Molecular growth of PAH-like systems induced by oxygen species: experimental and theoretical study of the reaction of naphthalene with HO ($^2\Pi_{3/2}$), O (^{3}P), and O$_2$ ($^3\Sigma_g^-$).

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Electronic Supplementary Information

CONTENT

Section 1.

Theoretical Method Validation.

We like to specify that our investigation is not aimed to reproduce very accurate computational results, but rather to offer the description of some reaction pathways which explain the formation of oxygen-containing products (some of them with significant mass increase). However, the comparisons presented in this section could be of some interest. Thermodynamic and kinetic experimental data are used to validate the computational level chosen for this study [DFT(M06-2X)/cc-pV*TZ*//DFT(M06-2X)/6-311G(d,p) for energies and geometries; DFT(M06-2X)/6-311G(d,p) for the assessment of the thermochemistry].

Four reactions are considered, and a comparison is drawn in **Table S1** between our DFT reaction enthalpies and the relevant experimental data. Reaction #1, the formation of the benzyl radical from propargyl and but-1-ene-3-yne, was considered in a previous study.[1] Reaction #2 is the formation of benzene starting by recombination of two propargyl radicals.[2] Reaction #3 sees seven ethyne molecules put into relation with two benzyl radicals: it is not to be considered as a real reaction, yet it allows a "reaction" enthalpy comparison. Reaction #4 is the radical coupling of propargyl with atomic hydrogen, to get propyne.

Then, another comparison can be drawn with experimental data for the **rate constants** of the propargyl radical + ethyne reaction, calculated at DFT(M06-2X)/cc-pV*TZ* // DFT(M06-2X)/6-311G(d,p) level by using TST theory, at four different temperatures.[3] Calculated rate constants show a rather satisfactory agreement with the experimental rate constants, as reported in **Table S2**.

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[1] D. Trogolo, A. Maranzana, G. Ghigo, G. Tonachini *J. Phys. Chem. A* 2014, **118**, 427–440.

[2] J. A. Miller, S. J. Klippenstein, *J. Phys. Chem. A* 2003, **107**, 7783–7799(and refs therein).

[3] V.D. Knyazev, I.R. Slagle, *J. Phys. Chem. A*, 2002, **106**, 5613-5617.

Table S1. Experimental vs. theoretically assessed **reaction enthalpies** for cases 1-4.

	ΔH /kcal mol^{-1}		
	experimental	theoretical DFT(M06-2X)[g]	
Reaction		a	b
1	-101.9 ± 1.5 [a,b,d]	-105.0	-103.7
2	-142.20 ± 1.43 [a,c]	-149.6	-148.4
3	-280 ± 1 [f,d]	-295.3	-291.3
4	-88.78 ± 1.02 [a,e,f]	-91.2	-91.1
	Mean Signed Error	*-7.04*	*-5.33*
	Mean Unsigned Error	*7.04*	*5.33*

[a]propargyl radical: ref 4; [b] but-1-ene-3-yne: ref 5; [c] benzene: ref 6; [d]benzyl radical: ref 4; [e]propyne: ref 7; [f]hydrogen atom and ethyne: ref 8; [g]column **a**: geometry optimization at 6-311G(d,p); column **b**: single point energy computation at cc-pV*TZ* on the 6-311G(d,p) optimum geometry; thermochemistry at 6-311G(d,p) for both columns

Table S2. Experimental vs. theoretically assessed rate constants for the propargyl radical + ethyne reaction.

	k / molec^{-1} cm^{3} s^{-1}	
T /K	experiment	DFT(M06-2X)
800	7.25 x 10^{-16}	6.89 x 10^{-16}
900	1.46 x 10^{-15}	1.92 x 10^{-15}
1000	2.55 x 10^{-15}	4.44 x 10^{-15}
1100	4.03 x 10^{-15}	8.98 x 10^{-15}

[4] W. Tsang, "Heats of Formation of Organic Free Radicals by Kinetic Methods", in: *Energetics of Organic Free Radicals*, J. A. Martinho Simoes, A. Greenberg, J. F. Liebman (Eds.), Blackie Academic and Professional, London, 1996, p. 22-58.

