500	0.62658400
	H	2.80820300	1.17951600	0.83372000
	O	0.99475600	-1.43716500	0.02839700
	O	-0.02206000	-0.82375100	-0.72977500
	C	0.64353600	1.06362200	0.80792200
	H	0.53012300	0.49125800	1.72722600
	H	0.50025400	2.12285600	1.02493000
59	C	1.67976800	-0.24028000	-0.30878400
	H	2.65781100	-0.29378800	0.17425500
	H	1.76217600	-0.64169600	-1.32279400
	C	1.07990300	1.18212600	-0.28434400
	H	0.89730000	1.53318100	-1.30244400
	H	1.76403300	1.89273200	0.18369200
	C	-0.24988300	1.15358300	0.49881000
	H	-0.05002600	1.01162400	1.56433800
	H	-0.82029700	2.07281200	0.37456400
	C	-1.11402800	0.00948800	0.02739600
	O	-2.26817700	0.03939700	-0.28183500
	O	-0.44196800	-1.18930800	-0.11497100
	O	0.88695100	-1.12563400	0.48804500
60	C	-0.02561600	0.64902700	0.32634100
	O	0.39941900	1.30084600	1.23149400
	O	1.20737100	-0.31665300	-0.49836100
	C	2.37053700	-0.50930700	0.26132200
	H	2.48297200	-1.57906700	0.46950400
	H	2.29661300	0.04928400	1.20063400
	C	-2.39198800	0.82959700	-0.35937500
	H	-2.58363600	1.39842200	0.55296700
	C	-2.63887400	-0.66988500	-0.11306100
	H	-3.17872900	-0.84693900	0.82160200
	H	-3.18693700	-1.13880600	-0.93284500
	H	-3.07845800	1.20353900	-1.12248200
	O	-1.41482100	-1.43210900	-0.09317400
	O	-0.50344300	-0.83183600	0.79960000
	C	-0.93905500	1.06931400	-0.80099400
	H	-0.70694100	0.50516000	-1.70298800
	H	-0.75861900	2.12906100	-0.98573000
	C	3.56280000	-0.00679400	-0.56845000
	H	4.48585600	-0.18874100	-0.01138100

H	3.61928200	-0.53022700	-1.52450300
H	3.47356100	1.06462600	-0.75595100

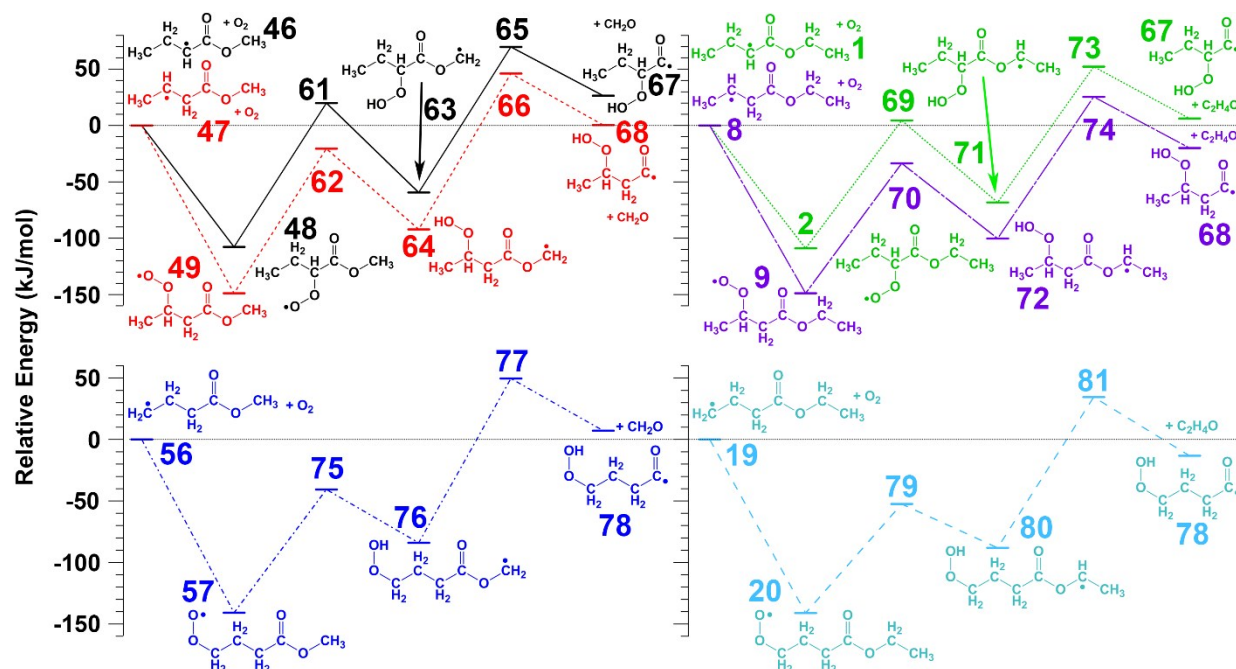


Figure S12. PES of the reaction of R_β , γ , or δ with O_2 , where the peroxy radical abstracts a hydrogen atom from C_m . The numbers correspond with the energies and geometries listed in the supporting information.

Table S11. Calculated 0 K CBS-QB3 energies for the structures in Figure S11.

Species	Energy (Hartrees)
61	-495.937614
62	-495.945610
63	-495.967854
64	-495.972898
65	-495.918681
66	-495.920169
67	-381.590953
68	-381.593456
69	-535.174031
70	-535.181074
71	-535.201790
72	-535.206445
73	-535.155889
74	-535.158617

75	-495.949112
76	-495.965605
77	-495.914710
78	-381.586707
79	-535.184128
80	-535.197730
81	-535.150967

Table S12. Optimized geometries for the structures in Figure S11.

Species	Optimized coordinates (Å)			
61	C	0.61871900	1.06006800	-0.16824500
	O	0.42866100	2.21933500	-0.39563100
	O	1.90787000	0.67406200	0.11728900
	C	2.28356600	-0.57086600	0.60587500
	H	1.81710100	-0.85273200	1.55072700
	H	1.67536000	-1.48380500	-0.18590200
	H	3.36477600	-0.65910900	0.55597300
	C	-0.53524400	0.04501000	-0.30670700
	C	-1.77395700	0.52084900	0.46021200
	H	-1.56165800	0.45529200	1.53259400
	C	-3.02974400	-0.28173200	0.11478700
	H	-3.88549100	0.08682000	0.68513800
	H	-3.27298700	-0.19119600	-0.94800500
	H	-2.89904600	-1.34083800	0.34201600
	H	-1.91012300	1.57751500	0.22508400
	H	-0.74894000	0.00725900	-1.38196300
	O	-0.27433200	-1.28615400	0.14345500
	O	0.69292100	-1.88714000	-0.69151200
62	C	0.96827500	-1.02751500	-0.00877500
	O	1.65068900	-1.47376300	-0.87857200
	O	1.41561300	-0.03263400	0.85933600
	C	1.99674200	1.08327200	0.27213700
	H	0.85044700	1.76613500	-0.10326500
	H	2.50462300	1.68429600	1.02018200
	H	2.53832500	0.87720600	-0.65006500
	C	-1.30149800	-0.06309100	0.32049700
	H	-1.11063800	0.48371900	1.24296500
	C	-2.78915600	-0.29847100	0.11713300
	H	-3.32952300	0.64788200	0.17422400
	H	-2.97627500	-0.74458500	-0.86271500
	H	-3.18185000	-0.97266700	0.88383500
	O	-0.29079400	1.99548700	-0.27773900
	O	-0.81879000	0.78632600	-0.76527800
	C	-0.47179800	-1.36511200	0.29824600

	H	-0.54382100	-1.86502600	1.26939700
	H	-0.82041800	-2.05476900	-0.47196600
63	C	3.07988600	0.50840300	-0.18895400
	H	3.25429600	-0.51142500	-0.53472400
	H	3.34376900	0.55641000	0.87160400
	H	3.75452200	1.17462300	-0.73184300
	C	1.62471300	0.92348300	-0.41201200
	H	1.44970500	1.93936600	-0.05011300
	H	1.38354300	0.91540300	-1.48011100
	C	0.62580700	0.00814700	0.31066500
	H	0.89579200	-0.07762800	1.37000900
	C	-0.77878600	0.60928500	0.26869500
	O	-1.07343200	1.67093500	0.74247100
	O	-1.67760800	-0.20270200	-0.38069400
	C	-2.97428500	0.22330200	-0.48640900
	H	-3.22128800	1.21126100	-0.13426200
	H	-3.59504900	-0.42104300	-1.08511200
	O	0.72154500	-1.26309500	-0.30571300
	O	0.04271400	-2.22968900	0.53174700
	H	-0.83505100	-2.22628100	0.12015200
64	C	2.45805900	1.35541900	0.14587300
	H	2.38828700	2.14580000	0.89879200
	H	2.48489200	1.81496800	-0.84568000
	H	3.39156000	0.81359400	0.30160000
	C	1.28436800	0.39299400	0.26206200
	H	1.22949700	-0.03561000	1.26746400
	C	-0.06105000	1.02463300	-0.08360300
	H	-0.10751300	1.27868600	-1.14454000
	H	-0.17650400	1.95999000	0.47536400
	C	-1.22331200	0.12732700	0.27646700
	O	-1.24611800	-0.69183000	1.15495300
	O	-2.30106500	0.39558000	-0.52717400
	C	-3.46768600	-0.27798600	-0.30024200
	H	-4.23733300	-0.06819000	-1.02300700
	H	-3.48059300	-1.05401200	0.44737700
	O	1.39816000	-0.68884200	-0.67817000
	O	2.47418600	-1.55299900	-0.23926200
	H	1.96413600	-2.28482000	0.13651900
65	C	-3.21631800	-0.20016800	0.22188900
	H	-3.30734000	0.81992500	-0.15320400
	H	-3.25974900	-0.16573300	1.31427500
	H	-4.07705000	-0.77432800	-0.12967200
	C	-1.91479600	-0.84388200	-0.25944600

