Low-Temperature Combustion Chemistry of Novel Biofuels: Resonance-Stabilized QOOH in the Oxidation of Diethyl Ketone

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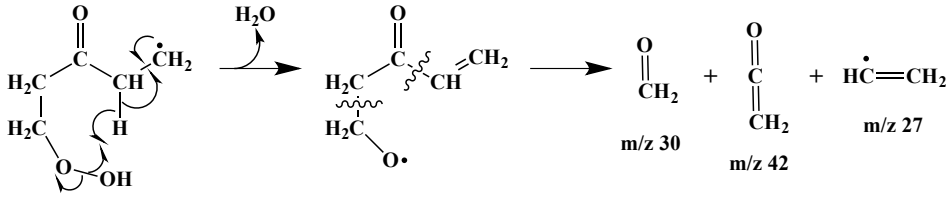
Supplementary Material

Discussion of Water Elimination Reactions:

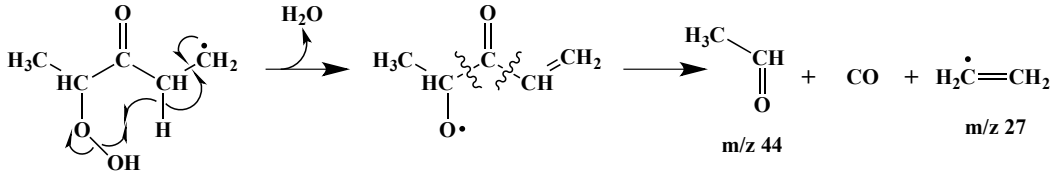
For example, the R_p QOOH radical with the radical center on the primary carbon (1,5 position) could eliminate water (reaction S1).



(S1)

The formed unsaturated alkoxy ketone can easily undergo a series of β-scission reactions, forming formaldehyde, ketene and a vinyl radical. The vinyl radical, in the presence of O_2, also forms formaldehyde.[1] A completely analogous reaction applies for the case when the –OOH and the radical centers are in 1,4 position. We did not consider the 1,2 case, because the barrier leading to that QOOH radical is too high for it to be relevant.

For the R_s QOOH radical with the radical center on the primary carbon (1,4 position) the water-elimination reaction proceeds by reaction S2.



(S2)

and as for R_p, the 1,3 case is entirely analogous. The products formed in the R_s case after the *β*-scissions are acetaldehyde, CO and the vinyl radical, which can further oxidize to

form formaldehyde. Again, we did not investigate the 1,2 case as the barrier leading to that QOOH is too high for this QOOH radical to be relevant.

Table S1. Kinetic Model[2-4]

Reactants	**Products**	**Rate Constant** [a] **(550 K)**	**Reference**
$Cl\bullet + C_2H_5C(O)CH_2CH_3$	$HCl + C_2H_5C(O)CH_2CH_2$	$4.0 \times 10^{-11}e^{-500/RT}$ (2.5×10^{-11}) [b]	1
$Cl\bullet + C_2H_5C(O)CH_2CH_3$	$HCl + C_2H_5C(O)CHCH_3$	6.3×10^{-11}	1
$Cl\bullet + C_2H_5C(O)CH_2CH_2$	$HCl + C_2H_5C(O)CHCH_2$	3×10^{-10} [c]	2
$Cl\bullet + C_2H_5C(O)CHCH_3$	$HCl + C_2H_5C(O)CHCH_2$	3×10^{-10} [c]	2
$Cl\bullet + C_2H_5C(O)CH_2CH_2$	$C_2H_5C(O)CH_2CH_2Cl$	4.55×10^{-10} [d]	3
$Cl\bullet + C_2H_5C(O)CHCH_3$	$C_2H_5C(O)CHClCH_3$	4.55×10^{-10} [d]	3
$Cl_2 + C_2H_5C(O)CH_2CH_2$	$Cl\bullet + C_2H_5C(O)CH_2CH_2Cl$	2.7×10^{-12}	1
$Cl_2 + C_2H_5C(O)CHCH_3$	$Cl\bullet + C_2H_5C(O)CHClCH_3$	1.85×10^{-12}	1
$O_2 + C_2H_5C(O)CH_2CH_2$	$C_2H_5C(O)CH_2CH_2O_2$	1×10^{-12}	1
$O_2 + C_2H_5C(O)CHCH_3$	$C_2H_5C(O)CH(O_2)ClCH_3$	1×10^{-12}	1
$C_2H_5C(O)CH(O_2)ClCH_3$	$O_2 + C_2H_5C(O)CHCH_3$	$6.76 \times 10^{10}e^{-14000/RT}$ (1.83×10^{5}) [b]	1

[a] in cm^3 $molecule^{-1}$, s, K and cal units. R = 1.986 cal K^{-1} mol^{-1}

[b] Rate constant includes estimations (see reference)

[c] Rate constant assumed to be equal to that for $Cl\bullet + C_2H_5 \rightarrow HCl + C_2H_4$

[d] Rate constant assumed to be equal to that for $Cl\bullet + C_2H_5 \rightarrow HCl + C_2H_5Cl$

Tables S2-S4: Absolute photoionization cross sections at the mass of the parent for the indicated species.

2-methyltetrahydrofuran-3-one

Energy(eV)	Photoionization Cross Section (Mb)
8.85	0.00
8.875	0.00
8.9	0.00
8.925	0.00
8.95	0.00
8.975	0.00
9	0.00
9.025	0.02
9.05	0.01
9.075	0.02
9.1	0.03
9.125	0.07
9.15	0.14
9.175	0.18
9.2	0.21
9.225	0.41
9.25	0.45
9.275	0.70
9.3	0.86
9.325	1.12
9.35	1.33
9.375	1.79
9.4	2.03
9.425	2.31
9.45	2.63
9.475	3.15
9.5	3.15
9.525	3.72
9.55	4.11
9.575	4.23
9.6	4.46
9.625	4.90
9.65	5.02
9.675	5.18
9.7	5.69
9.725	5.56

tetrahydro-4*H*-pyran-4-one

Energy(eV)	Photoionization Cross Section (Mb)
8.8	0.00
8.825	0.00
8.85	0.00
8.875	0.00
8.9	0.00
8.925	0.00
8.95	0.00
8.975	0.00
9	0.00
9.025	0.00
9.05	0.00
9.075	0.00
9.1	0.00
9.125	0.00
9.15	0.00
9.175	0.00
9.2	0.00
9.225	0.00
9.25	0.00
9.275	0.01
9.3	0.01
9.325	0.00
9.35	0.01
9.375	0.06
9.4	0.18
9.425	0.29
9.45	1.25
9.475	1.97
9.5	2.58
9.525	2.79
9.55	2.98
9.575	3.67
9.6	4.29
9.625	4.87
9.65	5.15
9.675	5.76

