Probing the Transition State-to-Intermediate Continuum: Mechanistic Distinction Between a Dry vs Wet Perepoxide in the Singlet Oxygen 'Ene' Reaction at the Air-Water Interface

Belaid Malek,[1] Wenchao Lu,[2,3] Prabhu Prasad Mohapatra,[1,3] Niluksha Walalawela,[1,3] Shakeela Jabeen,[1,3] Jianbo Liu,[2,3*] and Alexander Greer[1,3*]

[1] Department of Chemistry, Brooklyn College of the City University of New York, Brooklyn, New York 11210, United States

[2] Department of Chemistry and Biochemistry, Queens College of the City University of New York, 65-30 Kissena Blvd., Queens, New York, United States

[3] Ph.D. Program in Chemistry, The Graduate Center of the City University of New York, 365 Fifth Avenue, New York, New York 10016, United States

Supporting Information

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METHODS

Instrumentation and analysis. An NMR instrument was used that operated at 400 MHz for ^{1}H NMR and 100.6 MHz for ^{13}C NMR. After reaction of singlet oxygen with surfactants 7C, 9C, and 11C, the ratio of **1a** and **1b** or **2a** and **2b** or **3a** and **3b** was determined by ^{1}H NMR analysis of the 11.2 and 10.8 ppm proton signals of the 2° and 3° hydroperoxides, respectively, and is based on our previous work,[1] in which benzoic acid was used as an internal standard. Our photoreactor and bubbling reactor were tuned to generate near the same percent yield hydroperoxide products for comparison purposes. Compare entry 1 and 4 (Table 1, main manuscript), in which the percent yield of hydroperoxides from the photoreactor was 85% and from the $^{1}O_2$ bubbler was 67.4%. In the photoreactor, the concentrations of 7C, 9C, and 11C used ranged from 0.5-5.0 mM. In these experiments, the surfactants were below their CMCs. The CMC of 9C was measured previously in our laboratory to be 9.7 mM (26 °C).[2] In the photoreactor, evaporation of water in the cuvette was not discernable. In the bubble reactor, evaporation of water was discernable and replenishing of it was required during the reaction.

Water layer surface-to-volume (S/V) ratios. The photoreactor consisted of a 1 cm × 1 cm curvet with a 1.7 cm^2 of curved surface (meniscus), where the S/V ratio is estimated to be 2.72. For the bubbler, at any given instant, ~9 bubbles were present with an average diameter of 0.7 cm, where the S/V ratio is estimated to be 1.38. The number of surfactant molecules at the water interface was estimated. The surfactant molecule bears a cross-section of ~9 Å^2. Assuming the gas-liquid interface of the photoreactor is fully loaded, the maximum number of surfactants at the surface is 1.9×10^{15}. For the bubbler, the estimated total surface is 13.9 cm^2, in which the maximum number of surfactants that could be loaded at the surface is 1.5×10^{16}. Formation of a monolayer is calculated 2.5×10^{-3} mM surfactant in 10 mL, which was below the actual bulk concentration of 0.1 mM used in the experiment. This analysis leads us to conclude that water was fully covered by a monolayer in the bubbler. The proximity of the surfactant molecules at the air/water interface at equilibrium was estimated. The distance between the surfactant molecules at the air-water interface in the static cuvette photoreactor is ~3 Å from a side-to-side (cylinder length-to-cylinder length type of arrangement). It is longer when the surfactants are laying flat on the surface with a low-end value of 4.3 Å for laying down. The intermolecular distance is larger than 3 Å and is far less than CMC. If the molecule, with its own dimensions negligible, is placed at the center of each sphere, then the distance would be 2r = 15 Å =1.5 nm. The total area available

for 3.61×10^{17} surfactant molecules are 1 cm^2 = 1×10^{16} Å. In our case the molecules are well packed. We cannot exactly assume surface area of interface is 1 cm^2.

Area for 4 surfactant molecules = $\frac{1\times10^{16}}{3.61\times10^{17}} \times 4$

Distance between two surfactant molecules = $\sqrt{\frac{1\times10^{16}}{3.61\times10^{17}} \times 4}$ = 0.33 Å̄

The number of surfactant molecules per area is $\frac{3.61\times10^{17}}{1\times10^{16}}$ = 36 surfactant molecules per $Å^2$

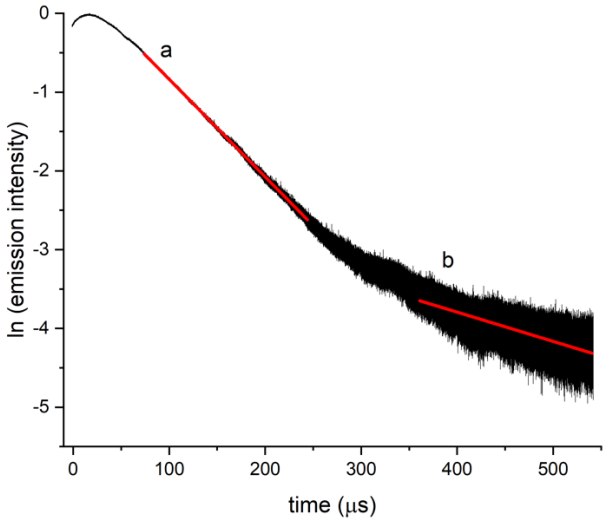

Figure S1. Phosphorescence from $^1O_2$ at 1270 nm was observed was observed with 355-nm pulsed irradiation into the cuvette reactor. Two $^1O_2$ decay curves are shown with 9C (1 mM) in D_2O (0.60 mL): (a) fast decay component attributed to $^1O_2$ at the air–D_2O interface [y = -12400x + 0.403, R^2 = 0.998, $1/k_{obs} = \tau_\Delta(^1O_2)$ is 81 μs], and (b) slow decay component attributed to $^1O_2$ in the air space [y = -3710x + 2.31, R^2 = 0.599, $1/k_{obs} = \tau_\Delta(^1O_2)$ = is 270 μs], in which the decay fitting are of higher quality in the former than the latter. Experimental data (black line) and fitting (red line) are shown.