[5] W. R. Roth, O. Adammczak, R. Breuckmann, *Chem. Ber.*, 1991, **124**, 2499-2521.

[6] M. V. Roux, M. Temprado, J. S. Chickos, Y. Nagano, *J. Phys. Chem. Ref. Data*, 2008, **37**, 1855-1996.

[7] D. D. Wagman, J. E. Kilpatrick, K. S. Pitzer, F. D. Rossini, *J. Res. NBS*, 1945, **35**, 467-496.

[8] M. W. Chase, Jr *NIST-JANAF Thermochemical Tables, Fourth Edition, J. Phys. Chem. Ref. Data*, 1998, Monograph **9**, 1-1951.

Finally, a test was carried out on the HO· addition to naphthalene, for which experimental measures of the kinetic constant are available[9] (ranging 2.17 – 2.39 x 10^{-11} molecule^{-1} cm^3 s^{-1}, which correspond to a ΔG barriers of 6.77– 6.72 kcal mol^{-1}). On the basis of our computed free energy barrier ($\Delta G^{\ddagger}$=7.42 kcal mol^{-1}), we estimate k = 1.09 x 10^{-11}. Also this comparison is encouraging within the declared scope of our investigation.

One can find in the literature that the M06-2X has been used oftentimes so far. Rayne and Forest reported some isomerization enthalpies of large[10] and small[11] organic molecules. They concluded that "M062X functional appears to offer comparable isomerization energy prediction performance to the best performing currently available dispersion corrected functionals…".

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[9] R. Atkinson, *Chem. Rev.*, 1986, **86**, 69-201. P. T. Phousongphouang, Arey, J., *Environ. Sci. Technol.*, 2002, **36**, 1947 – 1952.

[10] S. Rayne, K. Forest*, Nature Precedings,* doi:10.1038/npre.2010.5183.1

[11] S. Rayne, K. Forest*, Journal of Molecular Structure*: THEOCHEM, 2010, **948**, 102–107.

Section 2.

Reaction HO + naphthalene.

a) Definition of the addition "effective" rate constant, $k_{add,eff}$, to be reported with the H abstraction rate constant, k_{abs}, in a comparison to experimental data (in subsection b)
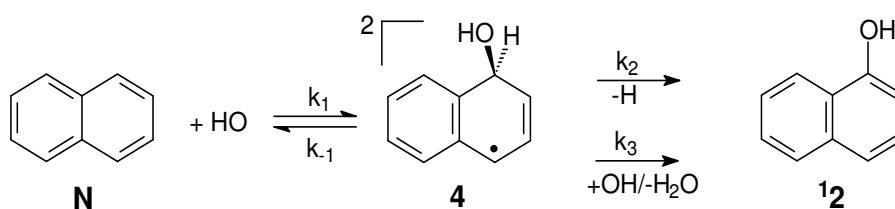
N = Naphthalene

$$-\frac{d[\mathbf{N}]}{dt} = k_1[\mathbf{N}][HO] - k_{-1}[\mathbf{4}]$$

$$-\frac{d[\mathbf{4}]}{dt} = k_{-1}[\mathbf{4}] + k_2[\mathbf{4}] + k_3[\mathbf{4}][HO] - k_1[\mathbf{4}][HO]$$