9.75	5.84	9.7	6.01
9.775	6.01	9.725	6.26
9.8	6.43	9.75	6.24
9.825	6.58	9.775	6.95
9.85	6.85	9.8	7.74
9.875	6.80	9.825	7.70
9.9	6.78	9.85	8.21
9.925	6.96	9.875	8.35
9.95	7.09	9.9	8.00
9.975	7.41	9.925	9.06
10	7.34	9.95	9.02
10.025	7.40	9.975	9.90
10.05	7.76	10	10.13
10.075	8.04	10.025	10.41
10.1	7.83	10.05	11.18
10.125	8.21	10.075	12.11
10.15	8.33	10.1	12.54
10.175	8.90	10.125	13.43
10.2	8.57	10.15	14.42
10.225	8.46	10.175	14.31
10.25	8.79	10.2	15.13
10.275	9.00	10.225	15.09
10.3	8.95	10.25	15.99
10.325	9.20	10.275	17.49
10.35	9.16	10.3	16.90
10.375	9.41	10.325	17.48
10.4	9.30	10.35	18.54
10.425	9.40	10.375	18.29
10.45	9.39	10.4	18.51
10.475	9.70	10.425	18.22
10.5	9.50	10.45	19.59
10.525	9.46	10.475	19.36
10.55	9.41	10.5	20.06
10.575	9.83	10.525	18.82
10.6	9.63	10.55	18.91
10.625	9.44	10.575	19.66
10.65	9.66	10.6	19.88
10.675	9.50	10.625	19.28
10.7	9.43	10.65	19.85
10.725	9.54	10.675	19.85
10.75	9.35	10.7	19.70
10.775	9.65	10.725	19.60
10.8	9.44	10.75	19.46

10.825	9.97	10.775	20.11
10.85	9.40	10.8	19.70
10.875	9.41	10.825	20.16
10.9	9.73	10.85	19.81
10.925	9.46	10.875	19.54
10.95	9.67	10.9	18.94
10.975	9.88	10.925	20.11
11	10.00	10.95	19.26
11.025	9.78	10.975	19.73
		11	19.86

vinyl ethyl ketone

Energy(eV)	Photoionization Cross Section (Mb)
9.2	0.00
9.225	0.02
9.25	0.00
9.275	0.01
9.3	0.00
9.325	0.00
9.35	0.03
9.375	0.07
9.4	0.17
9.425	0.41
9.45	0.72
9.475	1.47
9.5	2.40
9.525	3.14
9.55	3.80
9.575	4.48
9.6	5.33
9.625	5.41
9.65	6.52
9.675	7.61
9.7	7.52
9.725	7.87
9.75	8.26
9.775	8.41
9.8	8.92
9.825	9.64
9.85	10.46
9.875	10.62

9.9	10.48
9.925	10.84
9.95	11.48
9.975	11.70
10	12.29
10.025	12.05
10.05	13.05
10.075	13.29
10.1	13.63
10.125	13.90
10.15	14.27
10.175	14.88
10.2	14.76
10.225	15.06
10.25	15.21
10.275	15.72
10.3	16.16
10.325	16.63
10.35	16.22
10.375	16.11
10.4	16.84
10.425	16.69
10.45	16.96
10.475	17.38
10.5	17.41
10.525	16.97
10.55	16.85
10.575	16.71
10.6	16.69
10.625	16.97
10.65	17.18
10.675	16.72
10.7	16.96
10.725	16.97
10.75	17.20
10.775	16.89
10.8	17.35
10.825	17.08
10.85	17.11
10.875	16.96
10.9	16.82
10.925	16.66
10.95	16.74

10.975	17.10
11	16.36
11.025	15.94

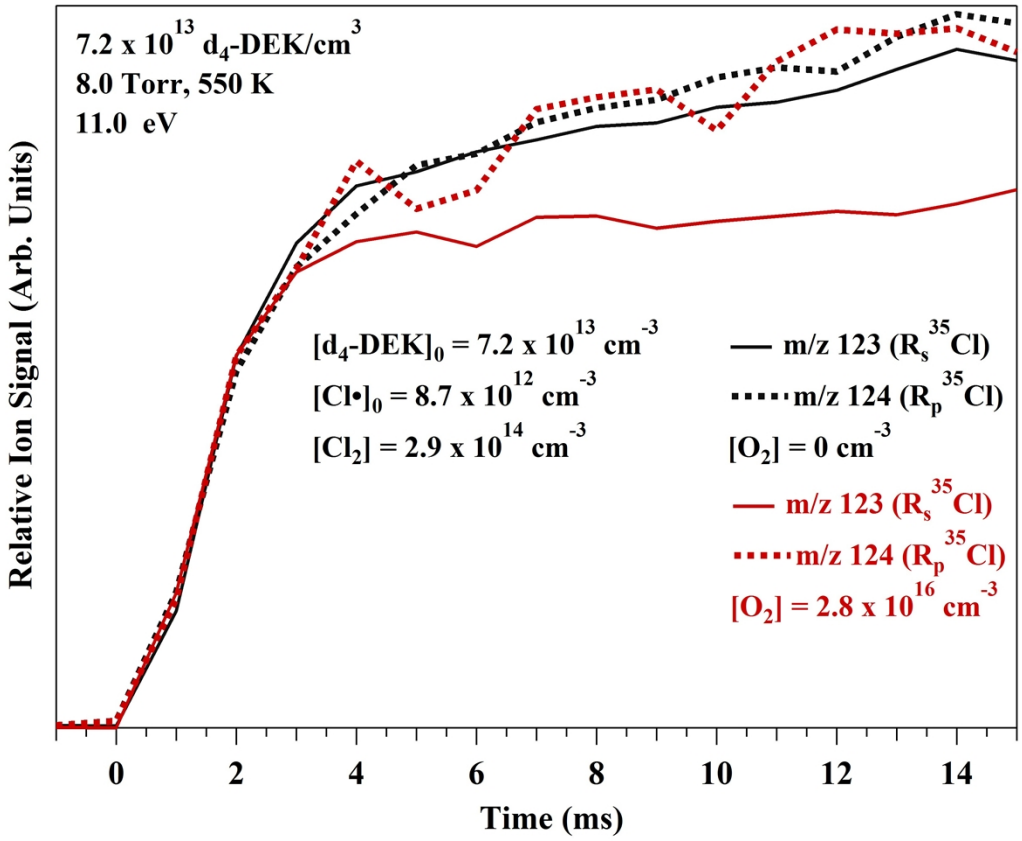


Figure S1. Accumulation of chlorinated products 1-Cl-3-pentanone ($R_p{}^{35}Cl$) and 2-Cl-3-pentanone ($R_s{}^{35}Cl$) as a function of reaction time for the Cl-initiated oxidation of diethyl ketone both in the presence (0.2 mole fraction; red traces) and absence (black traces) of O_2.