	H	-1.81421400	-1.86025100	0.13102500
	H	-1.90714600	-0.91916400	-1.35117300
	C	-0.67357200	-0.05200100	0.17364700
	H	-0.67442600	0.12679800	1.25620000
	C	0.58407300	-0.85954500	-0.15659300
	O	0.89043500	-1.96802100	0.09240700
	O	2.09251100	0.38398400	-0.00114900
	C	3.22688900	-0.13872400	0.04588000
	H	3.38831500	-1.06830700	0.60149700
	H	4.05367100	0.28290100	-0.53404400
	O	-0.70253700	1.18833100	-0.50350300
	O	0.04521300	2.16770300	0.25308000
	H	0.95531500	1.94810800	-0.01384300
66	C	-2.01166000	1.68751700	-0.27461900
	H	-1.46790100	2.52091500	-0.72798900
	H	-2.38051200	1.99867000	0.70635000
	H	-2.86832900	1.44861600	-0.90670700
	C	-1.11398800	0.46334000	-0.14522700
	H	-0.71535200	0.17835000	-1.12506600
	C	0.04359000	0.67349600	0.84607800
	H	-0.34790100	0.59253100	1.86607200
	H	0.47487800	1.66707000	0.73080600
	C	1.14687300	-0.33673400	0.71318700
	O	1.16385800	-1.47408500	0.39194400
	O	2.54353000	0.67923800	-0.16076300
	C	3.40782500	0.00394000	-0.74615200
	H	4.45374800	0.32957600	-0.74874000
	H	3.15255800	-0.95829500	-1.20624400
	O	-1.82949700	-0.65562600	0.39120800
	O	-2.73116400	-1.14163200	-0.63641400
	H	-2.31084400	-1.98994400	-0.83589100
67	C	2.49194800	-0.01645500	0.19160300
	H	2.51587300	-1.04801800	-0.16172600
	H	2.54708800	-0.03123400	1.28376200
	H	3.38210200	0.49540500	-0.18216500
	C	1.22681800	0.70136700	-0.28701300
	H	1.20990700	1.73530400	0.06841600
	H	1.19879800	0.73757400	-1.38024400
	C	-0.06011300	0.03495100	0.20837200
	H	-0.07532500	-0.05077600	1.30316200
	C	-1.30516500	0.87265500	-0.17055300
	O	-1.50517400	1.99506700	0.12752400
	O	-0.12425200	-1.25053000	-0.37420400
	O	-1.24112000	-1.94709900	0.22690500

	H	-1.93499900	-1.77287300	-0.42745700
68	C	1.54281200	1.41927300	-0.31255800
	H	1.74827900	1.84580200	0.67275900
	H	1.30950500	2.23112900	-1.00731000
	H	2.44282000	0.91308400	-0.66453800
	C	0.39364900	0.42249400	-0.23818500
	H	0.16107700	0.02510300	-1.23207200
	C	-0.87860100	1.00949500	0.38305500
	H	-0.73942700	1.18698300	1.45339400
	H	-1.11458100	1.98218100	-0.06103000
	C	-2.11843600	0.14585100	0.20448700
	O	-2.24639400	-0.81594300	-0.46824300
	O	0.70951900	-0.68039700	0.62266900
	O	1.70985800	-1.49207700	-0.04181900
	H	1.17191500	-2.25962800	-0.28285700
69	C	0.09024600	1.15045800	-0.21920400
	O	-0.22685300	2.28653000	-0.42796600
	O	1.41650700	0.89646700	0.02157200
	C	1.96035200	-0.32764200	0.43767400
	H	1.53522300	-0.67823400	1.38199000
	H	1.39351700	-1.24778800	-0.34846600
	C	-0.96762700	0.03126600	-0.31605000
	C	-2.19358600	0.36768200	0.54051300
	H	-1.90515100	0.30515900	1.59525000
	C	-3.38447700	-0.55056000	0.25867700
	H	-4.23246900	-0.27964200	0.89202600
	H	-3.70616400	-0.46689700	-0.78365100
	H	-3.13469200	-1.59499000	0.45154100
	H	-2.44865100	1.40922100	0.33936100
	H	-1.24624200	-0.00105500	-1.37637800
	O	-0.55179500	-1.27700900	0.07676500
	O	0.42387300	-1.75028100	-0.82658700
	C	3.45268500	-0.30548400	0.32865700
	H	3.87355300	0.45838400	0.99364900
	H	3.86631200	-1.27501000	0.61352900
	H	3.76535300	-0.06912000	-0.69071700
70	C	-0.21829000	1.39595000	-0.01257300
	O	-0.57362200	2.15100400	-0.86599300
	O	-1.09128600	0.52590600	0.62961100
	C	-1.91496700	-0.25440900	-0.19221400
	H	-0.99899200	-1.20152700	-0.56094700
	H	-2.16863800	0.24952700	-1.12623600
	C	1.55002600	-0.31581100	0.38224500

	H	1.05729100	-0.87349400	1.17768500
	C	3.04911800	-0.56901600	0.37924000
	H	3.24860800	-1.64106700	0.33696100
	H	3.51526000	-0.09664900	-0.48902800
	H	3.51206600	-0.16194900	1.28292300
	O	0.02430200	-1.80768300	-0.64570900
	O	1.00196000	-0.82159800	-0.87196500
	C	1.19122000	1.18218300	0.48828500
	H	1.27396300	1.50678500	1.53053200
	H	1.85454100	1.79959500	-0.11930500
	C	-3.02919500	-0.90073500	0.57178200
	H	-3.73174500	-0.14554900	0.94461300
	H	-3.57752900	-1.58918700	-0.07454700
	H	-2.64313100	-1.45649000	1.42920300
71	C	3.48982300	-0.25717800	-0.49164200
	H	3.88320600	-0.33727400	0.52600400
	H	3.53368700	0.79155800	-0.78906100
	H	4.14850600	-0.82814800	-1.15041300
	C	2.05896600	-0.79174300	-0.57058900
	H	1.69155000	-0.75117600	-1.60140200
	H	2.01502400	-1.83652700	-0.25454000
	C	1.07962900	-0.01028400	0.31626400
	H	1.46936700	0.05169500	1.33949200
	C	-0.26286900	-0.73814600	0.40590400
	O	-0.39209500	-1.85732200	0.82116800
	O	-1.30602800	0.02974900	-0.04000400
	C	-2.58177800	-0.50072100	0.00014800
	H	-2.64608600	-1.55112500	0.24217200
	C	-3.60801000	0.28793600	-0.71620100
	H	-3.43765500	0.30067900	-1.80385000
	H	-4.59695200	-0.13839000	-0.53840400
	H	-3.62109400	1.33218100	-0.38419300
	O	0.98777400	1.29293500	-0.23221200
	O	0.34601200	2.15560700	0.73691100
	H	-0.57942600	2.05958300	0.46397700
72	C	2.93538500	1.37838400	0.01793000
	H	2.92890600	2.15142500	0.79180800
	H	2.86092600	1.85951000	-0.96090800
	H	3.88618100	0.84683400	0.07086900
	C	1.79003800	0.39710400	0.22446800
	H	1.83720100	-0.05381300	1.22038800
	C	0.40923300	1.01566700	0.02517900
	H	0.25709300	1.29209200	-1.02005300
	H	0.33846800	1.93604700	0.61551800

	C	-0.70066100	0.09092600	0.47605400
	O	-0.62381600	-0.73069700	1.35124300
	O	-1.84431600	0.33478700	-0.22973100
	C	-2.97444100	-0.40042500	0.05741700
	H	-2.92746900	-1.02073400	0.94028300
	O	1.82668600	-0.66270400	-0.74671600
	O	2.94847400	-1.52244600	-0.43045400
	H	2.48402200	-2.26665100	-0.02135600
	C	-4.20930600	0.07060100	-0.60712900
	H	-5.01352900	-0.65329900	-0.46173300
	H	-4.55505200	1.03829500	-0.21017200
	H	-4.05445800	0.20522500	-1.68289800
73	C	-3.67292400	-0.09674900	-0.07310300
	H	-3.78290700	-0.08403700	-1.16137300
	H	-3.69866200	0.93435800	0.28161800
	H	-4.53298000	-0.62624700	0.34423500
	C	-2.37039000	-0.78256700	0.34257600
	H	-2.29938900	-0.83808800	1.43333600
	H	-2.33276700	-1.80927900	-0.03148000
	C	-1.12762500	-0.05039300	-0.17990700
	H	-1.19291900	0.10967500	-1.26370400
	C	0.11206400	-0.90256900	0.09815900
	O	0.35537600	-2.02360200	-0.18872200
	O	1.58594100	0.24446100	-0.12279600
	C	2.69790200	-0.32098600	-0.28764100
	H	2.72004400	-1.27476600	-0.82663200
	C	3.95167400	0.18661100	0.34141800
	H	4.28136300	-0.49723900	1.13606300
	H	4.76316700	0.22824200	-0.39229200
	H	3.79634600	1.17611500	0.77241100
	O	-1.07304100	1.20671400	0.46949200
	O	-0.34762000	2.14563300	-0.35703300
	H	0.56924400	1.89554300	-0.14870900
74	C	-3.12838200	-0.50598800	-0.71956500
	H	-3.55126900	-1.49028600	-0.49922100
	H	-2.97543400	-0.42207500	-1.79881600
	H	-3.84685000	0.25466800	-0.41115400
	C	-1.81524900	-0.30475600	0.02474700
	H	-1.95784800	-0.43266600	1.10381600
	C	-0.70388500	-1.25620800	-0.44362700
	H	-0.42627900	-1.04913100	-1.47739300
	H	-1.08529700	-2.28130000	-0.39628300
	C	0.52858300	-1.20769800	0.42220800
	O	0.63900500	-0.99932000	1.59097700

	O	1.72824800	-0.24039000	-0.59071200
	C	2.60290800	0.36705700	0.05734200
	H	2.38986900	0.63163900	1.10092800
	O	-1.27832500	1.00721100	-0.20209100
	O	-2.14651500	1.96286700	0.45956400
	H	-1.60653800	2.17803300	1.23306400
	C	3.95174400	0.66383800	-0.50793900
	H	4.17305600	1.73354400	-0.42684200
	H	4.72812100	0.13871400	0.06392700
	H	4.00484500	0.35844700	-1.55292600
75	C	-0.42655100	-1.25548600	0.07794500
	O	-0.92843100	-1.62413200	1.09881800
	O	-1.07960100	-0.44474300	-0.83985600
	C	-2.09361500	0.38005700	-0.37759400
	H	-2.73756700	0.68334300	-1.19740800
	H	-2.56788200	0.03870100	0.53980400
	H	-1.35026300	1.50366700	-0.02211700
	C	1.96784700	-0.43780900	-0.00493100
	H	2.16540100	-0.51396100	1.06830500
	C	1.50186800	0.98489800	-0.30085500
	H	2.32994700	1.69649300	-0.21676500
	H	1.04680900	1.07933200	-1.28791800
	H	2.91826500	-0.61697800	-0.51616400
	O	0.51280300	1.30385000	0.69983000
	O	-0.44581700	2.20261500	0.20604100
	C	0.96699800	-1.54592200	-0.42255600
	H	0.93794400	-1.62344800	-1.51165800
	H	1.28642700	-2.50229900	-0.00681400
76	C	2.03860300	-0.45260400	0.02291000
	H	2.11443600	-1.14421900	-0.82471000
	H	2.12372800	-1.03167400	0.95206200
	C	0.73737300	0.33827500	-0.02280800
	H	0.70296300	1.03657100	0.81668500
	H	0.71485300	0.94166800	-0.93330900
	C	-0.47841100	-0.58674400	0.02061400
	H	-0.48533300	-1.28076400	-0.82672500
	H	-0.46904500	-1.21724400	0.91725500
	C	-1.78623500	0.16787900	0.01046500
	O	-1.93100700	1.35939200	0.01899500
	O	-2.83765800	-0.71656000	-0.00595900
	C	-4.10941000	-0.21680100	0.00501500
	H	-4.87321900	-0.97040900	-0.08057500
	H	-4.24735900	0.85057200	-0.04870200
	O	3.08953800	0.50373300	-0.04879100