COMPUTATIONAL DATA

Energies and Cartesian Coordinates of structures at B3LYP/6-31+G(d) in Figure 5a:

singlet O_2
O1 0.000000 0.000000 0.607559
O2 0.000000 0.000000 -0.607559

Zero-point correction=	0.003714 (Hartree/Particle)
Thermal correction to Energy=	0.006077
Thermal correction to Enthalpy=	0.007021
Thermal correction to Gibbs Free Energy=	-0.015229
Sum of electronic and zero-point Energies=	-150.262338
Sum of electronic and thermal Energies=	-150.259975
Sum of electronic and thermal Enthalpies=	-150.259030
Sum of electronic and thermal Free Energies=	-150.281280

11C
C1 3.471381 -0.470007 0.083527
H2 3.585380 -0.253870 -0.988670
C3 2.127345 0.078913 0.581219
H4 2.025579 -0.133500 1.656742
H5 2.126015 1.175867 0.487022
C6 0.912583 -0.492782 -0.163463
H7 0.911937 -1.589558 -0.065075
H8 1.016516 -0.284211 -1.239670
C9 -0.430992 0.060817 0.331902
H10 -0.432308 1.156655 0.227695
H11 -0.531274 -0.141409 1.409327
C12 -1.649989 -0.515643 -0.402796
H13 -1.650336 -1.611949 -0.294431
H14 -1.549102 -0.315919 -1.481487
C15 -2.987038 0.050067 0.100384
H16 -2.998369 1.141222 -0.020687
H17 -3.093793 -0.147217 1.175078
C18 -4.196957 -0.534692 -0.625697
H19 -4.262008 -1.620556 -0.488517
H20 -4.162883 -0.322037 -1.700814
S21 -5.798856 0.145462 -0.028758
O22 -6.820763 -0.562094 -0.860149
O23 -5.840295 -0.208823 1.425130
O24 -5.705697 1.615904 -0.293608
C25 4.685196 0.104850 0.842916
H26 4.691388 1.196077 0.737936
H27 4.547132 -0.097003 1.917255
H28 3.474181 -1.566712 0.175756
C29 5.992930 -0.497363 0.400810
C30 7.056102 0.104161 -0.161976
H31 6.061099 -1.577374 0.555306
C32 7.155584 1.581295 -0.464065
H33 7.345100 1.745041 -1.534889

H34	6.255097	2.138824	-0.195776
H35	8.002693	2.031483	0.074221
C36	8.283008	-0.691691	-0.548302
H37	8.488711	-0.605305	-1.625526
H38	9.178363	-0.318442	-0.029106
H39	8.171702	-1.754944	-0.309288

Zero-point correction=	0.339250 (Hartree/Particle)
Thermal correction to Energy=	0.359083
Thermal correction to Enthalpy=	0.360027
Thermal correction to Gibbs Free Energy=	0.286784
Sum of electronic and zero-point Energies=	-1094.707141
Sum of electronic and thermal Energies=	-1094.687309
Sum of electronic and thermal Enthalpies=	-1094.686364
Sum of electronic and thermal Free Energies=	-1094.759607

TS1 (determined from relaxed 2D-PES in Figure 6)

C1	-2.70653200	-0.64718800	-0.36354200
H2	-2.64786200	-1.73477300	-0.20754000
C3	-1.42052600	0.00524800	0.16006500
H4	-1.46681200	1.09096900	-0.01110200
H5	-1.36704600	-0.12995200	1.25156200
C6	-0.14421900	-0.56034500	-0.47833100
H7	-0.17986300	-0.39707700	-1.56654800
H8	-0.12314400	-1.65205000	-0.33464600
C9	1.14922600	0.04510000	0.08467800
H10	1.18031400	-0.11733500	1.17295000
H11	1.13426100	1.13609800	-0.05946200
C12	2.42616500	-0.53031300	-0.54502600
H13	2.40500900	-0.35184900	-1.63180200
H14	2.42855500	-1.62438500	-0.41557600
C15	3.71665400	0.05617100	0.04766100
H16	3.74286100	-0.12330400	1.13046800
H17	3.72989400	1.14520600	-0.09042600
C18	4.98150000	-0.53227700	-0.57441200
H19	5.03705500	-0.32265600	-1.64915500
H20	5.03236600	-1.61794300	-0.42940600
S21	6.53006300	0.14453500	0.15272500
O22	7.61477000	-0.56444500	-0.59335400
O23	6.46158100	1.61533200	-0.11621700
O24	6.45118800	-0.21243400	1.60452400
C25	-3.97612600	-0.10559900	0.31003800
H26	-3.89209300	-0.17850900	1.40461600
H27	-4.08084500	0.99124500	0.11050900
H28	-2.78275500	-0.49186600	-1.44925500
C29	-5.23985600	-0.71175400	-0.16232800
C30	-6.49159300	-0.45927800	0.40523400
H31	-5.20109300	-1.37233500	-1.02674900
C32	-6.61824900	0.38682800	1.63153700
H33	-5.97948200	0.02786300	2.44794400
H34	-6.28454800	1.41245100	1.38699100

H35 -7.65157800 0.43284500 1.98801100
C36 -7.71462800 -1.16304800 -0.10956000
H37 -8.01624700 -1.96145300 0.58457000
H38 -8.55506200 -0.46341000 -0.18750000
H39 -7.54289500 -1.61321500 -1.09246700
O40 -6.23581300 0.97770200 -1.05554200
O41 -5.68808600 2.04654500 -0.61512000

TS2

C1 -2.691001 -0.670309 -0.223840
H2 -2.631070 -1.651003 0.271841
C3 -1.404759 0.114134 0.066346
H4 -1.445682 1.084626 -0.449577
H5 -1.357543 0.341828 1.142613
C6 -0.128894 -0.634252 -0.344163
H7 -0.157530 -0.833978 -1.426512
H8 -0.116177 -1.619752 0.147277
C9 1.165893 0.114509 0.001408
H10 1.187673 0.317580 1.083074
H11 1.162241 1.097858 -0.492589
C12 2.441432 -0.645106 -0.391498
H13 2.434501 -0.825226 -1.478220
H14 2.427230 -1.639415 0.082666
C15 3.733540 0.087457 0.001416
H16 3.746473 0.260390 1.085526
H17 3.762832 1.076232 -0.474557
C18 4.996500 -0.680516 -0.383680
H19 5.072983 -0.812485 -1.469406
H20 5.024322 -1.669386 0.089205
S21 6.545771 0.166099 0.133821
O22 7.628895 -0.750255 -0.338379
O23 6.508466 1.485718 -0.571313
O24 6.437277 0.269398 1.623492
C25 -3.958357 0.065393 0.238045
H26 -3.875765 0.363044 1.293682
H27 -4.102868 1.025572 -0.321250
H28 -2.764749 -0.869412 -1.302499
C29 -5.215555 -0.664977 -0.001546
C30 -6.538744 -0.175981 0.401670
H31 -5.184108 -1.627980 -0.506178
C32 -6.663083 0.933078 1.412982
H33 -6.279202 0.600252 2.384424
H34 -6.091552 1.801534 1.072961
H35 -7.709478 1.230781 1.534099
C36 -7.691606 -1.149677 0.322774
H37 -7.745254 -1.736044 1.249262
H38 -8.637908 -0.611975 0.199912
H39 -7.571413 -1.842858 -0.516221
O40 -6.270585 0.334200 -1.043743
O41 -5.823115 1.625904 -1.162578