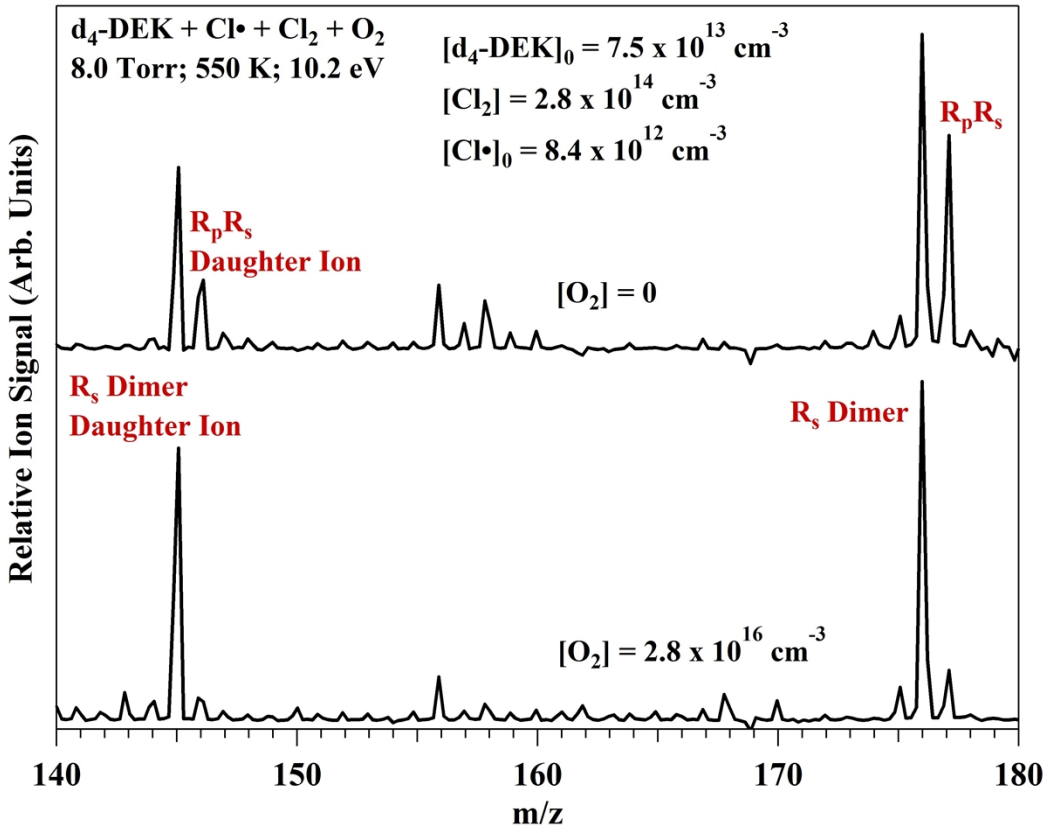


Figure S2. Difference mass spectra for the dimer products and their daughter ions observed during the Cl-initiated oxidation of d_4-DEK. Top: no O_2 is added to the reaction mixture. Bottom: $[O_2] = 2.8 \times 10^{16}$ cm^{-3}.

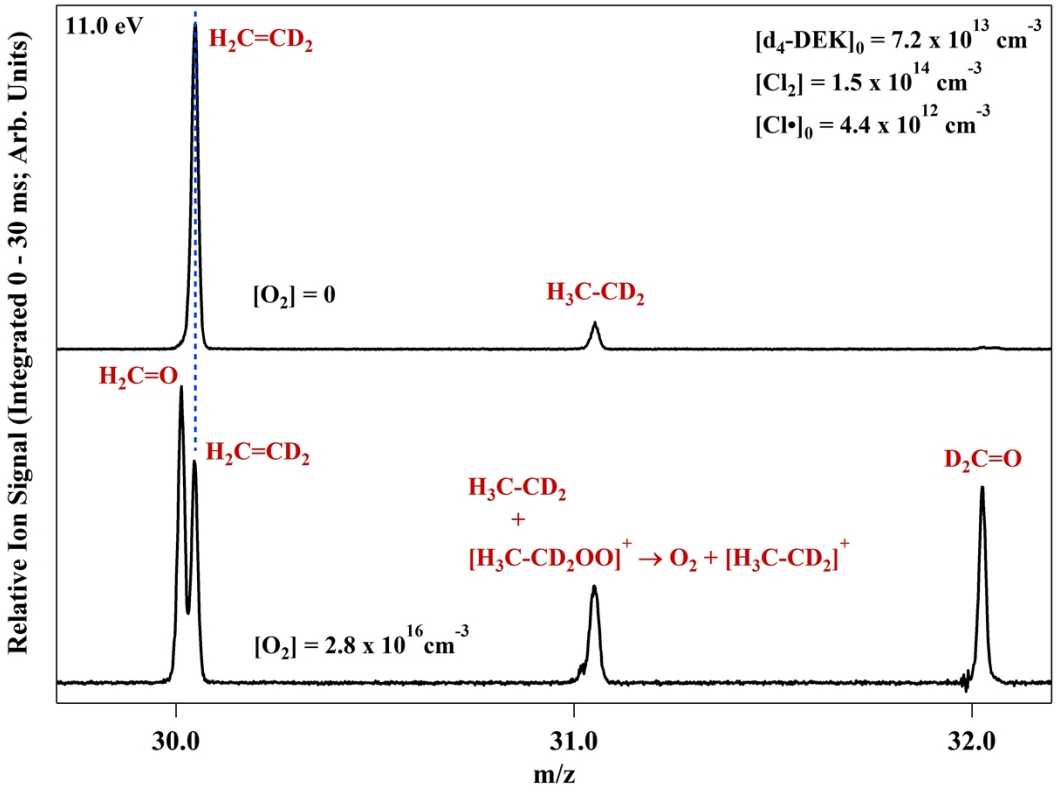


Figure S3. Difference mass spectra in the region of d_2-ethene and d_0- and d_2-formaldehyde observed during the Cl-initiated oxidation of d_4-DEK. Top: no O_2 is added to the reaction mixture. Bottom: $[O_2] = 2.8 \times 10^{16}$ cm^{-3}.