	O	4.33536400	-0.24465500	-0.07794800
	H	4.75757100	0.10019200	0.72047000
77	C	-1.99101900	0.07242000	0.42896000
	H	-2.31924700	1.00832600	0.89622500
	H	-2.00182300	-0.71994500	1.18874500
	C	-0.60912100	0.22315100	-0.19468300
	H	-0.33133600	-0.71108600	-0.68987900
	H	-0.63595000	1.00345100	-0.95856600
	C	0.45005500	0.57281100	0.86726600
	H	0.18610100	1.50687000	1.37679200
	H	0.53318400	-0.20747100	1.62441900
	C	1.81153600	0.80377300	0.27338800
	O	2.15942300	1.37326300	-0.70452200
	O	2.63399500	-0.93217200	0.42843300
	C	3.56034900	-1.14812600	-0.37018500
	H	4.40983800	-1.77157400	-0.07127900
	H	3.57445000	-0.66789500	-1.35590400
	O	-2.87461800	-0.26438700	-0.63499700
	O	-4.21046600	-0.34085400	-0.06491000
	H	-4.41268500	-1.27165200	-0.23106900
78	C	-1.08586800	0.45628100	0.01243900
	H	-1.23499900	1.10932300	-0.85567400
	H	-1.23553000	1.04933300	0.92422900
	C	0.29479400	-0.18786600	-0.01167200
	H	0.40347500	-0.85335300	0.84845100
	H	0.38815200	-0.80735800	-0.90687800
	C	1.40845300	0.86816900	0.00713200
	H	1.34678900	1.51619500	0.88887200
	H	1.35076300	1.54159900	-0.85524700
	C	2.81424000	0.28930500	0.00501300
	O	3.13499000	-0.84687800	0.00379200
	O	-2.02398300	-0.61249500	-0.02958100
	O	-3.34559500	-0.00709000	-0.07993100
	H	-3.73166300	-0.37936200	0.72452900
79	C	0.25872600	-1.32649800	0.17804800
	O	0.10322200	-1.80833900	1.26271800
	O	-0.75146100	-0.69702500	-0.52767300
	C	-1.81037300	-0.12858600	0.18710800
	H	-1.92512000	-0.56494300	1.17911800
	H	-1.26939600	1.10754000	0.43647100
	C	2.32688200	0.03126400	-0.35865500
	H	2.76187400	-0.00642100	0.64436300
	C	1.49934400	1.30891900	-0.46799100

	H	2.14438600	2.19226100	-0.52451700
	H	0.82948200	1.29981900	-1.32913400
	H	3.16082900	0.08358200	-1.06490500
	O	0.70858100	1.38961700	0.73537100
	O	-0.52251300	2.02209200	0.49861600
	C	1.53634700	-1.27508600	-0.62494200
	H	1.28636200	-1.34348700	-1.68600700
	H	2.14799500	-2.13469800	-0.34790500
	C	-3.03893000	0.03743200	-0.65538400
	H	-3.46255400	-0.93880600	-0.92189500
	H	-3.79742100	0.59897400	-0.10591200
	H	-2.81104500	0.57076100	-1.58103100
80	C	-2.42932000	-0.20269500	0.31146900
	H	-2.48004500	0.08280700	1.36872700
	H	-2.83537600	-1.21680100	0.20338600
	C	-1.00059400	-0.11829900	-0.21197100
	H	-0.99314200	-0.37406700	-1.27572800
	H	-0.64533200	0.91000500	-0.11914100
	C	-0.06536500	-1.06633600	0.55977800
	H	-0.05941700	-0.79290400	1.61986100
	H	-0.40053600	-2.10092900	0.47235900
	C	1.35532900	-1.02117400	0.04847800
	O	1.93917100	-1.91308100	-0.50682700
	O	1.91536600	0.20535700	0.29580300
	C	3.21969500	0.43197700	-0.08778000
	H	3.66877100	-0.32628600	-0.71254300
	O	-3.19323800	0.71188100	-0.46683300
	O	-4.54223700	0.69961400	0.07312400
	H	-5.02909900	0.36391400	-0.69189600
	C	3.66480900	1.83901500	0.01880700
	H	3.43116300	2.25574000	1.00416700
	H	4.74346700	1.90450400	-0.13714800
	H	3.17973400	2.48892500	-0.72684800
81	C	2.46427200	0.26078900	0.23661700
	H	2.47581800	0.16391400	1.32869500
	H	2.93088700	1.21795900	-0.03207600
	C	1.04645200	0.15709200	-0.31101500
	H	1.07448800	0.21705100	-1.40265500
	H	0.62714500	-0.81578400	-0.05237100
	C	0.15065200	1.26742000	0.24403800
	H	0.11143900	1.23119000	1.34027500
	H	0.53374900	2.25783300	-0.02498900
	C	-1.26899500	1.23468400	-0.26744300
	O	-2.13629200	2.04316700	-0.18704500

O	-1.85341400	-0.47785400	0.15850200
C	-3.09279100	-0.60013800	0.27339000
H	-3.68080000	0.27675800	0.57186700
O	3.19659100	-0.81374200	-0.34347200
O	4.53135800	-0.77269400	0.23022100
H	5.05334600	-0.60329100	-0.56575400
C	-3.80468700	-1.86108900	-0.08856400
H	-3.09107900	-2.65206200	-0.31972200
H	-4.45833500	-2.18237400	0.72926900
H	-4.45202100	-1.69476700	-0.96033200

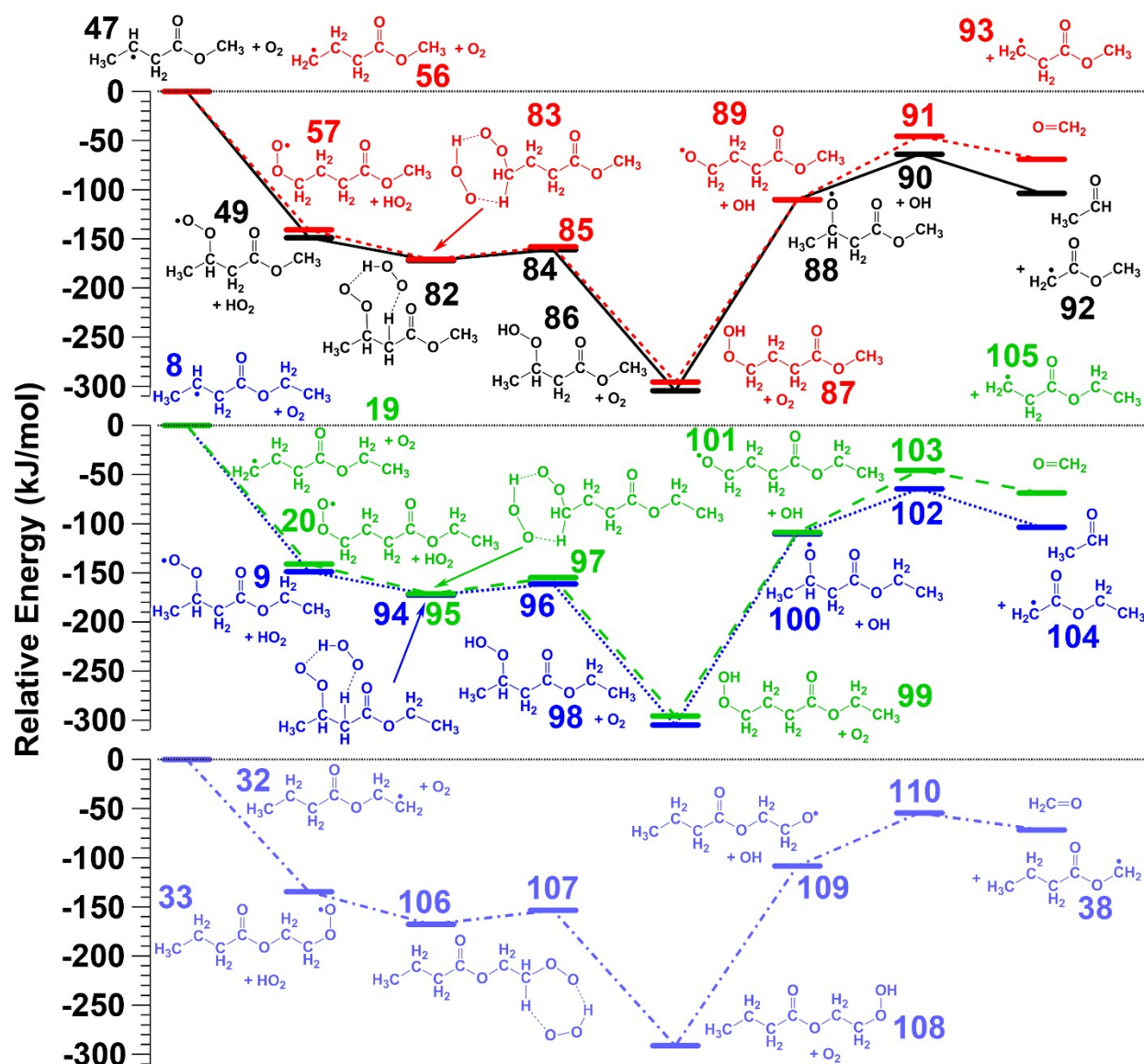


Figure S13. PES of the reactions of $R_\gamma O_2$, $R_\delta O_2$, and $R_\epsilon O_2$ with HO_2 . The top shows $R_\gamma O_2$ and $R_\delta O_2$ for MB, middle shows $R_\gamma O_2$ and $R_\delta O_2$ for EB, and the bottom shows $R_\epsilon O_2$ for EB. The numbers correspond with the energies and geometries listed in the supporting information.

Table S13. Calculated 0 K CBS-QB3 energies for the structures in Figure S12.