Zero-point correction=	0.344629 (Hartree/Particle)
Thermal correction to Energy=	0.365903
Thermal correction to Enthalpy=	0.366848
Thermal correction to Gibbs Free Energy=	0.290892
Sum of electronic and zero-point Energies=	-1244.987259
Sum of electronic and thermal Energies=	-1244.965984
Sum of electronic and thermal Enthalpies=	-1244.965040
Sum of electronic and thermal Free Energies=	-1245.040995

secondary R-OOH

C1 2.777025 -0.265390 -0.408020
H2 2.769117 -0.216560 -1.508231
C3 1.454715 0.298886 0.130496
H4 1.449064 0.223363 1.228592
H5 1.397063 1.374032 -0.100860
C6 0.209254 -0.401136 -0.431306
H7 0.260389 -1.475733 -0.197659
H8 0.218998 -0.327663 -1.530080
C9 -1.110870 0.173536 0.101473
H10 -1.152015 1.251067 -0.120246
H11 -1.126864 0.088988 1.198879
C12 -2.362917 -0.504158 -0.474043
H13 -2.326550 -1.581845 -0.248947
H14 -2.343962 -0.421189 -1.572433
C15 -3.675287 0.089292 0.061268
H16 -3.714308 1.163934 -0.160093
H17 -3.709145 -0.007145 1.154401
C18 -4.918443 -0.574748 -0.527516
H19 -4.958333 -1.643044 -0.284065
H20 -4.953536 -0.465749 -1.617995
S21 -6.491190 0.144445 0.100337
O22 -7.550629 -0.641596 -0.603904
O23 -6.444319 -0.079333 1.579705
O24 -6.431941 1.586335 -0.298337
C25 4.003986 0.488739 0.123711
H26 3.920638 1.553312 -0.135485
H27 4.026627 0.428389 1.217541
H28 2.860906 -1.327794 -0.146819
C29 5.328379 -0.021491 -0.444579
C30 6.587170 0.764625 -0.096676
H31 5.247063 -0.072688 -1.540937
C32 6.673289 1.571411 0.969684
H33 5.833894 1.745706 1.636035
H34 6.499900 -1.439831 1.497623
H35 7.595829 2.099453 1.203708
C36 7.756341 0.533267 -1.025769
H37 7.531375 0.908042 -2.034511
H38 8.662643 1.035769 -0.671557
H39 7.969686 -0.538390 -1.130079
O40 5.554390 -1.430314 -0.158587
O41 5.568089 -1.632911 1.279308

Zero-point correction=	0.347101 (Hartree/Particle)
Thermal correction to Energy=	0.369141
Thermal correction to Enthalpy=	0.370085
Thermal correction to Gibbs Free Energy=	0.291264
Sum of electronic and zero-point Energies=	-1245.042653
Sum of electronic and thermal Energies=	-1245.020613
Sum of electronic and thermal Enthalpies=	-1245.019669
Sum of electronic and thermal Free Energies=	-1245.098489

tertiary R-OOH

C1	-2.658559	-1.353871	-0.079075
H2	-2.514928	-2.334019	0.403104
C3	-1.438318	-0.470513	0.249464
H4	-1.559729	0.507815	-0.237989
H5	-1.415201	-0.272443	1.331621
C6	-0.106215	-1.098821	-0.182057
H7	-0.130113	-1.287394	-1.266634
H8	-0.001409	-2.085409	0.295902
C9	1.120636	-0.240624	0.155930
H10	1.149281	-0.059532	1.241219
H11	1.013905	0.748699	-0.314609
C12	2.450910	-0.867759	-0.285839
H13	2.423013	-1.042096	-1.373229
H14	2.552763	-1.861111	0.179587
C15	3.676267	-0.010078	0.064549
H16	3.715862	0.157466	1.148850
H17	3.584678	0.979211	-0.402747
C18	4.993768	-0.641128	-0.381075
H19	5.024798	-0.782128	-1.467966
H20	5.157439	-1.612839	0.099831
S21	6.465043	0.381546	0.036226
O22	7.615433	-0.420053	-0.482834
O23	6.242287	1.673279	-0.686460
O24	6.426988	0.504720	1.527561
C25	-3.963122	-0.768128	0.388547
H26	-4.026511	-0.555328	1.456973
H27	-4.832462	2.136740	-0.819478
H28	-2.701604	-1.542312	-1.160685
C29	-5.013736	-0.501471	-0.397617
C30	-6.350182	0.080860	0.014574
H31	-4.937969	-0.714017	-1.467226
C32	-6.522410	0.320033	1.515399
H33	-6.461703	-0.626003	2.064716
H34	-5.760388	1.001468	1.900894
H35	-7.504485	0.767570	1.701332
C36	-7.492694	-0.784605	-0.540114
H37	-7.467699	-1.772550	-0.067983
H38	-8.461683	-0.317453	-0.333158
H39	-7.393444	-0.915802	-1.623036
O40	-6.557042	1.331915	-0.718912

O41 -5.611563 2.334308 -0.264984

Zero-point correction=	0.346627 (Hartree/Particle)
Thermal correction to Energy=	0.368609
Thermal correction to Enthalpy=	0.369553
Thermal correction to Gibbs Free Energy=	0.291911
Sum of electronic and zero-point Energies=	-1245.051112
Sum of electronic and thermal Energies=	-1245.029131
Sum of electronic and thermal Enthalpies=	-1245.028187
Sum of electronic and thermal Free Energies=	-1245.105829

Energies and Cartesian Coordinates of structures at B3LYP/6-31+G(d) in Figure 5b:

***trans*-complex**

C1 -2.606106 -0.247443 -0.489269
H2 -2.637674 -1.343227 -0.403952
C3 -1.299253 0.277438 0.120913
H4 -1.268266 1.373257 0.022983
H5 -1.292603 0.067647 1.201407
C6 -0.041483 -0.326927 -0.519089
H7 -0.051365 -0.121247 -1.600718
H8 -0.075980 -1.422825 -0.417581
C9 1.270975 0.194587 0.082780
H10 1.278294 -0.003772 1.165405
H11 1.311034 1.289115 -0.025984
C12 2.526910 -0.421777 -0.550331
H13 2.518332 -0.224317 -1.633942
H14 2.485210 -1.516959 -0.439616
C15 3.836806 0.104132 0.056187
H16 3.853576 -0.095116 1.135596
H17 3.891451 1.194050 -0.063093
C18 5.078330 -0.521763 -0.576759
H19 5.135757 -0.305875 -1.650017
H20 5.094359 -1.609468 -0.440602
S21 6.650544 0.096548 0.143889
O22 7.710256 -0.641312 -0.609581
O23 6.635572 1.570625 -0.113837
O24 6.573734 -0.263464 1.594629
C25 -3.868387 0.346767 0.174241
H26 -3.860460 0.117463 1.245089
H27 -3.827578 1.443933 0.090981
H28 -2.622562 -0.022714 -1.566066
C29 -5.133476 -0.118099 -0.479243
C30 -6.152095 -0.849662 0.053979
H31 -5.220058 0.143384 -1.534747
C32 -6.219559 -1.314076 1.484629
H33 -6.276946 -2.410934 1.527660
H34 -5.366128 -0.993942 2.085441
H35 -7.131802 -0.927838 1.959575

C36 -7.354110 -1.163629 -0.780795
H37 -7.766561 -2.155504 -0.558300
H38 -8.147493 -0.423893 -0.547448
H39 -7.150643 -1.092038 -1.853789
O40 -6.704753 1.636795 0.282928
O41 -7.903798 1.664701 -0.087136

Zero-point correction=	0.343842 (Hartree/Particle)
Thermal correction to Energy=	0.367094
Thermal correction to Enthalpy=	0.368038
Thermal correction to Gibbs Free Energy=	0.285779
Sum of electronic and zero-point Energies=	-1244.981739
Sum of electronic and thermal Energies=	-1244.958487
Sum of electronic and thermal Enthalpies=	-1244.957543
Sum of electronic and thermal Free Energies=	-1245.039801

TS3
C1 2.662974 0.082408 -0.480091
H2 2.726269 1.169598 -0.329749
C3 1.341088 -0.439953 0.099693
H4 1.281008 -1.527379 -0.057852
H5 1.337769 -0.288572 1.189813
C6 0.102846 0.232659 -0.509422
H7 0.108599 0.080959 -1.599964
H8 0.168658 1.320646 -0.352974
C9 -1.224669 -0.280591 0.065904
H10 -1.229972 -0.130852 1.156335
H11 -1.292984 -1.367697 -0.092026
C12 -2.462399 0.396002 -0.540967
H13 -2.458167 0.242798 -1.631849
H14 -2.390523 1.484271 -0.385460
C15 -3.786297 -0.118350 0.044539
H16 -3.799481 0.040640 1.130774
H17 -3.868570 -1.201412 -0.115122
C18 -5.012579 0.559920 -0.562909
H19 -5.076064 0.383989 -1.643248
H20 -5.002013 1.642174 -0.387192
S21 -6.599110 -0.049448 0.141883
O22 -7.640322 0.738106 -0.586791
O23 -6.609748 -1.513878 -0.167553
O24 -6.505341 0.262770 1.602889
C25 3.905997 -0.590942 0.148590
H26 3.904777 -0.421387 1.230898
H27 3.837766 -1.676911 0.000269
H28 2.674264 -0.078592 -1.568003
C29 5.182830 -0.114912 -0.471746
C30 6.042036 0.855547 0.000692
H31 5.379650 -0.492235 -1.474905
C32 5.897420 1.540928 1.330294
H33 5.710534 2.614153 1.181787
H34 5.086927 1.137064 1.940001

H35 6.831549 1.455650 1.900531
C36 7.252765 1.179547 -0.799496
H37 7.711517 2.132013 -0.514872
H38 7.999145 0.370306 -0.599083
H39 7.068128 1.167963 -1.878403
O40 6.648249 -1.369170 0.512796
O41 7.790275 -1.502777 -0.026383

Zero-point correction=	0.344169 (Hartree/Particle)
Thermal correction to Energy=	0.366166
Thermal correction to Enthalpy=	0.367110
Thermal correction to Gibbs Free Energy=	0.288600
Sum of electronic and zero-point Energies=	-1244.981052
Sum of electronic and thermal Energies=	-1244.959055
Sum of electronic and thermal Enthalpies=	-1244.958110
Sum of electronic and thermal Free Energies=	-1245.036621

secondary R-OOH
C1 2.832475 -0.162508 -0.355847
H2 2.912586 0.916466 -0.162670
C3 1.481794 -0.670031 0.169214
H4 1.397212 -1.749999 -0.024527
H5 1.451820 -0.553778 1.263456
C6 0.277543 0.053847 -0.449269
H7 0.298574 -0.078329 -1.542229
H8 0.376962 1.136175 -0.272121
C9 -1.076829 -0.422896 0.093604
H10 -1.096861 -0.288945 1.186005
H11 -1.178940 -1.504765 -0.081589
C12 -2.280409 0.303985 -0.523684
H13 -2.267823 0.158976 -1.615646
H14 -2.169791 1.387615 -0.358689
C15 -3.630074 -0.163943 0.041817
H16 -3.650798 -0.010302 1.128724
H17 -3.750707 -1.242342 -0.124807
C18 -4.822807 0.562798 -0.576337
H19 -4.882707 0.390881 -1.657524
H20 -4.771446 1.643591 -0.398774
S21 -6.439040 0.016375 0.112371
O22 -7.441677 0.842987 -0.627309
O23 -6.503982 -1.446950 -0.195902
O24 -6.348474 0.326442 1.574121
C25 4.031681 -0.895627 0.264811
H26 4.010355 -0.793573 1.357548
H27 3.962932 -1.969449 0.050486
H28 2.864401 -0.277321 -1.449687
C29 5.383417 -0.405412 -0.271411
C30 5.699960 1.052034 0.023547
H31 5.439890 -0.584456 -1.351977
C32 5.594663 1.508372 1.459626
H33 4.551001 1.513574 1.800419

H34 6.141536 0.834085 2.130758
H35 5.991875 2.521088 1.583745
C36 6.082733 1.873189 -0.964197
H37 6.321288 2.919084 -0.780176
H38 8.007995 -0.353846 0.029244
H39 6.154578 1.529707 -1.993886
O40 6.362125 -1.265746 0.363267
O41 7.615237 -1.157855 -0.362333