Table S5: Stationary point energies (0K) for small molecules computed in this work (CBS-QB3)

Small Molecules

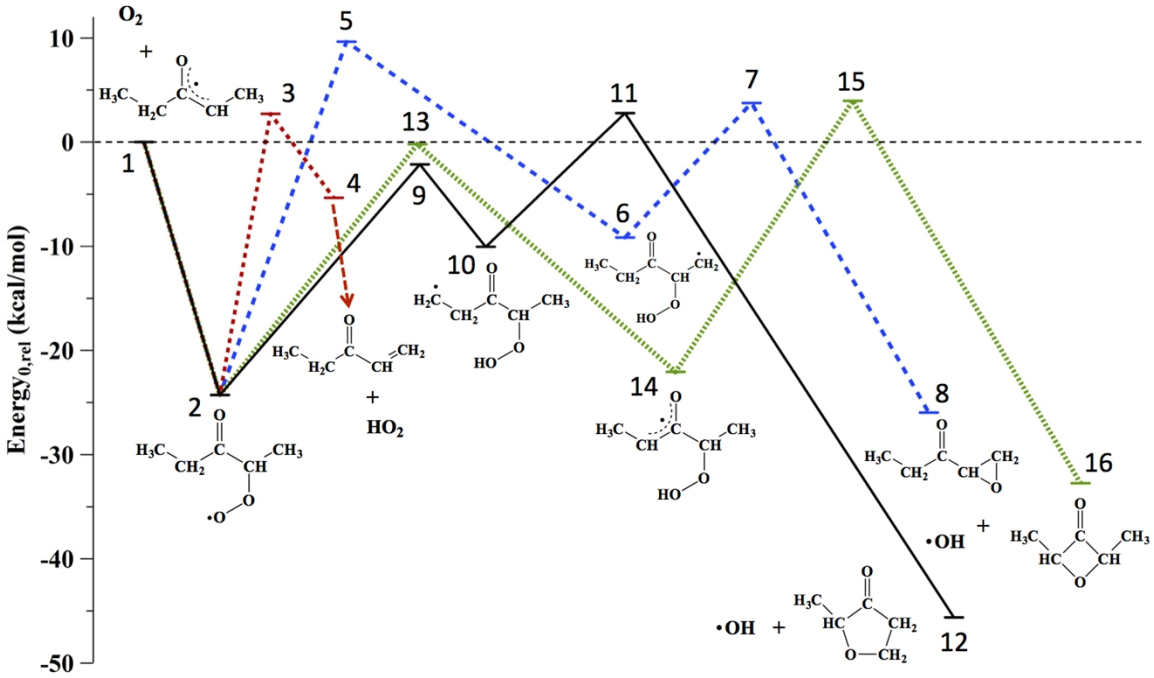
Species	Energy (Hartrees)
O_2	-150.164746
HO_2	-150.741102
OH	-75.649720

Table S6: Optimized stationary point geometries (0K) for small molecules computed in this work (CBS-QB3)

Small Molecules

O_2	O	1.214152	0.856009	-0.97843
	O	0.945073	1.930622	-0.50268
HO_2	O	2.048407	-0.976401	0.701909
	O	2.387916	-1.586283	-0.42797
	H	1.966058	-0.031512	0.474045
OH	O	2.054226	-0.968508	0.670989
	H	1.956918	-0.012814	0.503025

Table S7-8: Stationary point energies and geometries (0K; CBS_QB3) along with the T1 diagnostic of Lee et al.[5] for the $R_s + O_2$ reaction in reference to the given potential energy surface replicated from the main text.



$R_s + O_2$

Stationary Point	Energy (Hartrees)	T1 Diognostic	
1	-270.628779	0.0213	
2	-420.832221	0.0219	
3	-420.789185	0.0301	
4	-270.060951	0.0138	
5	-420.778141	0.0193	
6	-420.808091	0.0136	
7	-420.78751	0.0326	
8	-345.18519	0.013	
9	-420.796948	0.017	
10	-420.809545	0.0139	
11	-420.789064	0.0351	
12	-345.218401	0.0128	
13	-420.793845	0.0201	
14	-420.828683	0.0199	
15	-420.787193	0.0353	
16	-345.195995	Cis	0.0132
	-345.195618	Trans	0.0132

$R_s + O_2$

Stationary Point				
1	C	0.024006	0.046391	-0.33255
	O	0.42873	0.684746	0.641549
	C	0.83363	-0.985525	-0.93972
	C	2.183353	-1.333966	-0.43336
	H	0.434898	-1.521778	-1.79684
	H	2.233433	-2.390351	-0.13899
	H	2.943788	-1.200616	-1.21379
	H	2.439599	-0.712211	0.424234
	C	-1.350532	0.315097	-0.94356
	C	-2.125657	1.420352	-0.23242
	H	-1.21007	0.558953	-2.00427
	H	-1.574494	2.362341	-0.25835
	H	-3.099012	1.575106	-0.70442
	H	-2.285988	1.170703	0.818182
	H	-1.916877	-0.624835	-0.93483
2	C	0.268704	0.100645	-0.11138
	O	0.526566	0.219835	1.062698
	C	-0.71615	0.991764	-0.83989
	C	-1.220453	2.153519	0.011406
	H	-0.240989	1.337433	-1.7662
	H	-0.399234	2.804884	0.317788
	H	-1.942411	2.75056	-0.54985
	H	-1.704194	1.790653	0.919656
	C	1.033317	-0.969693	-0.92309
	C	1.28179	-2.253558	-0.15131
	H	1.945589	-2.913933	-0.71166
	H	1.739102	-2.004809	0.805982
	H	0.337392	-2.766317	0.032956
	O	0.391625	-1.235422	-2.21398
	O	-0.777228	-1.833338	-2.07447
	H	-1.544006	0.357029	-1.17578
	H	1.976765	-0.508578	-1.23465
3	C	0.430997	0.472646	-0.01053
	O	0.680844	1.240088	-0.91802
	C	1.446866	-0.512633	0.537791
	C	2.789546	-0.475547	-0.18468
	H	1.567671	-0.299608	1.608764
	H	3.235979	0.519062	-0.12975

	H	3.484871	-1.19255	0.257635
	H	2.669061	-0.719126	-1.2419
	C	-0.921558	0.459849	0.629773
	C	-1.935562	1.293333	0.186002
	H	-2.776752	1.492848	0.844219
	H	-1.649502	2.08978	-0.49713
	H	-2.460445	0.407523	-0.66437
	O	-1.527666	-1.306527	-0.69655
	O	-2.513931	-0.740153	-1.24203
	H	0.995822	-1.511413	0.491013
	H	-1.055225	-0.166185	1.504956
4	C	0.621486	0.63423	0.186695
	O	1.105151	1.699135	-0.13898
	C	1.431207	-0.653546	0.192371
	C	2.881341	-0.473871	-0.24345
	H	1.368886	-1.078246	1.2034
	H	3.400634	0.228228	0.411567
	H	3.413814	-1.427594	-0.22055
	H	2.936376	-0.071027	-1.25654
	C	-0.810447	0.510856	0.607371
	C	-1.61785	1.569543	0.642155
	H	-2.655579	1.492657	0.944774
	H	-1.237905	2.546062	0.361214
	H	0.908648	-1.374919	-0.45027
	H	-1.168881	-0.476682	0.884303
5	C	0.495012	0.554771	0.196463
	O	0.88221	1.656059	-0.12069
	C	1.370914	-0.677386	0.19443
	C	2.823159	-0.388376	-0.17339
	H	1.285603	-1.156673	1.177443
	H	3.281262	0.302801	0.53718
	H	3.406409	-1.311742	-0.18008
	H	2.892005	0.069244	-1.16197
	C	-0.962555	0.385196	0.675977
	C	-1.94369	1.192427	-0.16651
	H	-2.932312	1.342524	0.261942
	H	-1.540161	2.03136	-0.72359
	H	-2.084363	0.083998	-0.93896
	O	-1.447665	-0.959952	0.584857
	O	-1.741067	-1.082613	-0.81076
	H	0.910285	-1.390859	-0.49828