Species	Energy (Hartrees)
82 (triplet state)	-646.744378
83 (triplet state)	-646.739843
84 (triplet state)	-646.740238
85 (triplet state)	-646.734876
86	-496.630330
87	-496.622683

88	-420.906520
89	-420.902387
90	-420.888872
91	-420.877750
92	-267.321558
93	-306.542474
94 (triplet state)	-685.975146
95 (triplet state)	-685.970484
96 (triplet state)	-685.970890
97 (triplet state)	-685.964246
98	-535.860862
99	-535.853326
100	-460.137086
101	-460.132475
102	-460.119623
103	-460.108242
104	-306.552030
105	-345.773012
106 (triplet state)	-685.966976
107 (triplet state)	-685.961575
108	-535.849427
109	-460.130095
110	-460.109534

Table S14. Optimized geometries for the structures in Figure S12.

Species	Optimized coordinates (Å)			
82 (triplet state)	C	1.79820900	-1.61911900	-1.08824600
	H	2.44030100	-0.73943100	-1.03727200
	H	1.58807200	-1.82439100	-2.14048400
	H	2.33435600	-2.47510600	-0.67450900
	C	0.48843000	-1.40520100	-0.34943100
	H	-0.15490800	-2.28325600	-0.40760000
	C	-0.29173100	-0.16753500	-0.76569300
	H	-0.35235800	-0.14837900	-1.85966400
	H	0.22204000	0.75089500	-0.47612600
	C	-1.71545200	-0.18024200	-0.23882500
	O	-2.33312300	-1.17164200	0.06064700
	O	-2.21366100	1.06487600	-0.17995200
	C	-3.58130300	1.17435700	0.26368300
	H	-3.80484000	2.23820100	0.24984000
	H	-4.24490600	0.63127700	-0.41059200
	H	-3.68596200	0.77059000	1.27132700
	O	0.73475300	-1.36848700	1.12115800
	O	1.50866400	-0.38950800	1.52203100
	O	3.02575400	1.57574300	0.23816400

	O	2.14767300	2.21560000	-0.52643000
	H	2.50880300	0.85338300	0.67121500
83 (triplet state)	C	1.41479200	0.90368800	1.01062300
	H	1.17947700	1.60978500	1.80893800
	C	0.25617000	-0.02410700	0.68647100
	H	0.11443200	-0.68869200	1.54331200
	H	0.53685600	-0.67190900	-0.14765800
	O	1.71575400	1.79081600	-0.12520800
	O	2.37662600	1.18914500	-1.08788000
	O	3.45079900	-1.38758700	-0.82598600
	O	3.61809200	-1.48470200	0.48678900
	H	3.04508200	-0.49592400	-0.96777000
	C	-4.47021400	-0.36327300	-0.51477700
	H	-4.76393800	-0.90634200	0.38464900
	H	-5.24522300	0.34075700	-0.80836800
	H	-4.27630500	-1.07841500	-1.31533200
	H	2.32660700	0.35020000	1.23875000
	C	-1.04636100	0.71187100	0.37335300
	H	-0.94073200	1.36096500	-0.50009700
	H	-1.33713700	1.37017400	1.20012100
	C	-2.19913000	-0.23869400	0.12205200
	O	-2.15778600	-1.43633100	0.25010700
	O	-3.29981700	0.43771900	-0.26068200
84 (triplet state)	C	-1.47635200	1.84542800	-0.59649800
	H	-1.80422800	1.33067900	-1.50149200
	H	-1.11316800	2.84153900	-0.86080700
	H	-2.32875400	1.95965300	0.07345000
	C	-0.37242000	1.06711500	0.09880800
	H	-0.03950600	1.56218100	1.01270200
	C	0.81800800	0.73524000	-0.78697200
	H	1.13857400	1.64582400	-1.30370300
	H	0.53774000	0.01170200	-1.55455200
	C	2.00858000	0.22356500	0.00485900
	O	2.26602800	0.53576400	1.13981100
	O	2.76369000	-0.60070600	-0.74094900
	C	3.94891200	-1.11492300	-0.10049900
	H	4.42414000	-1.75308500	-0.84148000
	H	4.61150600	-0.29759300	0.18737900
	H	3.68061300	-1.68804300	0.78766300
	O	-0.87021000	-0.25359700	0.52693900
	O	-1.83142600	-0.14874800	1.45028400
	H	-2.94620200	-0.73867900	0.78972500
	O	-3.67741900	-1.08461300	0.11323100
	O	-3.11580000	-1.12469200	-1.05270000

85 (triplet state)	C	1.23752400	-0.66604700	1.05035100
	H	1.10702100	-1.70025000	1.38025400
	H	1.97009300	-0.16890200	1.68704400
	C	-0.06649000	0.10112900	0.96604100
	H	-0.45162100	0.22620500	1.98151000
	H	0.13584400	1.10694200	0.58938700
	C	-1.12193300	-0.58581400	0.09795000
	H	-1.28618000	-1.61924600	0.42684900
	H	-0.80585100	-0.65062100	-0.94556900
	C	-2.46176400	0.11896200	0.15595900
	O	-2.76562400	0.97924300	0.94398900
	O	-3.29435900	-0.35763000	-0.79037500
	C	-4.61435000	0.21873900	-0.81084900
	H	-5.13537300	-0.27850700	-1.62561700
	H	-5.12393500	0.04086800	0.13731800
	H	-4.55835100	1.29351400	-0.98878800
	O	1.80749200	-0.72049000	-0.29477100
	O	2.98363700	-1.34649600	-0.30156400
	O	4.37294800	0.71797200	-0.59884100
	O	3.44431400	1.58223000	-0.31192900
	H	3.92318800	-0.21045300	-0.57117200
86	C	2.53164900	-1.33254800	0.12990800
	H	2.57590600	-1.77362000	-0.86945400
	H	2.47107400	-2.13779200	0.86778100
	H	3.45304300	-0.77541800	0.30351100
	C	1.33783200	-0.39603300	0.25330300
	H	1.26516200	0.01293700	1.26566900
	C	0.00726000	-1.04440300	-0.11413500
	H	-0.09731000	-1.99023300	0.42818100
	H	-0.02690900	-1.28084700	-1.17959800
	C	-1.17735600	-0.17096700	0.25262900
	O	-1.20055300	0.63227800	1.15151800
	O	-2.23218400	-0.43093400	-0.54375400
	C	-3.43046200	0.31478900	-0.25766900
	H	-4.16413900	-0.02427800	-0.98531500
	H	-3.77359400	0.11305900	0.75818300
	H	-3.24741000	1.38471000	-0.36587900
	O	1.44039500	0.70630600	-0.66522800
	O	2.48907600	1.58731800	-0.19480600
	H	1.95678100	2.28670800	0.21086500
87	C	-2.10309600	-0.45036700	0.02326400
	H	-2.19310600	-1.02503400	0.95473600
	H	-2.18552000	-1.14480000	-0.82144500

	C	-0.79472300	0.32822000	-0.02576900
	H	-0.76709200	0.92876100	-0.93803500
	H	-0.75291500	1.02940700	0.81092800
	C	0.41269700	-0.60735200	0.01997300
	H	0.41446500	-1.30192800	-0.82651500
	H	0.39672500	-1.23622300	0.91729600
	C	1.73323600	0.13493500	0.01076400
	O	1.87027500	1.33170200	0.02270400
	O	2.76602900	-0.73504300	-0.00817300
	C	4.07898400	-0.14487100	-0.01069800
	H	4.77391000	-0.98144400	-0.02381900
	H	4.21519400	0.48167000	-0.89349100
	H	4.22698100	0.46384700	0.88263600
	O	-3.14678400	0.51433800	-0.05169000
	O	-4.39944100	-0.22320200	-0.07493300
	H	-4.81186600	0.12000900	0.72924500
88	C	3.03822200	-0.47112500	0.18571100
	H	3.20231600	-1.15316800	-0.65284900
	H	3.11929700	-1.04112300	1.11463700
	H	3.81969300	0.28972100	0.16688700
	C	1.66117500	0.19900900	0.06373700
	H	1.51549900	0.87110700	0.93758800
	C	0.48180200	-0.79628400	0.07441400
	H	0.61072200	-1.51693300	0.88945400
	H	0.45041000	-1.35493700	-0.86228200
	C	-0.83462400	-0.08468300	0.30526600
	O	-0.99673300	0.80981800	1.09821600
	O	-1.81584600	-0.58981300	-0.46435300
	C	-3.11462000	0.01007100	-0.29225500
	H	-3.76942700	-0.51195600	-0.98602700
	H	-3.46084100	-0.11672300	0.73453700
	H	-3.07440000	1.07457400	-0.52629500
	O	1.58695500	1.06968400	-0.98847400
89	C	1.42146200	0.31388000	-0.00019700
	H	1.39661600	0.96829200	-0.87524900
	H	1.39640600	0.96906400	0.87427100
	C	0.20291800	-0.60693600	0.00011500
	H	0.20254100	-1.27075000	0.87240000
	H	0.20239300	-1.27119900	-0.87182100
	C	-1.11319900	0.14351600	0.00007900
	O	-1.24214100	1.34110300	0.00025500
	O	-2.15181700	-0.71984700	-0.00014300
	C	-3.46102900	-0.12093800	-0.00012500
	H	-3.59887300	0.49775700	-0.88818000

	H	-4.16149300	-0.95297300	-0.00029200
	H	-3.59897400	0.49748600	0.88810300
	C	2.73752800	-0.46657200	0.00030000
	H	2.80239100	-1.15682900	-0.86639400
	H	2.80221400	-1.15632100	0.86737500
	O	3.87279500	0.29096500	-0.00026700
90	C	3.08193100	0.08263600	0.20622500
	H	3.16604800	-0.46882400	1.14405900
	H	3.25149500	1.14771900	0.37767300
	H	3.86668200	-0.27767900	-0.46784200
	C	1.74291100	-0.19576300	-0.45745900
	H	1.47228700	0.49433000	-1.27919000
	C	0.41301100	0.77468200	0.77444100
	H	0.84850800	1.76224800	0.68596500
	H	0.57206900	0.23478200	1.69888700
	C	-0.88463300	0.59970000	0.09304500
	O	-1.24030800	1.24668200	-0.86657900
	O	-1.60866400	-0.38564300	0.65444400
	C	-2.84418600	-0.70312000	-0.01070200
	H	-3.29664900	-1.49553400	0.58070000
	H	-3.49532400	0.17141600	-0.04960200
	H	-2.64487900	-1.04804500	-1.02643700
	O	1.24966700	-1.34469300	-0.45005500
91	C	1.27828400	0.53439900	-0.00008400
	H	1.47238500	1.08422000	-0.91281600
	H	1.47233000	1.08426700	0.91263200
	C	0.16930500	-0.46892300	-0.00008600
	H	0.21379200	-1.12380000	0.87609600
	H	0.21374300	-1.12374800	-0.87630800
	C	-1.21150200	0.18446600	-0.00002300
	O	-1.42822500	1.36808400	-0.00000100
	O	-2.17171600	-0.76038300	0.00000600
	C	-3.52842900	-0.27270200	0.00007000
	H	-3.71587100	0.33156100	-0.88851300
	H	-4.15540500	-1.16114800	0.00005200
	H	-3.71581300	0.33148300	0.88871800
	C	3.14260000	-0.61976300	-0.00000100
	H	2.83224200	-1.12972900	-0.93318400
	H	2.83210100	-1.12984600	0.93307000
	O	4.03106100	0.22878400	0.00012000
92	C	1.78673200	-0.58191600	0.00000000
	H	1.81860000	-1.66238600	0.00000300
	H	2.69730400	-0.00064800	-0.00000200