Zero-point correction=	0.347341 (Hartree/Particle)
Thermal correction to Energy=	0.369297
Thermal correction to Enthalpy=	0.370241
Thermal correction to Gibbs Free Energy=	0.292237
Sum of electronic and zero-point Energies=	-1245.046109
Sum of electronic and thermal Energies=	-1245.024153
Sum of electronic and thermal Enthalpies=	-1245.023209
Sum of electronic and thermal Free Energies=	-1245.101213

tertiary R-OOH
C1 -2.633975 -1.230284 -0.546807
H2 -2.491431 -2.322430 -0.568645
C3 -1.403676 -0.594059 0.131334
H4 -1.532480 0.497611 0.157154
H5 -1.357574 -0.921866 1.180808
C6 -0.082459 -0.939962 -0.569076
H7 -0.131620 -0.605999 -1.617173
H8 0.032938 -2.034572 -0.603665
C9 1.152002 -0.321577 0.101684
H10 1.210874 -0.668277 1.144649
H11 1.029692 0.771170 0.151100
C12 2.471095 -0.648086 -0.613623
H13 2.413500 -0.290675 -1.654086
H14 2.588296 -1.741857 -0.672956
C15 3.703168 -0.037428 0.071301
H16 3.779817 -0.410085 1.101148
H17 3.589887 1.052428 0.139916
C18 5.008516 -0.347501 -0.658626
H19 5.009307 0.065844 -1.674127
H20 5.187261 -1.427372 -0.722897
S21 6.488353 0.358087 0.176227
O22 7.625299 -0.050765 -0.704471
O23 6.235763 1.833239 0.206563
O24 6.498378 -0.285060 1.527950
C25 -3.927162 -0.916482 0.155872
H26 -3.983338 -1.240798 1.196251
H27 -5.343907 2.562314 -0.685896
H28 -2.691252 -0.901928 -1.593720
C29 -4.965436 -0.278707 -0.399039
C30 -6.289417 0.062704 0.255590
H31 -4.888533 0.028680 -1.442951
C32 -6.452171 -0.478711 1.678907

H33 -6.434965 -1.573406 1.668312
H34 -5.655695 -0.119579 2.337531
H35 -7.411855 -0.150952 2.091077
C36 -7.457327 -0.378270 -0.638044
H37 -8.411301 -0.078201 -0.189792
H38 -7.380929 0.080099 -1.628455
H39 -7.449928 -1.467709 -0.759740
O40 -6.384287 1.506803 0.490881
O41 -6.253822 2.223076 -0.769712

Zero-point correction=	0.346620 (Hartree/Particle)
Thermal correction to Energy=	0.368630
Thermal correction to Enthalpy=	0.369574
Thermal correction to Gibbs Free Energy=	0.290903
Sum of electronic and zero-point Energies=	-1245.049356
Sum of electronic and thermal Energies=	-1245.027346
Sum of electronic and thermal Enthalpies=	-1245.026402
Sum of electronic and thermal Free Energies=	-1245.105073

Energies and Cartesian Coordinates of structures at B3LYP/6-31+G(d) in Figure 7a

singlet O_2
O1 0.000000 0.000000 0.607284
O2 0.000000 0.000000 -0.607284

Zero-point correction=	0.003716 (Hartree/Particle)
Thermal correction to Energy=	0.006079
Thermal correction to Enthalpy=	0.007023
Thermal correction to Gibbs Free Energy=	-0.015226
Sum of electronic and zero-point Energies=	-150.263247
Sum of electronic and thermal Energies=	-150.260884
Sum of electronic and thermal Enthalpies=	-150.259940
Sum of electronic and thermal Free Energies=	-150.282189

11C surfactant
C1 3.469551 -0.442265 0.084640
H2 3.580514 -0.261951 -0.994600
C3 2.132052 0.135126 0.567198
H4 2.033314 -0.039398 1.649540
H5 2.137623 1.227366 0.431071
C6 0.913193 -0.458187 -0.152956
H7 0.907919 -1.550114 -0.014696
H8 1.011139 -0.285473 -1.235551
C9 -0.424125 0.118665 0.331927
H10 -0.424483 1.209091 0.183372
H11 -0.516857 -0.044660 1.416335
C12 -1.644080 -0.488390 -0.374933

H13 -1.645465 -1.578132 -0.223978
H14 -1.555364 -0.325784 -1.459391
C15 -2.976577 0.095926 0.120239
H16 -2.985761 1.180449 -0.047298
H17 -3.066332 -0.062094 1.202438
C18 -4.177029 -0.537490 -0.584029
H19 -4.221326 -1.617404 -0.405602
H20 -4.142535 -0.370567 -1.666177
S21 -5.792027 0.112073 -0.042303
O22 -6.811357 -0.654699 -0.835926
O23 -5.886774 -0.156299 1.432131
O24 -5.792700 1.578750 -0.364973
C25 4.688952 0.148268 0.821949
H26 4.711492 1.233358 0.668762
H27 4.543472 -0.006970 1.903070
H28 3.462827 -1.534655 0.216358
C29 5.989041 -0.493345 0.409628
C30 7.068233 0.072345 -0.162976
H31 6.037522 -1.567976 0.604337
C32 7.196921 1.536904 -0.512487
H33 7.408346 1.659237 -1.584303
H34 6.302929 2.119772 -0.277900
H35 8.044411 1.987927 0.023442
C36 8.286243 -0.756506 -0.507240
H37 8.507464 -0.704421 -1.583096
H38 9.179391 -0.379323 0.011688
H39 8.154591 -1.809779 -0.236579

Zero-point correction=	0.339183 (Hartree/Particle)
Thermal correction to Energy=	0.358941
Thermal correction to Enthalpy=	0.359885
Thermal correction to Gibbs Free Energy=	0.287384
Sum of electronic and zero-point Energies=	-1094.807034
Sum of electronic and thermal Energies=	-1094.787276
Sum of electronic and thermal Enthalpies=	-1094.786332
Sum of electronic and thermal Free Energies=	-1094.858833

***cis*-perepoxide**

C1 -2.743602 -0.579893 -0.129991
H2 -2.724509 -1.677283 -0.061090
C3 -1.433607 -0.010841 0.430312
H4 -1.448573 1.085842 0.342909
H5 -1.372399 -0.234048 1.506210
C6 -0.183576 -0.558994 -0.271637
H7 -0.251072 -0.349588 -1.349896
H8 -0.163537 -1.654689 -0.170781
C9 1.126619 0.023888 0.275550
H10 1.185836 -0.169863 1.357203
H11 1.113399 1.117962 0.158404
C12 2.379453 -0.542638 -0.407118
H13 2.319825 -0.357462 -1.489885