	H	-0.989542	0.64188	1.742669
6	C	0.478075	0.47648	0.113593
	O	0.793832	1.569427	-0.29329
	C	1.439868	-0.688537	0.208122
	C	2.882343	-0.308741	-0.11483
	H	1.345925	-1.127178	1.208658
	H	3.258403	0.445989	0.579377
	H	3.530704	-1.185677	-0.05299
	H	2.960664	0.107693	-1.1206
	C	-0.964918	0.244258	0.625303
	C	-1.961325	1.142762	-0.00338
	H	-3.010724	1.01614	0.231779
	H	-1.635244	1.961818	-0.62726
	H	-2.311291	-1.503607	-0.99234
	O	-1.34765	-1.141087	0.601009
	O	-1.368261	-1.574295	-0.78805
	H	1.067218	-1.464719	-0.46902
	H	-0.916019	0.415657	1.716015
7	O	0.987049	1.547629	0.284727
	C	0.52668	0.498178	-0.10173
	C	1.338892	-0.755286	-0.33047
	C	2.816848	-0.592984	0.009324
	H	0.875705	-1.568536	0.243107
	H	2.956427	-0.335385	1.061474
	H	3.361241	-1.517989	-0.1938
	H	3.266371	0.207171	-0.58182
	C	-1.82686	-0.020903	0.751233
	H	-1.449798	-0.727622	1.477784
	H	-2.867863	0.267017	0.786377
	O	-1.448814	-0.739781	-1.00713
	C	-0.981425	0.418103	-0.37965
	H	1.178586	-1.042205	-1.37619
	H	-1.314312	1.341587	-0.86129
	O	-0.926267	-0.665766	-2.67384
	H	-1.570121	-1.325737	-2.96941
8	O	0.832791	1.626679	0.058963
	C	0.291735	0.55095	-0.0722
	C	1.047343	-0.762792	-0.132
	C	2.541578	-0.611755	0.13608
	H	0.583227	-1.473334	0.56158

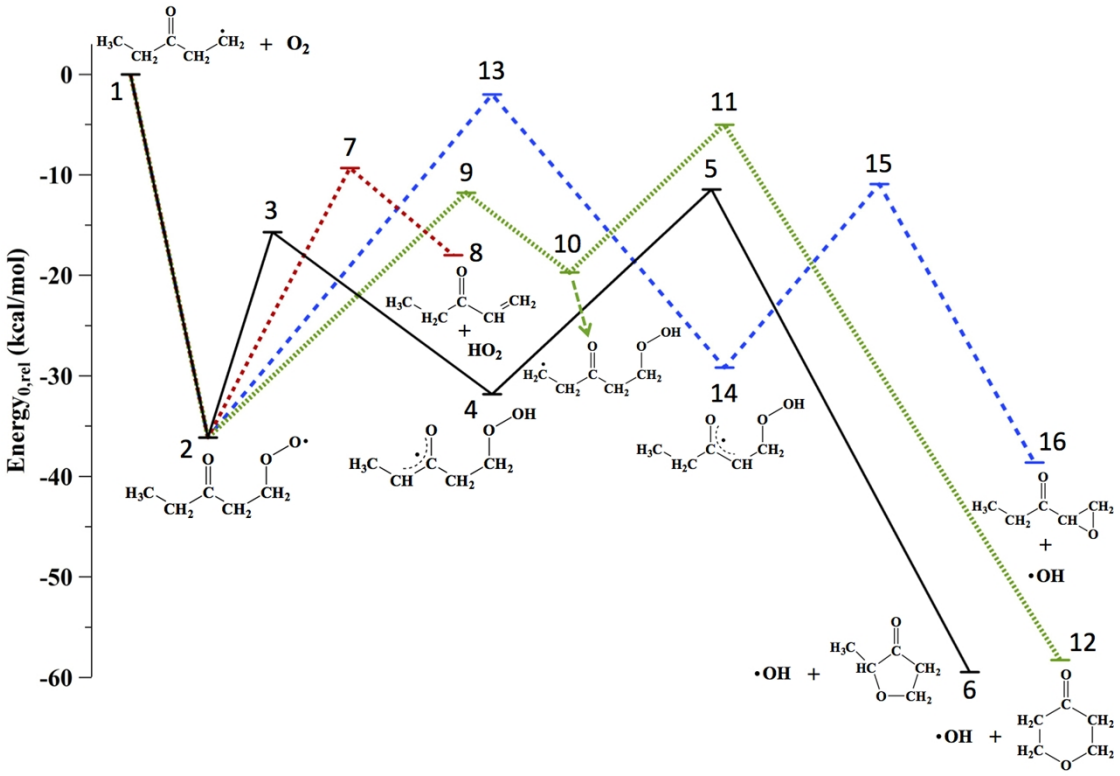
	H	2.724488	-0.222674	1.140028
	H	3.047647	-1.575299	0.043363
	H	2.995008	0.086959	-0.56894
	C	-2.034286	-0.282916	0.731752
	H	-1.55359	-0.872989	1.508168
	H	-3.0383	0.065818	0.958554
	O	-1.82032	-0.728488	-0.60294
	C	-1.209231	0.504071	-0.20765
	H	0.857321	-1.190694	-1.12425
	H	-1.637841	1.405929	-0.63777
9	C	-0.358595	-0.692922	-0.17456
	O	-0.514002	-1.671592	-0.86533
	C	1.673233	-1.237701	1.219545
	H	1.095086	-1.27218	2.14616
	H	1.685952	-2.233396	0.774829
	H	2.693836	-0.935639	1.458614
	C	-1.527511	0.138878	0.35061
	C	-1.646119	1.472944	-0.3551
	H	-1.39457	0.303572	1.424288
	H	-0.342359	1.980044	-0.22118
	H	-1.754584	1.432959	-1.43737
	H	-2.276948	2.216589	0.126811
	C	1.059562	-0.253431	0.228204
	O	1.053336	1.02815	0.87522
	O	0.790229	2.023506	-0.09233
	H	-2.437546	-0.454938	0.200809
	H	1.665774	-0.186807	-0.68004
10	C	-0.414737	-0.59422	-0.23315
	O	-0.638568	-1.68642	-0.69697
	C	-1.523212	0.443219	0.019505
	H	-1.213949	1.392646	-0.42367
	C	1.027515	-0.244822	0.181169
	C	1.429362	-0.995915	1.449596
	H	1.280415	-2.064157	1.287273
	H	2.479379	-0.81005	1.682402
	H	0.817738	-0.679588	2.296905
	C	-1.772305	0.597402	1.48018
	H	-1.226374	1.330794	2.057918
	H	1.996287	2.231726	-0.85901
	H	-2.405315	-0.109606	2.001644
	O	1.221786	1.138265	0.467287