$$-\frac{d[\mathbf{4}]}{dt} = 0 \quad \text{Steady State}$$

$$[\mathbf{4}](k_{-1} + k_2 + k_3[HO] = k_1[\mathbf{N}][HO]$$

$$[\mathbf{4}] = \frac{k_1[\mathbf{N}][HO]}{k_{-1} + k_2 + k_3[HO]}$$

$$-\frac{d[\mathbf{N}]}{dt} = k_1\left(1 - \frac{k_{-1}}{k_{-1} + k_2 + k_3[HO]}\right)[\mathbf{N}][HO] = \mathbf{k_{add,eff}}[\mathbf{N}][HO]$$
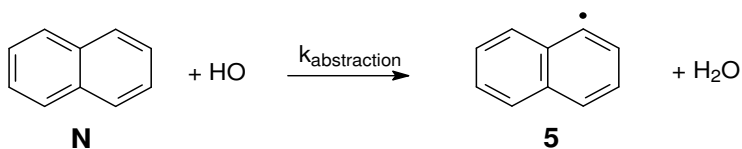
b) Comparison with experimental data.
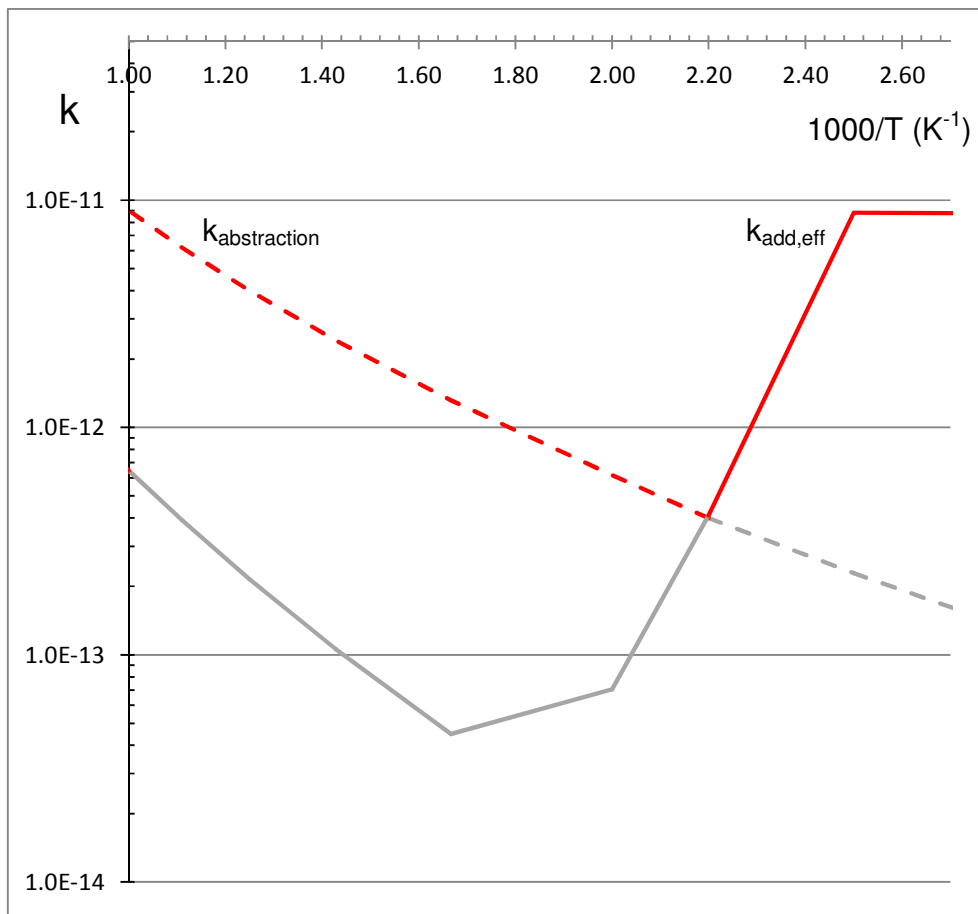
Figure S1. Rate constants (molecule^{-1} cm^3 s^{-1}) for HO addition to naphthalene ($k_{add,eff}$, continuous line) vs H-abstraction (k_{abs}) from its position 1 (broken line). At lower temperatures, addition is easier. Then, the two different slopes bring about a crossing at ca. 400-500 K.

The information conveyed by this plot can be compared with the kinetic results by Lorenz and Zellner[12] on the same system, later on integrated by further data gathered by other researchers.[13] All these data suggest a change in mechanism in the same temperature zone. The agreement seems fairly good, and supports the computational data reported in the main text.