H14 2.399141 -1.635185 -0.279865
C15 3.683588 0.058176 0.140839
H16 3.743363 -0.120379 1.221923
H17 3.675008 1.145850 -0.004696
C18 4.918482 -0.534739 -0.538725
H19 4.909616 -0.351399 -1.618741
H20 4.985246 -1.615891 -0.375595
S21 6.500734 0.147106 0.057446
O22 7.560685 -0.575966 -0.723811
O23 6.468745 1.619276 -0.237069
O24 6.565698 -0.147569 1.528498
C25 -3.981635 -0.046539 0.607210
H26 -3.925631 -0.313355 1.673245
H27 -4.023428 1.044303 0.548270
H28 -2.825718 -0.332057 -1.196564
C29 -5.266346 -0.628115 0.095231
C30 -6.602834 -0.069414 0.355210
H31 -5.231901 -1.693206 -0.131616
C32 -6.757371 1.260694 1.024467
H33 -6.293983 1.247622 2.017239
H34 -6.248260 2.018191 0.414548
H35 -7.812831 1.525788 1.129127
C36 -7.800929 -0.969328 0.259262
H37 -8.049593 -1.325028 1.268103
H38 -8.668024 -0.423426 -0.126738
H39 -7.610206 -1.841787 -0.371853
O40 -5.918168 0.048677 -1.124238
O41 -5.392330 1.323315 -1.496213

Zero-point correction=	0.346237 (Hartree/Particle)
Thermal correction to Energy=	0.367976
Thermal correction to Enthalpy=	0.368920
Thermal correction to Gibbs Free Energy=	0.291900
Sum of electronic and zero-point Energies=	-1245.101285
Sum of electronic and thermal Energies=	-1245.079545
Sum of electronic and thermal Enthalpies=	-1245.078601
Sum of electronic and thermal Free Energies=	-1245.155621

TS2′a

C1 -2.765187 -0.223064 -0.459855
H2 -2.766630 -0.933675 -1.299792
C3 -1.448498 -0.359406 0.316632
H4 -1.453584 0.340880 1.165578
H5 -1.385384 -1.369028 0.750002
C6 -0.205855 -0.098494 -0.545603
H7 -0.268571 0.914036 -0.972269
H8 -0.204336 -0.792873 -1.399605
C9 1.114051 -0.241479 0.224420
H10 1.184884 -1.258897 0.637781
H11 1.106632 0.441914 1.087085
C12 2.354582 0.043754 -0.633507

H13 2.287144 1.063467 -1.040775
H14 2.362675 -0.635528 -1.498978
C15 3.671050 -0.107687 0.144782
H16 3.749827 -1.129852 0.536264
H17 3.664936 0.567363 1.010050
C18 4.890149 0.197484 -0.726239
H19 4.867757 1.226633 -1.100897
H20 4.948868 -0.478461 -1.586303
S21 6.488269 0.026749 0.134260
O22 7.526641 0.380318 -0.891960
O23 6.460668 0.991970 1.284228
O24 6.581070 -1.403829 0.581720
C25 -4.001296 -0.468262 0.417045
H26 -3.946118 -1.468522 0.870190
H27 -4.026832 0.255260 1.237206
H28 -2.829161 0.781142 -0.898872
C29 -5.298080 -0.416500 -0.366704
C30 -6.621342 -0.482303 0.300456
H31 -5.252125 -1.057683 -1.250714
C32 -6.804182 0.318321 1.477195
H33 -6.071104 0.151382 2.273153
H34 -6.440769 1.360570 1.061663
H35 -7.825776 0.360190 1.858499
C36 -7.765327 -1.123835 -0.406979
H37 -7.851933 -2.161853 -0.046200
H38 -8.714846 -0.625927 -0.186190
H39 -7.612921 -1.171756 -1.489355
O40 -5.643083 0.918635 -0.944515
O41 -5.432211 1.983165 -0.068914

Zero-point correction=	0.344174 (Hartree/Particle)
Thermal correction to Energy=	0.365091
Thermal correction to Enthalpy=	0.366036
Thermal correction to Gibbs Free Energy=	0.290803
Sum of electronic and zero-point Energies=	-1245.101772
Sum of electronic and thermal Energies=	-1245.080854
Sum of electronic and thermal Enthalpies=	-1245.079910
Sum of electronic and thermal Free Energies=	-1245.155143

secondary R-OOH

C1 2.779719 -0.234282 -0.423459
H2 2.786173 -0.259628 -1.523674
C3 1.461516 0.385767 0.060307
H4 1.458187 0.417687 1.160429
H5 1.406287 1.431818 -0.277665
C6 0.216113 -0.368152 -0.426419
H7 0.267145 -1.412246 -0.081924
H8 0.221747 -0.406222 -1.526365
C9 -1.100996 0.258815 0.050885
H10 -1.154305 1.300618 -0.299788
H11 -1.103620 0.303506 1.150475

C12 -2.348726 -0.497953 -0.425891
H13 -2.301576 -1.537886 -0.070057
H14 -2.347339 -0.545920 -1.524978
C15 -3.658490 0.147173 0.054076
H16 -3.709293 1.182584 -0.305937
H17 -3.665933 0.188175 1.150700
C18 -4.889529 -0.617938 -0.433390
H19 -4.898445 -1.646981 -0.057804
H20 -4.932462 -0.652413 -1.527463
S21 -6.477017 0.107713 0.092958
O22 -7.533144 -0.781032 -0.499815
O23 -6.480199 0.085897 1.594543
O24 -6.514231 1.501123 -0.465710
C25 4.012996 0.531716 0.075579
H26 3.947153 1.578412 -0.249710
H27 4.022285 0.540868 1.171403
H28 2.836246 -1.278188 -0.088647
C29 5.335369 -0.029800 -0.448392
C30 6.606952 0.730030 -0.094703
H31 5.277436 -0.108005 -1.544535
C32 6.655309 1.666458 0.862598
H33 5.784562 1.955877 1.443316
H34 6.468864 -1.542638 1.518947
H35 7.583372 2.185734 1.092501
C36 7.825484 0.344159 -0.901289
H37 7.670260 0.560187 -1.967531
H38 8.715322 0.887093 -0.567756
H39 8.029312 -0.731415 -0.825735
O40 5.498723 -1.442946 -0.126448
O41 5.515927 -1.616840 1.318063