	O	1.104194	1.864536	-0.79023
	H	1.674016	-0.536302	-0.65346
	H	-2.405376	0.063585	-0.50116
11	C	-1.042772	1.766916	-0.23988
	H	-0.820204	2.604944	0.403295
	H	-1.067604	1.953923	-1.30537
	C	-0.713952	-0.687444	-0.0063
	O	-1.123938	-1.784655	-0.27603
	C	-1.627754	0.514585	0.29367
	H	-1.74019	0.562245	1.382443
	C	1.312223	-0.825633	1.471173
	H	2.384182	-0.639352	1.52345
	H	0.82262	-0.254529	2.264303
	H	1.122228	-1.890004	1.627123
	C	0.795882	-0.395589	0.094471
	O	2.654933	1.126921	-0.17438
	H	2.675699	1.642492	-0.99217
	O	1.000537	0.987767	-0.15421
	H	1.282042	-0.981774	-0.69126
	H	-2.606673	0.274435	-0.1333
12	C	1.642363	-0.728945	-0.10159
	O	0.372403	-1.37943	0.039223
	H	2.35358	-1.262478	0.527672
	H	1.984919	-0.784906	-1.14493
	C	-0.068699	0.925492	-0.07079
	O	-0.678556	1.961244	-0.11898
	C	1.395581	0.723025	0.314227
	H	1.479071	0.847058	1.398996
	C	-1.960933	-0.765662	0.278539
	H	-2.329323	-1.748439	-0.0206
	H	-1.845784	-0.75354	1.364636
	H	-2.692274	-0.00697	-0.00724
	C	-0.632946	-0.466617	-0.39251
	H	-0.744418	-0.517292	-1.49024
	H	2.036067	1.46508	-0.16409
13	C	0.197687	0.767213	0.014752
	O	0.245525	1.975188	-0.06478
	C	1.424174	-0.096653	0.044714
	H	0.902579	-1.069426	-0.76712
	C	-1.159945	0.029832	0.005102

	C	1.755839	-0.832795	1.322805
	H	0.91129	-1.431911	1.669315
	H	2.617645	-1.487893	1.182616
	H	2.008096	-0.115723	2.115014
	C	-2.074133	0.531594	-1.10657
	H	-3.058443	0.06954	-1.01673
	H	-2.174573	1.615395	-1.03599
	H	-1.65197	0.278382	-2.08012
	O	-0.932343	-1.392271	-0.056
	O	-0.065589	-1.644893	-1.14287
	H	2.262881	0.373148	-0.46737
	H	-1.630393	0.166493	0.984684
14	C	-0.379645	-0.794252	-0.0373
	O	-0.426651	-2.014883	-0.23082
	C	-1.545549	0.038797	-0.0627
	H	1.642819	2.066007	-1.34323
	C	0.990526	-0.173018	0.277733
	C	1.43707	-0.536703	1.692473
	H	1.419584	-1.622149	1.798466
	H	2.448346	-0.172295	1.881177
	H	0.762609	-0.099735	2.432793
	C	-2.893285	-0.512815	-0.33987
	H	-2.848723	-1.592176	-0.4835
	H	-3.584623	-0.284309	0.48122
	H	-3.324936	-0.048241	-1.23587
	O	1.002679	1.254046	0.231954
	O	0.789254	1.652789	-1.15342
	H	1.700131	-0.56578	-0.4586
	H	-1.422621	1.101674	0.106345
15	C	0.455523	1.01297	0.003269
	O	0.768825	2.151789	-0.2576
	C	-1.471753	0.229368	1.547531
	H	-2.378746	-0.374611	1.512056
	H	-0.747844	-0.273366	2.193696
	H	-1.710328	1.204777	1.980255
	C	-0.927315	0.405397	0.137989
	C	2.447289	-0.271239	-1.04316
	H	2.605442	-1.310187	-1.3449
	H	2.253325	0.344188	-1.92217
	H	3.387204	0.075498	-0.59094
	C	1.347707	-0.171557	-0.051

	O	-2.014498	-1.716211	-0.64259
	H	-1.808305	-1.997508	-1.54514
	O	-0.523498	-0.836655	-0.48334
	H	-1.642891	0.93018	-0.5004
	H	1.39167	-0.809311	0.824209
16 Cis	O	0.000011	-1.198049	-0.54647
	C	-0.000006	0.867996	-0.22285
	O	-0.000016	2.025259	0.07101
	C	1.066636	-0.211621	-0.44888
	C	2.062963	-0.485582	0.660466
	H	2.603157	-1.413713	0.459744
	H	2.786642	0.331721	0.720843
	H	1.559187	-0.580145	1.624591
	C	-2.062949	-0.485617	0.660474
	H	-2.603128	-1.413758	0.459754
	H	-1.559169	-0.580172	1.624596
	H	-2.786642	0.331674	0.720853
	C	-1.066632	-0.211639	-0.44888
	H	1.575442	-0.092572	-1.4148
	H	-1.575443	-0.092599	-1.4148
16 Trans	O	0	-1.273362	0
	C	0	0.819592	0
	O	0	2.013507	0
	C	-0.95122	-0.282627	0.483795
	C	-2.317197	-0.3705	-0.17095
	H	-2.79339	-1.320434	0.082604
	H	-2.954703	0.444104	0.183192
	H	-2.235288	-0.305184	-1.25823
	C	0.95122	-0.282627	-0.4838
	C	2.317197	-0.3705	0.170948
	H	2.235288	-0.305184	1.258225
	H	2.79339	-1.320434	-0.0826
	H	2.954703	0.444104	-0.18319
	H	1.034388	-0.323957	-1.57712
	H	-1.034388	-0.323957	1.577122

Table S9-10: Stationary point energies and geometries (0K; CBS_QB3) along with the T1 diagnostic of Lee et al.[5] for the $R_s + O_2$ reaction in reference to the given potential energy surface replicated from the main text.