	C	0.52561800	0.12610800	0.00000000
	O	0.40808600	1.33674400	0.00000000
	O	-0.53269900	-0.72708600	0.00000000
	C	-1.82458200	-0.10112900	0.00000000
	H	-2.54442300	-0.91675200	-0.00000400
	H	-1.95059600	0.52206700	0.88749100
	H	-1.95059300	0.52207400	-0.88748600
93	C	2.52308000	0.10499500	0.00022800
	H	3.48822800	-0.38377200	0.00084000
	H	2.46926100	1.18440200	0.00041600
	C	1.28212700	-0.71043900	-0.00017800
	H	1.23578800	-1.38795000	0.86580500
	H	1.23625000	-1.38779100	-0.86625100
	C	0.00579500	0.10915900	-0.00021800
	O	-0.06454600	1.31250800	-0.00018800
	O	-1.07593500	-0.70007900	-0.00013000
	C	-2.35739800	-0.04344600	0.00027400
	H	-2.46751600	0.57845000	-0.88913900
	H	-3.09354300	-0.84419600	0.00137300
	H	-2.46623600	0.57982400	0.88886200
94 (triplet state)	C	2.54786800	-1.29918700	-1.02447200
	H	2.94995900	-0.28612900	-0.99550400
	H	2.41647800	-1.58139600	-2.07165100
	H	3.27170600	-1.98192100	-0.57578400
	C	1.21139900	-1.39658000	-0.30924800
	H	0.80764000	-2.40846000	-0.34564800
	C	0.15614100	-0.40549800	-0.77576500
	H	0.11534700	-0.43416500	-1.87047200
	H	0.41872600	0.62004900	-0.51010800
	C	-1.23095600	-0.75897700	-0.26711100
	O	-1.58582500	-1.86779700	0.04889800
	O	-2.02226900	0.32360700	-0.24658200
	C	-3.39587500	0.11277300	0.17660100
	H	-3.85762700	-0.61621700	-0.49321200
	H	-3.38603500	-0.31574400	1.18098600
	O	1.41155200	-1.25647000	1.16227900
	O	1.90937500	-0.10417900	1.53965300
	O	2.91277700	2.13883700	0.20975100
	O	1.91679600	2.52275500	-0.58127700
	H	2.58278600	1.32241200	0.65842300
	C	-4.09397900	1.45561000	0.13214400
	H	-4.08145900	1.86852800	-0.87871900
	H	-5.13506300	1.34144200	0.44494500
	H	-3.60928900	2.16872500	0.80205900

95 (triplet state)	C	1.91398900	0.84284500	1.05812800
	H	1.69451300	1.48220500	1.91505400
	C	0.77437400	-0.10523600	0.72583900
	H	0.69897700	-0.83118600	1.54017200
	H	1.03628200	-0.68388200	-0.16352200
	O	2.12441300	1.81785900	-0.02498200
	O	2.75620700	1.31097800	-1.05906400
	O	3.93469800	-1.23217200	-1.03405300
	O	4.17606000	-1.41266100	0.25824300
	H	3.48974900	-0.34977600	-1.09126600
	C	-4.00595900	-0.55031400	-0.27187100
	H	-4.20656200	-1.14062800	0.62516800
	H	-3.78323600	-1.24546600	-1.08437800
	H	2.85578800	0.31160900	1.20181600
	C	-0.56801600	0.59811100	0.52673500
	H	-0.53393100	1.30095600	-0.30982800
	H	-0.83442400	1.19495200	1.40691300
	C	-1.70055100	-0.37990200	0.28319700
	O	-1.61340200	-1.57942800	0.36784400
	O	-2.83489100	0.27264900	-0.03282300
	C	-5.15165200	0.37966300	-0.61255900
	H	-6.05777300	-0.20198700	-0.80054200
	H	-5.35083700	1.07047200	0.20953400
	H	-4.92634300	0.96393600	-1.50726100
96 (triplet state)	C	-2.07325700	1.55276700	-1.06713300
	H	-2.26436000	0.79306400	-1.82737300
	H	-1.82418900	2.49687200	-1.55776800
	H	-2.98017800	1.70183100	-0.48081100
	C	-0.93162300	1.13408300	-0.15638900
	H	-0.72871200	1.88297200	0.61115300
	C	0.35032200	0.76164400	-0.88407500
	H	0.58533100	1.54813100	-1.60872100
	H	0.21912700	-0.16480900	-1.44604200
	C	1.54014100	0.64264900	0.05351700
	O	1.67393400	1.27128400	1.07330000
	O	2.44234300	-0.23024600	-0.42246800
	C	3.65139700	-0.40035600	0.36446700
	H	4.15181600	0.56727200	0.44581200
	H	3.36738900	-0.71513500	1.37074700
	O	-1.28798600	-0.09404300	0.57849900
	O	-2.31298100	0.10471900	1.41376100
	H	-3.29682700	-0.78145500	0.89512500
	O	-3.93234000	-1.38602900	0.30875400
	O	-3.29360800	-1.64139600	-0.78807500

	C	4.50796900	-1.43177100	-0.33921700
	H	4.76862600	-1.10088700	-1.34683200
	H	5.43301000	-1.58914200	0.22133500
	H	3.98436800	-2.38712100	-0.41380600
97 (triplet state)	C	-2.26998800	-1.65074000	-0.51993800
	H	-2.09778000	-2.07484100	-1.51160400
	C	-0.98573200	-1.48764500	0.27821600
	H	-0.65997700	-2.48468500	0.58994400
	H	-1.20888300	-0.94197500	1.19785200
	O	-2.90313600	-0.36966900	-0.81794700
	O	-3.52630900	0.11367500	0.26827700
	O	-2.37800300	2.24506900	0.64258300
	O	-1.43113300	2.23902600	-0.23617800
	H	-2.95218400	1.35978900	0.49400500
	C	3.62411700	0.18150200	0.28422200
	H	4.01302500	-0.77718900	0.63542900
	H	3.43692600	0.80559800	1.16094300
	H	-3.00826700	-2.24707600	0.01765700
	C	0.13108600	-0.79099100	-0.49771600
	H	-0.18369000	0.20382800	-0.82439800
	H	0.39151200	-1.34419300	-1.40673200
	C	1.39129800	-0.63255100	0.32692500
	O	1.52111500	-0.97560900	1.47624100
	O	2.36542400	-0.04932100	-0.39729100
	C	4.55793200	0.84997300	-0.70332000
	H	5.52317500	1.04419900	-0.22848100
	H	4.72509700	0.21276800	-1.57448600
	H	4.14510500	1.80112000	-1.04594000
98	C	-2.99426800	1.34612500	-0.03145700
	H	-2.92538600	1.80061400	-1.02335200
	H	-3.00990000	2.14119600	0.71968600
	H	-3.93302300	0.79455400	0.03226500
	C	-1.82747100	0.39832100	0.20870700
	H	-1.86981800	-0.02643300	1.21625400
	C	-0.45974400	1.04090200	0.00174400
	H	-0.40876300	1.97370700	0.57352100
	H	-0.30771200	1.29881400	-1.04827100
	C	0.67064200	0.14723200	0.47811900
	O	0.58876300	-0.65804800	1.37241700
	O	1.80153400	0.39061200	-0.20991700
	C	2.96908500	-0.37528900	0.18089800
	H	3.17841200	-0.18058400	1.23538300
	H	2.73800600	-1.43789200	0.07859800
	O	-1.83479200	-0.68903300	-0.73310800

	O	-2.93530700	-1.56818600	-0.39667500
	H	-2.45687800	-2.27656500	0.05761300
	C	4.11190200	0.05032600	-0.71736700
	H	4.31902800	1.11684400	-0.60576600
	H	5.01635200	-0.50521500	-0.45611600
	H	3.87722000	-0.14749900	-1.76542000
99	C	-2.59624800	-0.50068600	0.02784900
	H	-2.64659100	-1.06587700	0.96806400
	H	-2.62459300	-1.21225900	-0.80602800
	C	-1.34877700	0.37155400	-0.03074000
	H	-1.36191300	0.95715200	-0.95302100
	H	-1.36224100	1.08788100	0.79391800
	C	-0.07540200	-0.47083900	0.03448700
	H	-0.01823300	-1.17759000	-0.79988300
	H	-0.04918400	-1.08383600	0.94259200
	C	1.18707500	0.36773100	0.01771300
	O	1.23036200	1.57203700	0.02142500
	O	2.28154800	-0.42173200	0.00298600
	C	3.56172500	0.25773300	-0.00512100
	H	3.60901800	0.90444200	-0.88439200
	H	3.62506900	0.89623100	0.87917700
	O	-3.70810400	0.38308700	-0.06428800
	O	-4.90297500	-0.44516300	-0.07697800
	H	-5.34242400	-0.11858600	0.71975500
	C	4.64042200	-0.80547100	-0.01990300
	H	4.55433500	-1.43564200	-0.90777600
	H	5.62662400	-0.33404000	-0.02686300
	H	4.57071800	-1.44383200	0.86358900
100	C	-3.49563200	-0.44018200	-0.42023100
	H	-3.51763400	-1.53317100	-0.40629400
	H	-3.65119900	-0.10547800	-1.44892400
	H	-4.31419100	-0.07256200	0.20010100
	C	-2.15707800	0.07106100	0.13388200
	H	-2.15458100	1.18211500	0.08688200
	C	-0.92815500	-0.40251700	-0.67088500
	H	-1.10908300	-0.26024200	-1.74190700
	H	-0.75190700	-1.46570900	-0.50043100
	C	0.30520800	0.39986200	-0.31015800
	O	0.31204100	1.59507700	-0.14349100
	O	1.39869000	-0.37734000	-0.22306400
	C	2.64239500	0.29871100	0.09508400
	H	2.84484000	1.04036800	-0.68120500
	H	2.51515400	0.83178300	1.03963100
	O	-2.01302900	-0.16400100	1.47349500