Zero-point correction=	0.347063 (Hartree/Particle)
Thermal correction to Energy=	0.369059
Thermal correction to Enthalpy=	0.370003
Thermal correction to Gibbs Free Energy=	0.291906
Sum of electronic and zero-point Energies=	-1245.148342
Sum of electronic and thermal Energies=	-1245.126346
Sum of electronic and thermal Enthalpies=	-1245.125402
Sum of electronic and thermal Free Energies=	-1245.203499

TS2′b

C1 -2.705939 -0.907194 -0.036027
H2 -2.638767 -1.856653 0.513230
C3 -1.443326 -0.078364 0.236193
H4 -1.500022 0.867177 -0.323225
H5 -1.412109 0.194305 1.301837
C6 -0.149333 -0.814409 -0.136436
H7 -0.179240 -1.081065 -1.203805
H8 -0.101696 -1.764316 0.417228
C9 1.121001 -0.001000 0.146375
H10 1.155904 0.256508 1.215719

H11 1.071610 0.953107 -0.399565
C12 2.412095 -0.736834 -0.238978
H13 2.385794 -0.978309 -1.311963
H14 2.455163 -1.698122 0.294240
C15 3.680571 0.073543 0.070975
H16 3.718119 0.296941 1.144779
H17 3.640105 1.035325 -0.455772
C18 4.951104 -0.673239 -0.337264
H19 4.973887 -0.865269 -1.415506
H20 5.037139 -1.633221 0.183352
S21 6.496408 0.220377 0.032795
O22 7.596838 -0.672164 -0.466031
O23 6.426319 1.522784 -0.711337
O24 6.534485 0.406556 1.522374
C25 -3.993578 -0.180257 0.364378
H26 -3.980155 0.164024 1.407881
H27 -4.123612 0.846111 -0.193744
H28 -2.753601 -1.164404 -1.103123
C29 -5.243449 -0.776113 -0.011916
C30 -6.528911 -0.075627 0.178627
H31 -5.258029 -1.625598 -0.692483
C32 -6.737032 0.799935 1.396402
H33 -6.887975 0.157573 2.271117
H34 -5.887310 1.456865 1.584415
H35 -7.631689 1.416555 1.263927
C36 -7.755044 -0.876990 -0.218143
H37 -7.965828 -1.626837 0.552667
H38 -8.626086 -0.221123 -0.312861
H39 -7.596953 -1.396697 -1.168603
O40 -6.152343 0.714289 -1.068941
O41 -5.341066 1.806085 -0.848511

Zero-point correction=	0.344160 (Hartree/Particle)
Thermal correction to Energy=	0.364911
Thermal correction to Enthalpy=	0.365855
Thermal correction to Gibbs Free Energy=	0.292313
Sum of electronic and zero-point Energies=	-1245.098602
Sum of electronic and thermal Energies=	-1245.077851
Sum of electronic and thermal Enthalpies=	-1245.076907
Sum of electronic and thermal Free Energies=	-1245.150449

tertiary R-OOH

C1 -2.664536 -1.365875 -0.110818
H2 -2.517936 -2.359932 0.339850
C3 -1.450809 -0.486399 0.249636
H4 -1.576128 0.504644 -0.209853
H5 -1.431713 -0.324377 1.337516
C6 -0.115384 -1.095346 -0.198201
H7 -0.137257 -1.256007 -1.286676
H8 -0.000775 -2.090332 0.258057
C9 1.100850 -0.231038 0.161540

H10 1.123554 -0.071858 1.250140
H11 0.986956 0.764326 -0.293711
C12 2.434969 -0.843374 -0.287473
H13 2.414953 -1.000088 -1.376179
H14 2.548104 -1.839021 0.166738
C15 3.649423 0.023830 0.080045
H16 3.670909 0.182308 1.165656
H17 3.549598 1.012078 -0.386754
C18 4.964103 -0.618176 -0.364529
H19 4.992158 -0.765004 -1.449762
H20 5.117028 -1.590769 0.115845
S21 6.451220 0.358922 0.031724
O22 7.604650 -0.461769 -0.470620
O23 6.311445 1.664800 -0.696217
O24 6.468058 0.527105 1.523743
C25 -3.969236 -0.795864 0.376879
H26 -4.040062 -0.637570 1.453938
H27 -4.822567 2.136029 -0.850620
H28 -2.705960 -1.514478 -1.198226
C29 -5.009061 -0.484482 -0.407141
C30 -6.344456 0.082952 0.024956
H31 -4.926814 -0.647677 -1.484513
C32 -6.508476 0.302069 1.528761
H33 -6.449577 -0.652385 2.062250
H34 -5.739533 0.969794 1.925364
H35 -7.489413 0.746055 1.728705
C36 -7.489936 -0.773358 -0.537311
H37 -7.465878 -1.763432 -0.070590
H38 -8.459197 -0.310485 -0.322031
H39 -7.391677 -0.900090 -1.620675
O40 -6.558288 1.350152 -0.692564
O41 -5.582490 2.341697 -0.271857

Zero-point correction=	0.346516 (Hartree/Particle)
Thermal correction to Energy=	0.368498
Thermal correction to Enthalpy=	0.369442
Thermal correction to Gibbs Free Energy=	0.292406
Sum of electronic and zero-point Energies=	-1245.155393
Sum of electronic and thermal Energies=	-1245.133411
Sum of electronic and thermal Enthalpies=	-1245.132467
Sum of electronic and thermal Free Energies=	-1245.209503

Energies and Cartesian Coordinates of structures at B3LYP/6-31+G(d) in Figure 7b:

***trans*-perepoxide**
O1 6.135237 2.084995 -0.525178
O2 5.749379 0.707623 -0.733995
C3 6.567120 -0.431431 0.050642
C4 5.232884 0.010516 0.499638