$R_p + O_2$

Stationary Point	Energy (Hartrees)	T1 Diognostic
1	-270.6086	0.0137
2	-420.830932	0.0216
3	-420.798387	0.0227
4	-420.824073	0.0201
5	-420.7916	0.0356
6	-345.218401	0.013
7	-420.788217	0.0248
8	-270.060951	0.0138
9	-420.792153	0.0176
10	-420.804769	0.0137
11	-420.781352	0.0353
12	-345.216488	0.0128
13	-420.776517	0.0443
14	-420.819837	0.0197
15	-420.790756	0.0362
16	-345.18519	0.013

$R_p + O_2$

Stationary Point				
1	C	0.08588	0.070029	0.287947
	O	0.154515	0.132184	1.492073
	C	1.355235	0.163561	-0.59275
	C	1.7599	-1.196785	-1.04171
	H	1.147736	0.810462	-1.45155
	H	1.43427	-1.597029	-1.99332
	H	2.26396	-1.863281	-0.35345
	C	-1.244209	-0.09841	-0.43332
	C	-1.904257	1.270552	-0.68066
	H	-1.095447	-0.621279	-1.38245
	H	-1.282745	1.910328	-1.31357
	H	-2.868418	1.146066	-1.17858
	H	-2.073088	1.789639	0.265215
	H	-1.890068	-0.709642	0.201166
	H	2.12706	0.624902	0.028209
2	C	-0.613293	0.413409	0.260178
	O	-0.708821	0.704797	1.43005
	C	-1.787838	-0.096518	-0.55504
	H	-1.820263	0.465179	-1.49751
	C	0.713658	0.566019	-0.4886
	H	0.813226	-0.183282	-1.278
	C	1.925636	0.513353	0.42225
	H	1.752263	1.0592	1.348607
	H	2.830394	0.86126	-0.0772
	C	-3.124051	-0.041074	0.179192
	H	-3.385634	0.986519	0.440426
	H	-3.922849	-0.451408	-0.44259
	H	-3.0798	-0.611385	1.10828
	O	2.183238	-0.85655	0.868646
	O	2.551492	-1.630058	-0.13245
	H	0.68565	1.541892	-0.99022
	H	-1.541272	-1.126104	-0.84835
3	C	-0.055328	-0.908567	-0.07724
	O	-0.073784	-1.916235	-0.75575
	C	-1.312894	-0.149901	0.197056
	H	-0.958694	0.968877	-0.49231

	C	1.259113	-0.336248	0.451958
	H	1.190043	-0.160726	1.5296
	C	1.675308	0.978811	-0.23629
	H	1.815159	0.838227	-1.31073
	H	2.599381	1.357123	0.207258
	C	-1.620914	0.37369	1.580617
	H	-0.83247	1.031055	1.953948
	H	-2.555949	0.937029	1.575332
	H	-1.737951	-0.451716	2.29485
	O	0.723788	2.029147	-0.02974
	O	-0.330021	1.873543	-0.93854
	H	2.03462	-1.084213	0.270753
	H	-2.154638	-0.57589	-0.34831
4	C	0.66688	0.917634	0.139411
	O	1.102806	1.923931	-0.43372
	C	1.502267	-0.221174	0.407144
	H	-2.294261	-2.456385	-0.31741
	C	-0.804254	0.846928	0.53663
	H	-0.953663	0.212251	1.412897
	C	-1.671898	0.320031	-0.60925
	H	-1.504055	0.90679	-1.51754
	H	-2.734816	0.361501	-0.34583
	C	2.934272	-0.257832	0.025446
	H	3.243195	0.698273	-0.39667
	H	3.566394	-0.4981	0.889314
	H	3.11758	-1.04834	-0.71441
	O	-1.326332	-1.001483	-1.01569
	O	-1.631257	-1.889945	0.099672
	H	1.050171	-1.095621	0.864123
	H	-1.133149	1.860803	0.778542
5	C	0.434318	1.512994	0.011427
	H	0.397798	2.329951	0.733042
	H	0.782012	1.901419	-0.95029
	C	0.746486	-0.870126	-0.21315
	O	1.334113	-1.532265	-1.04964
	C	1.322318	0.351122	0.483445
	H	1.249468	0.23128	1.568732
	C	-0.684453	-1.033599	0.086955
	O	-1.802435	2.403963	-0.34563
	H	-2.182425	2.14019	-1.19558
	O	-0.903411	0.983554	-0.15146

	H	2.366922	0.496278	0.207629
	H	-0.993998	-0.94611	1.121618
	C	-1.590948	-1.735503	-0.85665
	H	-1.712439	-2.783939	-0.55405
	H	-2.585808	-1.282146	-0.84371
	H	-1.190288	-1.724446	-1.87031
6	C	1.642363	-0.728945	-0.10159
	O	0.372403	-1.37943	0.039223
	H	2.35358	-1.262478	0.527672
	H	1.984919	-0.784906	-1.14493
	C	-0.068699	0.925492	-0.07079
	O	-0.678556	1.961244	-0.11898
	C	1.395581	0.723025	0.314227
	H	1.479071	0.847058	1.398996
	C	-1.960933	-0.765662	0.278539
	H	-2.329323	-1.748439	-0.0206
	H	-1.845784	-0.75354	1.364636
	H	-2.692274	-0.00697	-0.00724
	C	-0.632946	-0.466617	-0.39251
	H	-0.744418	-0.517292	-1.49024
	H	2.036067	1.46508	-0.16409
7	C	0.871213	0.214341	-0.00289
	O	0.951138	1.023714	-0.90241
	C	2.07381	-0.577033	0.489256
	H	2.200664	-0.35305	1.556617
	C	-0.436034	-0.077083	0.682401
	H	-1.019841	-0.95981	-0.21542
	C	-1.468384	0.853409	0.559762
	H	-1.341077	1.694585	-0.11057
	H	-2.268924	0.913677	1.284853
	C	3.356009	-0.294633	-0.28744
	H	3.619972	0.762883	-0.23189
	H	4.186484	-0.880714	0.112965
	H	3.235599	-0.543073	-1.34361
	O	-2.657814	-0.17875	-0.79798
	O	-1.963941	-1.229457	-0.97663
	H	-0.395249	-0.687059	1.58295
	H	1.810993	-1.642261	0.450783
8	C	0.621486	0.63423	0.186695
	O	1.105151	1.699135	-0.13898