	C	3.72491200	-0.75752100	0.17403100
	H	3.82755800	-1.28320000	-0.77783800
	H	4.68319700	-0.28949000	0.41380800
	H	3.49632900	-1.49078700	0.95031700
101	C	-1.97752000	0.28559100	-0.02778100
	H	-2.01299100	0.99718600	0.80093100
	H	-2.01509300	0.87918100	-0.94477300
	C	-0.67794000	-0.51477800	0.02988800
	H	-0.59968200	-1.21659000	-0.80798100
	H	-0.63116500	-1.13326500	0.93418300
	C	0.56221100	0.35670000	0.01621800
	O	0.57322300	1.56161200	0.02438700
	O	1.67731000	-0.40333000	-0.00200600
	C	2.93920400	0.30996300	-0.00705500
	H	2.98410800	0.94832900	0.87841200
	H	2.97044700	0.95922800	-0.88516300
	C	-3.21480300	-0.61299500	0.03307800
	H	-3.21373700	-1.25724800	0.93521200
	H	-3.21392900	-1.35044200	-0.79811800
	O	-4.41529800	0.03159500	-0.04349700
	C	4.04574900	-0.72417000	-0.02205300
	H	3.97793000	-1.35488300	-0.91115000
	H	5.01906800	-0.22669800	-0.02664000
	H	3.99175600	-1.36568100	0.86025300
102	C	3.45759300	-0.41389700	0.28253100
	H	3.37195000	-1.13318400	1.09865300
	H	3.81461500	0.54610300	0.66128500
	H	4.20323500	-0.79384100	-0.42437200
	C	2.13795000	-0.29270400	-0.46252800
	H	2.06137800	0.57520400	-1.14489700
	C	0.93969500	0.68600000	0.89134400
	H	1.56049000	1.56587400	1.00670900
	H	0.93072900	-0.03390900	1.69952300
	C	-0.31831300	0.90019000	0.14844200
	O	-0.47675700	1.77547600	-0.67377500
	O	-1.24826300	-0.01303300	0.47731500
	C	-2.48028800	0.02955100	-0.28332900
	H	-2.94905500	1.00588200	-0.13818900
	H	-2.23253600	-0.06883700	-1.34264200
	O	1.43493800	-1.30119900	-0.69111800
	C	-3.35419400	-1.10571500	0.20721400
	H	-3.58173800	-0.99224300	1.26948700
	H	-4.29607300	-1.11495300	-0.34745100
	H	-2.85698900	-2.06660500	0.06047300

103	C	1.84909900	0.48962400	-0.22031900
	H	2.10342300	0.71220600	-1.24953500
	H	2.07917900	1.27613300	0.48744900
	C	0.65156800	-0.36554900	0.04660100
	H	0.71501900	-0.84023300	1.03381800
	H	0.55075600	-1.17458100	-0.68043600
	C	-0.65144500	0.43480300	0.04700500
	O	-0.73339600	1.63450100	0.10139900
	O	-1.70814800	-0.39689100	-0.00313500
	C	-3.01927600	0.22727000	0.02736100
	H	-3.08511600	0.93762800	-0.79945300
	H	-3.11480700	0.78998400	0.95880300
	C	3.59699500	-0.76436300	0.19480600
	H	3.19635000	-1.55179400	-0.47351400
	H	3.28482100	-0.85165900	1.25417200
	O	4.56015500	-0.07595900	-0.13370800
	C	-4.04944100	-0.87717800	-0.08195400
	H	-3.95834800	-1.58001400	0.74897700
	H	-5.05480000	-0.44875700	-0.06140100
	H	-3.93037600	-1.42976900	-1.01632800
104	C	2.13077600	-0.93130200	0.00018100
	H	1.88353200	-1.98366000	-0.00036400
	H	3.16042200	-0.60422000	0.00048700
	C	1.09472200	0.07820900	-0.00006900
	O	1.29787100	1.27795800	0.00013200
	O	-0.14738500	-0.47165500	-0.00034900
	C	-1.25016100	0.46205900	-0.00021200
	H	-1.16910100	1.10382300	0.88101700
	H	-1.16964500	1.10338100	-0.88178000
	C	-2.53123800	-0.34681400	0.00029100
	H	-2.58934500	-0.98286200	0.88628100
	H	-3.39464700	0.32363800	0.00021700
	H	-2.58970200	-0.98343800	-0.88527400
105	C	-3.04551800	-0.19542200	-0.00032600
	H	-3.92625100	-0.82353600	-0.00054900
	H	-3.15273500	0.87966200	-0.00033300
	C	-1.69407700	-0.80957800	0.00022500
	H	-1.54039600	-1.47168900	-0.86546800
	H	-1.54076100	-1.47086200	0.86663700
	C	-0.56389300	0.20444100	0.00005200
	O	-0.69143000	1.40221500	0.00004200
	O	0.63123200	-0.42186200	0.00020600
	C	1.80225400	0.43162300	0.00022900

	H	1.76690300	1.07511900	0.88239800
	H	1.76643600	1.07583800	-0.88138700
	C	3.02018900	-0.46904400	-0.00042800
	H	3.03192500	-1.10753900	-0.88641700
	H	3.93042200	0.13639200	-0.00035400
	H	3.03230300	-1.10832400	0.88498700
106 (triplet state)	C	1.78136300	0.86885500	1.01754100
	H	1.42649500	1.49798200	1.83315000
	C	0.78304400	-0.20556700	0.66330200
	H	0.76716300	-0.96269100	1.45205400
	H	1.05297700	-0.70453700	-0.26970400
	O	1.96047000	1.81656000	-0.08857000
	O	2.68874800	1.33028300	-1.06690500
	O	4.06528700	-1.11343400	-0.91581800
	O	4.14298400	-1.29183300	0.39641700
	H	3.57101400	-0.26379500	-1.03045600
	C	-4.02014700	-0.51532600	-0.30028200
	H	-4.13318600	-1.31054100	0.44209200
	H	-3.80743800	-1.01900200	-1.24745400
	H	2.75438800	0.42907700	1.24081200
	C	-1.52984900	-0.41191300	0.19549800
	O	-1.38079300	-1.59208300	0.01494400
	C	-5.31767500	0.28867800	-0.41176800
	H	-6.15599700	-0.35671200	-0.68496600
	H	-5.56922200	0.77504500	0.53595600
	H	-5.23912800	1.07014500	-1.17400500
	O	-0.50621200	0.41528300	0.54117600
	C	-2.82486300	0.35860400	0.08044800
	H	-2.66839800	1.15880000	-0.65195100
	H	-2.99378500	0.86803000	1.03608300
107 (triplet state)	C	-1.67680700	-0.02534600	1.17551300
	H	-1.40685100	-0.73351800	1.96071300
	C	-0.50545300	0.81378100	0.73873200
	H	-0.26693600	1.54862600	1.51194200
	H	-0.73442900	1.35309600	-0.18273200
	O	-2.12748400	-0.79488200	0.02330500
	O	-3.20677600	-1.51816100	0.32254600
	O	-4.82736600	-0.05016100	-0.88162200
	O	-4.03849800	0.97236700	-1.02250300
	H	-4.26376300	-0.79303800	-0.43171800
	C	4.22059600	0.12570400	-0.39677800
	H	4.52632900	0.80590400	0.40348000
	H	4.10747200	0.74687600	-1.28967400
	H	-2.50973400	0.60041900	1.49884100

	C	1.78006300	0.53749200	0.18109100
	O	1.89137500	1.73104400	0.07175600
	C	5.30025500	-0.93456400	-0.62627500
	H	6.25717800	-0.47114100	-0.87843200
	H	5.45442900	-1.54805400	0.26696900
	H	5.03140400	-1.60702100	-1.44688000
	O	0.61348200	-0.06476900	0.53276200
	C	2.86679300	-0.48928500	-0.04145700
	H	2.52042400	-1.16736300	-0.82997200
	H	2.93394600	-1.10499400	0.86255500
108	C	-4.74343900	-0.78448500	0.00784300
	H	-4.72235900	-1.44202600	0.88269300
	H	-4.73352000	-1.42008000	-0.88324400
	H	-5.69520600	-0.24765300	0.02052400
	C	-3.56295400	0.18955200	0.01230900
	H	-3.62306900	0.85748900	-0.85165300
	H	-3.61249300	0.83643500	0.89290300
	C	-2.21369100	-0.52883700	-0.00482400
	H	-2.12045400	-1.17570300	-0.88467900
	H	-2.10782900	-1.19505800	0.85892100
	C	-1.03061900	0.41449800	-0.00405800
	O	-1.08132100	1.61718600	0.00081900
	O	0.13538500	-0.27883800	-0.01026500
	C	1.33864900	0.51224500	-0.01707600
	H	1.37299100	1.13425600	-0.91339400
	H	1.35886800	1.16814600	0.85542800
	C	2.48792500	-0.48256000	0.00619200
	H	2.45551000	-1.12768800	-0.87712400
	H	2.44321000	-1.10634200	0.90622500
	O	3.67075600	0.30602900	-0.00165300
	O	4.78673400	-0.61800800	-0.08352700
	H	5.23670200	-0.41521300	0.74809800
109	C	-4.17383400	-0.64407700	0.00011100
	H	-4.18780500	-1.29038200	-0.88316600
	H	-5.10012200	-0.06430000	0.00036300
	H	-4.18760300	-1.29082900	0.88306300
	C	-2.95011500	0.27517000	0.00020000
	H	-2.97481300	0.93462200	-0.87199600
	H	-2.97464000	0.93420800	0.87271800
	C	-1.63525600	-0.50471000	-0.00011900
	H	-1.56675900	-1.16515100	-0.87214900
	H	-1.56651400	-1.16549400	0.87162700
	C	-0.40953500	0.38226600	-0.00014300
	O	-0.40432700	1.58586700	-0.00023000