C5 6.749429 -1.628899 -0.839284
H6 6.937210 -2.507216 -0.208337
H7 5.874266 -1.835160 -1.458008
H8 7.619805 -1.489124 -1.488011
C9 7.775276 0.084077 0.772636
H10 8.674932 -0.010005 0.157009
H11 7.632799 1.131031 1.050875
H12 7.914902 -0.509643 1.684390
H13 5.249015 0.729905 1.316202
C14 3.933381 -0.728328 0.328764
H15 3.848966 -1.406639 1.190949
H16 3.957812 -1.359172 -0.565393
C17 2.717475 0.211575 0.283211
H18 2.715042 0.846006 1.180907
H19 2.815210 0.887219 -0.577621
C20 1.386713 -0.547108 0.191534
H21 1.393383 -1.187973 -0.702697
H22 1.295999 -1.222419 1.055565
C23 0.165488 0.381070 0.142079
H24 0.248685 1.042848 -0.733237
H25 0.173151 1.036614 1.025914
C26 -1.171628 -0.370482 0.084010
H27 -1.258359 -1.023207 0.965754
H28 -1.178996 -1.034285 -0.793562
C29 -2.389211 0.562303 0.023369
H30 -2.314910 1.198567 -0.871016
H31 -2.369675 1.241109 0.888844
C32 -3.727550 -0.193134 0.002510
H33 -3.812512 -0.810613 0.905768
H34 -3.752393 -0.875574 -0.856501
C35 -4.918908 0.762485 -0.073318
H36 -4.902659 1.351186 -0.996958
H37 -4.929223 1.456504 0.774187
S38 -6.546251 -0.058190 -0.045579
O39 -7.548571 1.056250 -0.143911
O40 -6.584329 -0.977129 -1.232906
O41 -6.628623 -0.796085 1.259678

Zero-point correction=	0.346541 (Hartree/Particle)
Thermal correction to Energy=	0.368348
Thermal correction to Enthalpy=	0.369292
Thermal correction to Gibbs Free Energy=	0.292616
Sum of electronic and zero-point Energies=	-1245.102556
Sum of electronic and thermal Energies=	-1245.080749
Sum of electronic and thermal Enthalpies=	-1245.079805
Sum of electronic and thermal Free Energies=	-1245.156481

TS3′
O1 -6.299664 2.034630 0.526511
O2 -5.532984 0.907033 0.827602
C3 -6.570124 -0.620007 -0.205529

C4 -5.266554 0.072060 -0.369417
C5 -6.705606 -1.847362 0.629134
H6 -6.531923 -2.725993 -0.012519
H7 -5.970365 -1.896292 1.437190
H8 -7.712776 -1.939336 1.045502
C9 -7.706381 0.124852 -0.662567
H10 -8.682996 -0.303970 -0.433252
H11 -7.515381 1.138714 -0.079253
H12 -7.633284 0.482301 -1.696051
H13 -5.239006 0.740200 -1.234807
C14 -3.959594 -0.677351 -0.185019
H15 -3.927109 -1.476849 -0.938360
H16 -3.945848 -1.168489 0.795359
C17 -2.729211 0.230414 -0.332575
H18 -2.738473 0.691053 -1.331074
H19 -2.795949 1.052970 0.392275
C20 -1.405868 -0.519910 -0.130945
H21 -1.401672 -0.987800 0.864961
H22 -1.339025 -1.342349 -0.859049
C23 -0.173209 0.384070 -0.270132
H24 -0.241718 1.201937 0.463075
H25 -0.182054 0.859034 -1.262833
C26 1.156774 -0.357248 -0.076882
H27 1.238161 -1.159870 -0.825277
H28 1.158307 -0.850740 0.906720
C29 2.382708 0.560799 -0.182235
H30 2.306306 1.354358 0.575801
H31 2.376490 1.064955 -1.160043
C32 3.713672 -0.186882 -0.004890
H33 3.805520 -0.961029 -0.777316
H34 3.721013 -0.699184 0.965553
C35 4.912996 0.758169 -0.087814
H36 4.884657 1.511383 0.706987
H37 4.947701 1.278509 -1.051213
S38 6.531276 -0.064368 0.076862
O39 7.544457 1.040476 -0.018611
O40 6.534918 -0.737615 1.418981
O41 6.630947 -1.039930 -1.060600

Zero-point correction=	0.344032 (Hartree/Particle)
Thermal correction to Energy=	0.364932
Thermal correction to Enthalpy=	0.365877
Thermal correction to Gibbs Free Energy=	0.290612
Sum of electronic and zero-point Energies=	-1245.103874
Sum of electronic and thermal Energies=	-1245.082974
Sum of electronic and thermal Enthalpies=	-1245.082029
Sum of electronic and thermal Free Energies=	-1245.157294

secondary R-OOH
C1 2.828838 -0.102759 -0.319136
H2 2.921294 0.964806 -0.077538

C3 1.483402 -0.625486 0.203758
H4 1.396365 -1.698227 -0.024865
H5 1.463551 -0.540797 1.300707
C6 0.275518 0.116574 -0.384700
H7 0.290333 0.018641 -1.480811
H8 0.369749 1.191876 -0.170063
C9 -1.071464 -0.388880 0.150117
H10 -1.093745 -0.273174 1.244266
H11 -1.158745 -1.467889 -0.047813
C12 -2.279987 0.334781 -0.459906
H13 -2.265199 0.207479 -1.552544
H14 -2.190647 1.415145 -0.272376
C15 -3.622516 -0.168186 0.093869
H16 -3.647886 -0.021169 1.181094
H17 -3.712600 -1.246933 -0.086030
C18 -4.811167 0.551581 -0.544332
H19 -4.841990 0.390285 -1.627412
H20 -4.773891 1.630804 -0.359953
S21 -6.436929 0.007701 0.075944
O22 -7.442604 0.817979 -0.691390
O23 -6.535177 -1.461935 -0.216183
O24 -6.454559 0.307907 1.547274
C25 4.026304 -0.873863 0.256194
H26 4.031855 -0.794891 1.350745
H27 3.925445 -1.939553 0.014494
H28 2.845693 -0.174196 -1.416499
C29 5.375717 -0.398586 -0.302749
C30 5.736264 1.039956 0.022650
H31 5.397334 -0.549755 -1.388537
C32 5.739628 1.449366 1.476627
H33 4.726669 1.433939 1.900217
H34 6.344786 0.763451 2.082629
H35 6.139231 2.460756 1.598733
C36 6.048557 1.891079 -0.964918
H37 6.309668 2.928220 -0.764360
H38 8.057179 -0.499571 0.071063
H39 6.046470 1.580395 -2.007631
O40 6.337533 -1.318020 0.283388
O41 7.599229 -1.202971 -0.429022

Zero-point correction=	0.347313 (Hartree/Particle)
Thermal correction to Energy=	0.369260
Thermal correction to Enthalpy=	0.370204
Thermal correction to Gibbs Free Energy=	0.292562
Sum of electronic and zero-point Energies=	-1245.151029
Sum of electronic and thermal Energies=	-1245.129083
Sum of electronic and thermal Enthalpies=	-1245.128139
Sum of electronic and thermal Free Energies=	-1245.205781

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