	C	1.431207	-0.653546	0.192371
	C	2.881341	-0.473871	-0.24345
	H	1.368886	-1.078246	1.2034
	H	3.400634	0.228228	0.411567
	H	3.413814	-1.427594	-0.22055
	H	2.936376	-0.071027	-1.25654
	C	-0.810447	0.510856	0.607371
	C	-1.61785	1.569543	0.642155
	H	-2.655579	1.492657	0.944774
	H	-1.237905	2.546062	0.361214
	H	0.908648	-1.374919	-0.45027
	H	-1.168881	-0.476682	0.884303
9	C	0.439877	-0.726914	0.17187
	O	0.632806	-1.354302	1.184667
	C	1.547224	0.095909	-0.50074
	H	1.570118	-0.150631	-1.56714
	C	-0.93536	-0.701546	-0.49709
	H	-0.882695	-0.257771	-1.49148
	C	-1.964206	0.057227	0.347572
	H	-2.127432	-0.444713	1.303419
	H	-2.911388	0.135472	-0.19585
	C	1.369108	1.584762	-0.31352
	H	-0.000845	1.92873	-0.43503
	H	1.500851	1.944324	0.705807
	H	1.821786	2.223264	-1.0691
	O	-1.521213	1.361488	0.738608
	O	-1.127669	2.087887	-0.40497
	H	-1.277243	-1.736157	-0.5962
	H	2.493561	-0.227107	-0.05147
10	C	-0.632795	0.429139	0.265059
	O	-0.764622	0.753518	1.421046
	C	-1.771679	-0.253954	-0.51709
	H	-1.818891	0.173908	-1.52464
	C	0.674278	0.667707	-0.48881
	H	0.746012	0.03095	-1.37205
	C	1.904506	0.480188	0.391218
	H	1.746801	0.956593	1.362021
	H	2.800222	0.894395	-0.08389
	C	-1.508335	-1.719613	-0.57263
	H	3.375735	-1.883446	-0.25817
	H	-1.741965	-2.336898	0.285275

	H	-0.885988	-2.146314	-1.34864
	O	2.125243	-0.885089	0.729987
	O	2.490849	-1.578677	-0.49978
	H	-2.698947	-0.03277	0.015922
	H	0.641369	1.706439	-0.84413
11	C	0.930182	0.661011	-0.17503
	O	1.811933	1.472496	-0.00951
	C	1.241252	-0.835463	-0.29765
	H	0.934529	-1.173771	-1.29353
	C	0.558968	-1.670529	0.737152
	H	0.380929	-2.71813	0.537507
	H	0.637824	-1.390782	1.781854
	C	-1.446566	0.284117	0.669958
	H	-1.106201	0.349999	1.708289
	H	-2.46874	0.66037	0.627333
	C	-0.531135	1.073652	-0.27097
	H	-0.882866	0.903677	-1.2948
	O	-2.730605	-1.172267	-0.7426
	H	-2.972619	-2.086018	-0.5391
	O	-1.48146	-1.105945	0.328574
	H	2.333087	-0.931836	-0.23158
	H	-0.587681	2.143798	-0.05965
12	O	-1.724059	0.000004	0.16926
	C	1.143418	-0.000004	0.066721
	O	2.281124	-0.000007	-0.34316
	C	0.357698	1.274388	0.334865
	C	0.357691	-1.27439	0.334868
	H	0.909858	-2.12702	-0.06531
	H	0.26469	1.395944	1.420468
	C	-1.057194	-1.175102	-0.26593
	H	-0.997902	-1.188593	-1.36493
	H	-1.674296	-2.016771	0.050593
	C	-1.057187	1.175106	-0.26593
	H	-1.674285	2.016779	0.050589
	H	-0.997895	1.188594	-1.36493
	H	0.909869	2.127014	-0.06531
	H	0.264682	-1.395944	1.420471
13	C	0.812374	0.220421	0.094986
	O	0.897157	1.123655	-0.72582
	C	2.02412	-0.612439	0.498168

	H	2.227776	-0.397418	1.555749
	C	-0.471903	-0.123083	0.722367
	H	-1.310717	-1.104937	-0.00728
	C	-1.61543	0.820545	0.521329
	H	-1.329017	1.762771	0.05856
	H	-2.183311	0.975194	1.442441
	C	3.261019	-0.346075	-0.35474
	H	3.535888	0.709284	-0.32156
	H	4.108259	-0.938607	-0.00148
	H	3.077072	-0.599637	-1.40093
	O	-2.558983	0.216864	-0.46769
	O	-2.383449	-1.130988	-0.42011
	H	-0.433401	-0.690273	1.650069
	H	1.741826	-1.671641	0.467751
14	C	0.852485	0.177733	-0.03133
	O	1.044953	1.34365	-0.38714
	C	2.009277	-0.780192	0.235582
	H	1.919575	-1.141205	1.267998
	C	-0.489809	-0.320088	0.14976
	C	-1.669595	0.564043	-0.05178
	H	-1.452134	1.323763	-0.80783
	H	-1.931109	1.087999	0.880612
	C	3.381885	-0.158426	-0.00392
	H	3.532007	0.714676	0.63392
	H	4.174023	-0.881144	0.205735
	H	3.48451	0.176409	-1.03798
	O	-2.810644	-0.128687	-0.54844
	O	-3.250828	-1.036257	0.501742
	H	-0.668177	-1.341707	0.466407
	H	1.865414	-1.667153	-0.39418
	H	-4.118288	-0.657143	0.699052
15	O	0.824035	1.579774	-0.32428
	C	0.233907	0.563437	0.006814
	C	0.956681	-0.731189	0.343002
	C	2.438597	-0.700331	-0.02224
	H	0.832383	-0.907044	1.420115
	H	2.949059	0.123358	0.478891
	H	2.921942	-1.63685	0.264819
	H	2.573518	-0.56108	-1.09708
	C	-2.076882	-0.520767	0.553346
	H	-1.597535	-1.23636	1.223633

	H	-3.088095	-0.273494	0.883258
	O	-1.989798	-0.88881	-0.79494
	C	-1.235216	0.608593	0.102592
	H	0.435171	-1.557185	-0.15117
	H	-1.704136	1.507411	-0.2784
	O	-2.325195	-2.611366	-0.89685
	H	-2.102074	-2.658096	-1.8385
16	O	0.832791	1.626679	0.058963
	C	0.291735	0.55095	-0.0722
	C	1.047343	-0.762792	-0.132
	C	2.541578	-0.611755	0.13608
	H	0.583227	-1.473334	0.56158
	H	2.724488	-0.222674	1.140028
	H	3.047647	-1.575299	0.043363
	H	2.995008	0.086959	-0.56894
	C	-2.034286	-0.282916	0.731752
	H	-1.55359	-0.872989	1.508168
	H	-3.0383	0.065818	0.958554
	O	-1.82032	-0.728488	-0.60294
	C	-1.209231	0.504071	-0.20765
	H	0.857321	-1.190694	-1.12425
	H	-1.637841	1.405929	-0.63777

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