	O	0.72431200	-0.36347300	-0.00007500
	C	1.96688200	0.36671300	-0.00014100
	H	2.02693000	1.00492200	0.88409800
	H	2.02709700	1.00448200	-0.88468800
	C	3.08128700	-0.67423100	0.00021500
	H	2.98687400	-1.35601900	-0.86748800
	H	2.98674300	-1.35558900	0.86823600
	O	4.33676900	-0.14705100	0.00013600
110	C	-4.12296800	-0.08960100	0.56943000
	H	-4.42910700	-0.97121900	-0.00213800
	H	-4.92896100	0.64479600	0.50207700
	H	-4.03417300	-0.38885400	1.61833500
	C	-2.80911500	0.49035500	0.04049700
	H	-2.93185400	0.81396500	-0.99699400
	H	-2.54003800	1.38774000	0.60489600
	C	-1.65885300	-0.51394500	0.11850200
	H	-1.88490600	-1.42459700	-0.44841200
	H	-1.49076700	-0.84959200	1.14847900
	C	-0.35334500	0.03025300	-0.39888700
	O	-0.14212500	1.12249700	-0.84190900
	O	0.63726200	-0.93746800	-0.30016100
	C	1.89432800	-0.61962800	-0.73685700
	H	1.96772000	0.19758700	-1.44270900
	H	2.51177600	-1.49861400	-0.85207800
	C	2.98541200	0.27696700	0.87646800
	H	2.64087300	-0.51545300	1.56955500
	H	2.33712100	1.17302000	0.83851800
	O	4.15105900	0.31307200	0.47276400

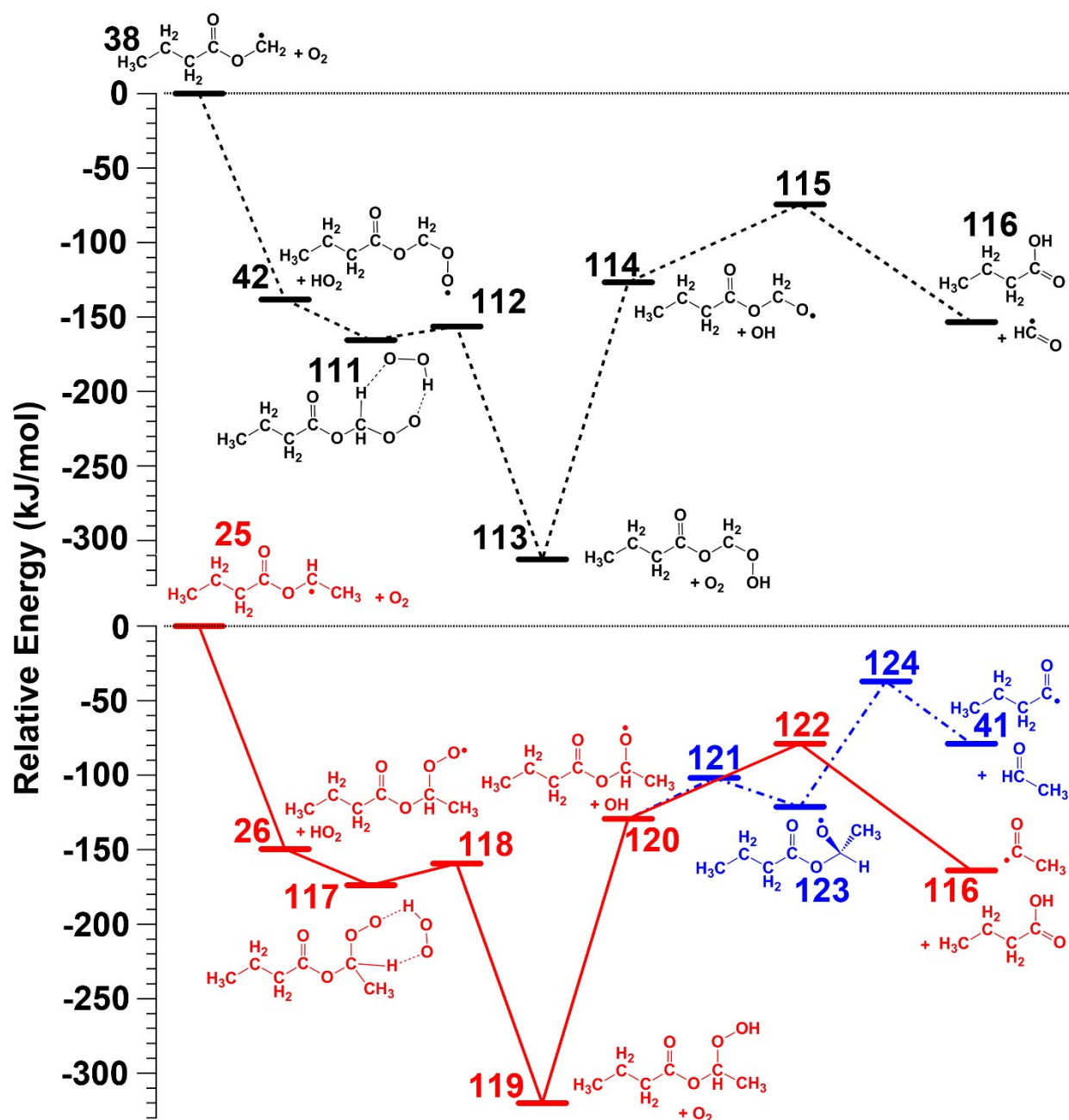


Figure S14. PES of the reactions of R_mO_2 with HO_2 . The top shows R_mO_2 for MB and the bottom shows R_mO_2 for EB. The numbers correspond with the energies and geometries listed in the supporting information.

Table S15. Calculated 0 K CBS-QB3 energies for the structures in Figure S13.

Species	Energy (Hartrees)
111 (triplet state)	-646.740652
112 (triplet state)	-646.737179

113	-496.632082
114	-420.911585
115	-420.891691
116	-307.216964
117 (triplet state)	-685.977085
118 (triplet state)	-685.971603
119	-535.868242
120	-460.145804
121	-460.135335
122	-460.126673
123	-460.142733
124	-460.110732

Table S16. Optimized geometries for the structures in Figure S13.

Species	Optimized coordinates (Å)			
111 (triplet state)	C	3.77378100	1.42398800	-0.29855600
	H	3.50681000	1.84489300	-1.27249100
	H	4.62448800	0.75218100	-0.44634800
	H	4.10625200	2.24682900	0.33873600
	C	2.58739100	0.69195100	0.33219300
	H	2.87237800	0.30733100	1.31722000
	H	1.75888900	1.38635900	0.49116100
	C	2.10006300	-0.47895600	-0.54372900
	H	2.89954800	-1.20221500	-0.71227100
	H	1.77663700	-0.09268200	-1.51643500
	C	0.94564500	-1.23254800	0.05986200
	O	0.92162200	-2.38307100	0.39004200
	O	-0.14473400	-0.38825500	0.21821300
	C	-1.31146100	-0.93721200	0.75610200
	H	-1.11634700	-1.83085100	1.34441300
	H	-1.83744900	-0.13973000	1.27690800
	O	-2.17171700	-1.41457600	-0.32478300
	O	-2.66547900	-0.42223600	-1.03599100
	H	-2.14574300	1.32774300	-0.72059800
	O	-1.99197300	2.25178000	-0.40531400
	O	-2.07496600	2.18096000	0.91589000
112 (triplet state)	C	-3.76842000	0.79571500	-0.22947100
	H	-3.47605400	1.72523200	0.26756200
	H	-4.43812200	0.25164800	0.44314800
	H	-4.33806000	1.06125600	-1.12333700
	C	-2.54114900	-0.04240100	-0.59380300
	H	-2.85548200	-0.94913700	-1.12196900
	H	-1.89648100	0.51667100	-1.27578000
	C	-1.72734200	-0.43880100	0.65255400

	H	-2.33712500	-1.00877400	1.35550300
	H	-1.38023600	0.46882100	1.15854300
	C	-0.51363900	-1.27511000	0.34860900
	O	-0.26178900	-2.36805700	0.76886300
	O	0.32714400	-0.60086000	-0.52561600
	C	1.55353500	-1.20524200	-0.83455600
	H	1.52496900	-2.28375800	-0.69240800
	H	1.83319700	-0.88815700	-1.83625700
	O	2.56989400	-0.74977700	0.08531700
	O	2.87547700	0.53529000	-0.14363400
	H	1.86795300	1.46238500	0.37027200
	O	1.18636100	2.12721800	0.78918900
	O	0.48760400	2.63604100	-0.17477900
113	C	-4.03243200	-0.05296900	-0.16340300
	H	-4.17201900	0.52095200	-1.08475200
	H	-4.30743600	0.59471700	0.67494200
	H	-4.73833800	-0.88670200	-0.18269100
	C	-2.59308200	-0.55633600	-0.03099000
	H	-2.48492300	-1.15363100	0.87840000
	H	-2.35295900	-1.22696400	-0.86119900
	C	-1.57934500	0.58789900	-0.00208100
	H	-1.78741200	1.27762000	0.82481600
	H	-1.63640500	1.19811300	-0.90980200
	C	-0.14730200	0.13149100	0.14839300
	O	0.19283300	-1.01526900	0.34892600
	O	0.70543500	1.16428100	0.03112200
	C	2.13019700	0.95913900	0.27205700
	H	2.54312300	1.95081400	0.09416300
	H	2.27846400	0.62069600	1.29843700
	O	2.73692000	0.09425400	-0.61966300
	O	2.87201000	-1.22066900	-0.02392600
	H	1.93210800	-1.49173700	0.03216400
114	C	3.63759000	-0.41226200	-0.13343500
	H	3.64061400	-1.12117900	-0.96727900
	H	3.79192600	-0.98387700	0.78714600
	H	4.49725900	0.25044500	-0.25938500
	C	2.33206100	0.38518700	-0.08457000
	H	2.36554200	1.11002000	0.73408500
	H	2.21569400	0.97258900	-0.99955500
	C	1.10799000	-0.51345700	0.09096200
	H	1.17098400	-1.10144700	1.01335200
	H	1.03714100	-1.25010300	-0.71794300
	C	-0.20038500	0.24061500	0.11825800
	O	-0.33273600	1.42953100	-0.03677900

	O	-1.24024800	-0.60424200	0.34602800
	C	-2.56790700	-0.02363000	0.32456900
	H	-3.03616100	-0.28177900	1.28963600
	H	-2.45826000	1.07970400	0.28071900
	O	-3.31212200	-0.41692500	-0.69118400
115	C	3.70515200	-0.13558900	-0.06885400
	H	3.85187000	-0.28227600	-1.14335600
	H	3.88328600	-1.09602000	0.42448900
	H	4.47110600	0.56232300	0.27804500
	C	2.30232800	0.39685400	0.23164600
	H	2.19600700	0.57172500	1.30754700
	H	2.15207400	1.36477900	-0.25264900
	C	1.20400000	-0.56685100	-0.23315100
	H	1.27816800	-1.53871400	0.25938100
	H	1.29970800	-0.75111700	-1.31073600
	C	-0.20531100	-0.05299500	-0.02396000
	O	-0.44198700	1.18412400	-0.16583900
	O	-1.11999700	-0.88138100	0.26699900
	C	-2.66516500	0.15822600	0.36924700
	H	-2.79624700	0.06405500	1.45790500
	H	-1.84258100	1.04571100	0.07966400
	O	-3.50544200	-0.14503500	-0.44489300
116	C	2.73377000	-0.21180700	0.00000000
	H	2.87071900	-0.84384200	-0.88306000
	H	2.87072900	-0.84374000	0.88313000
	H	3.53263200	0.53386600	-0.00004800
	C	1.35750900	0.45780500	-0.00003000
	H	1.25653400	1.10971200	0.87234800
	H	1.25652800	1.10961700	-0.87248000
	C	0.21486900	-0.55702800	0.00003000
	H	0.27090000	-1.21924700	0.87166800
	H	0.27087500	-1.21933100	-0.87154400
	C	-1.15648900	0.07738200	0.00002700
	O	-1.39619100	1.25753200	0.00001000
	O	-2.13511500	-0.86285800	-0.00002700
	H	-2.97642300	-0.38253800	-0.00004300
117 (triplet state)	C	3.95173100	0.13396300	-0.83918100
	H	4.14471700	-0.67951000	-1.54534900
	H	4.58141600	-0.03104600	0.04005100
	H	4.27532000	1.06604200	-1.30867400
	C	2.47108600	0.20085000	-0.45866200
	H	2.30054100	1.03796100	0.22502600
	H	1.86557700	0.39444000	-1.34808200

	C	1.98539900	-1.10198600	0.20302600
	H	2.57783800	-1.33558800	1.08925300
	H	2.09318700	-1.93193100	-0.50454200
	C	0.54523000	-1.05668900	0.64757300
	O	0.13204700	-1.21639700	1.76352700
	O	-0.28777000	-0.81294400	-0.41795400
	C	-1.66218100	-0.61833400	-0.11813400
	H	-1.76497900	0.04608900	0.74125500
	O	-2.19436200	0.07900300	-1.28919500
	O	-1.76077600	1.31413200	-1.40254300
	H	-0.61577400	2.10381500	-0.23365400
	O	-0.16006800	2.53899700	0.52807900
	O	-0.81462900	2.10595600	1.60014600
	C	-2.43975900	-1.90519500	-0.01291300
	H	-2.29017400	-2.50936500	-0.90941700
	H	-2.08877800	-2.45426900	0.86066100
	H	-3.50345700	-1.69227300	0.10674300
118 (triplet state)	C	-4.14692500	1.83455700	0.07732800
	H	-4.29001200	1.88574800	1.16083200
	H	-5.01588600	1.32647200	-0.35103800
	H	-4.13757500	2.85783000	-0.30580800
	C	-2.84751700	1.10890300	-0.27704800
	H	-2.71395500	1.09542800	-1.36346900
	H	-1.99138800	1.64653700	0.13922000
	C	-2.83162100	-0.34252200	0.24720500
	H	-3.65689800	-0.91339000	-0.18177400
	H	-2.93351700	-0.33786100	1.33632700
	C	-1.55701200	-1.05395400	-0.11845500
	O	-1.41123200	-1.87881000	-0.97461300
	O	-0.51619300	-0.60664200	0.67937100
	C	0.77011100	-1.06987500	0.37723500
	H	0.73774900	-2.04198000	-0.11347700
	O	1.24988500	-0.12297600	-0.65132100
	O	2.40334400	-0.54679300	-1.17839100
	H	3.31276500	0.51209100	-0.83360800
	O	3.85080500	1.29734300	-0.39153000
	O	3.04211700	1.88355800	0.43321400
	C	1.64217800	-1.01362000	1.60545600
	H	1.62778900	-0.00865900	2.02733900
	H	1.27141300	-1.72704000	2.34374200
	H	2.66442900	-1.28154400	1.33754700
119	C	4.31371600	0.29018300	-0.16344000
	H	4.49366700	1.00084700	0.64931000
	H	4.37600700	0.84274600	-1.10608100

	H	5.12845100	-0.43782600	-0.15244400
	C	2.95757200	-0.40256800	-0.00958800
	H	2.81659200	-1.13248000	-0.81210700
	H	2.93018100	-0.97340900	0.92264200
	C	1.79440300	0.58921800	-0.02387400
	H	1.76968100	1.16412300	-0.95595400
	H	1.90152800	1.33444400	0.77345200
	C	0.43791300	-0.05605700	0.14624000
	O	0.26414300	-1.23731100	0.36315900
	O	-0.54554900	0.84958300	0.02821500
	C	-1.94518700	0.46303800	0.26510400
	H	-2.01797600	0.06872400	1.27981600
	O	-2.37959900	-0.50603800	-0.63627300
	O	-2.34946400	-1.81716400	-0.02082600
	H	-1.38238800	-1.95236300	0.06241100
	C	-2.74367000	1.72785100	0.03958600
	H	-2.35351600	2.53681200	0.65821900
	H	-2.67836700	2.02043100	-1.00984500
	H	-3.78859300	1.54539500	0.29220600
120	C	4.01324000	-0.33934800	0.27888900
	H	4.11586800	-1.33536500	-0.16305400
	H	4.05198600	-0.45491200	1.36664600
	H	4.88422300	0.24772600	-0.02263000
	C	2.71410400	0.33728700	-0.16517500
	H	2.64936600	1.34261000	0.26087400
	H	2.71290100	0.47238700	-1.25048900
	C	1.47457400	-0.45993600	0.24081100
	H	1.43100100	-0.60191000	1.32672600
	H	1.49408600	-1.47042200	-0.18300700
	C	0.17276800	0.18028900	-0.18605100
	O	0.06900400	1.22282900	-0.79019100
	O	-0.88631200	-0.56623400	0.19418600
	C	-2.21230500	-0.07086200	-0.19371400
	H	-2.04637300	0.67237600	-1.00197400
	C	-2.84284600	0.64555400	1.01599100
	H	-2.20408400	1.47720000	1.31464800
	H	-3.82938900	1.01949300	0.74229800
	H	-2.93522400	-0.06003100	1.84238600
	O	-2.96288800	-1.03997600	-0.67611100
121	C	-4.00948500	-0.37368300	-0.09226600
	H	-4.15875100	-0.92633500	0.84070600
	H	-4.03915200	-1.09727700	-0.91296300
	H	-4.85937200	0.30216000	-0.21605700
	C	-2.68869300	0.40000200	-0.07875100

	H	-2.57719600	0.96987400	-1.00541800
	H	-2.69566400	1.13964600	0.72729900
	C	-1.47805800	-0.51718100	0.09272100
	H	-1.43402500	-1.26828100	-0.70439300
	H	-1.53849600	-1.08819100	1.02566100
	C	-0.15311300	0.22016200	0.08783000
	O	-0.02287100	1.40372700	-0.09056200
	O	0.85188200	-0.66139600	0.31953800
	C	2.29051400	-0.38642200	0.29505100
	H	2.61192100	-0.60780600	1.33091500
	C	2.74633400	1.05621900	-0.04536300
	H	2.26811300	1.76619900	0.62366300
	H	3.83035800	1.08252100	0.06881200
	H	2.47810100	1.30406100	-1.07013200
	O	2.90463500	-1.23872600	-0.51190400
122	C	-4.06354600	0.07987900	-0.17926600
	H	-4.29588300	-0.98949800	-0.16409900
	H	-4.18600100	0.43083800	-1.20864900
	H	-4.80955900	0.58975400	0.43540200
	C	-2.64885000	0.34756700	0.33964100
	H	-2.45674200	1.42567200	0.35051400
	H	-2.55432900	0.01090400	1.37489300
	C	-1.57825500	-0.34707400	-0.50745800
	H	-1.59308100	-0.00619300	-1.54532700
	H	-1.76148500	-1.42878400	-0.53365100
	C	-0.15999900	-0.18208500	0.01047700
	O	0.03970200	-0.04736700	1.24650900
	O	0.78733800	-0.21287200	-0.83844600
	C	2.34963100	-0.10535800	0.15927700
	H	1.57278700	-0.07144100	1.07705700
	C	2.85149300	1.26998300	-0.24268400
	H	2.09428000	2.02859900	-0.05403300
	H	3.74729400	1.48812100	0.34372100
	H	3.11039600	1.25888700	-1.30234800
	O	3.00164500	-1.12905300	0.06026200
123	C	-3.98249400	-0.17945100	0.08159600
	H	-4.10667300	-0.75499600	1.00436400
	H	-4.14612200	-0.86210800	-0.75818100
	H	-4.77276900	0.57483900	0.05335300
	C	-2.59891300	0.47119300	0.00984400
	H	-2.50859100	1.06547500	-0.90344500
	H	-2.47271900	1.17503300	0.83797700
	C	-1.46855900	-0.55710700	0.04890900
	H	-1.56054900	-1.27506900	-0.77476600

	H	-1.50386300	-1.15742000	0.96457900
	C	-0.08828300	0.05600800	-0.05123500
	O	0.14905600	1.22128500	-0.24178700
	O	0.86969600	-0.89511800	0.09889200
	C	2.26085300	-0.48033100	-0.08507900
	H	2.78700600	-1.45594100	-0.08983200
	C	2.76714100	0.34091000	1.11592800
	H	2.55100900	-0.19656400	2.04015300
	H	3.84353900	0.48572900	1.01936000
	H	2.26739200	1.30749500	1.12177600
	O	2.51673200	0.07210800	-1.26149400
124	C	-3.97077100	-0.14539000	0.17028300
	H	-4.14899800	-1.15812900	-0.20419500
	H	-4.27875200	0.55650100	-0.61072200
	H	-4.62493800	0.00930000	1.03199100
	C	-2.50265800	0.05947600	0.55357900
	H	-2.35010400	1.06813000	0.94498000
	H	-2.23356000	-0.62862400	1.36194600
	C	-1.56389700	-0.16422300	-0.63398200
	H	-1.79251200	0.54265900	-1.44004300
	H	-1.65621000	-1.17179500	-1.04344900
	C	-0.06156800	0.04636000	-0.32783800
	O	0.19101800	0.98023400	0.47769800
	O	0.75463200	-0.70501100	-0.90955000
	C	2.58306100	-0.03535700	-0.27243200
	H	3.04515600	-0.40890800	-1.20273000
	C	2.69544000	-0.93677400	0.92813700
	H	2.48355100	-1.97162000	0.66188500
	H	3.72722900	-0.86984900	1.29269100
	H	2.02490400	-0.59235700	1.71477500
	O	2.39517400	1.18479500	-0.19484900