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[12] K. Lorenz, R. Zellner *Ber. Bunsenges. Phys. Chem.* 1983, **87**, 629-636.

[13] R. Atkinson *J Phys Chem Ref Data*, Monograph 1, 1989; in particular page 237.

Section 3.

Possible roles of ozone and $^1\Delta_g$ dioxygen.

(A) **Ozone** is known to form under the experiment conditions (from O + O$_2$). Its reactivity is generally deemed less pronounced than those of HO or the O atom. Its reaction with PAHs has been the subject of some previous studies,[14] and a variety of poly-functional oxidized product species was suggested by a theoretical modelistic study, such as epoxy, ether, ketone, aldehyde, etc.
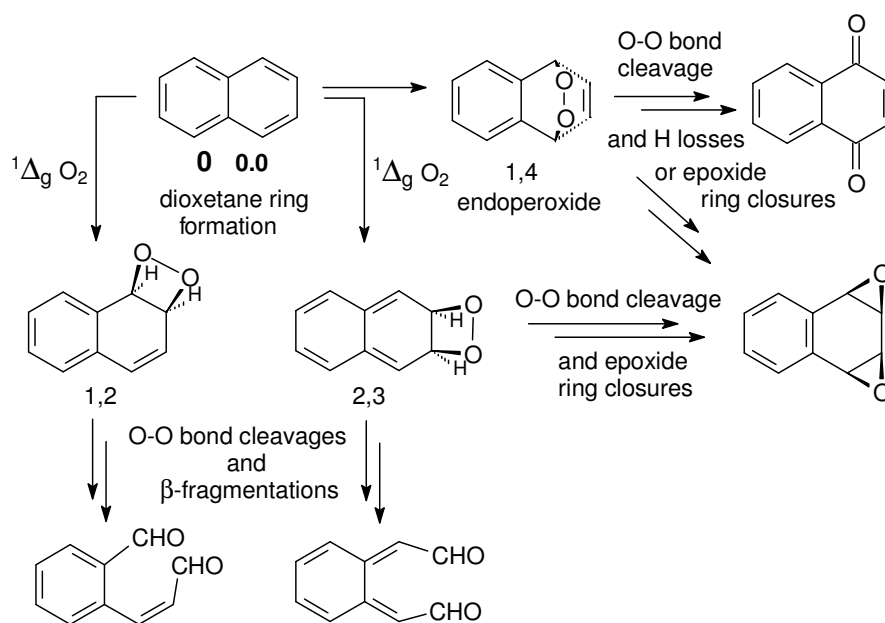
Scheme S1. Additions of $^1\Delta_g$ dioxygen to naphthalene.

(B) $^1\Delta_g$ **dioxygen** is expected to give [π2+π2] or [π4+π2] cycloadditions (Scheme S1). The former involves one couple of adjacent sites, with formation of a 4-membered ring, a dioxetane-like ring. The latter produces a 1,4-endoperoxide. From the dioxetane-like inter-mediates, an oxygen-oxygen bond cleavage usually induces the cleavage of the opposed carbon-carbon bond (a sort of β–fragmentation in each of the oxyl radicals potentially obtained). The final result would be a dialdehyde. Similarly *conceivable* is the formation of a diepoxide from the 2,3-dioxetane, following the cleavage of the oxygen-oxygen bond.

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[14] A. Giordana, A. Maranzana, G. Ghigo, M. Causa`, G. Tonachini, *J. Phys. Chem.* A, 2011, **115**, 470-481 and references therein.

However, none of these compounds has been detected in the experiment at 400 K. The Diels-Alder-like reaction could similarly be followed by oxygen-oxygen bond cleavage. The final stable product might again be a diepoxide, or, alternatively naphto-1,4-quinone could form through subsequent H losses.

Section 4.

Possible formation of a hydroperoxide. Considering the step in which the O atom reacts with the intermediate **1** (Scheme 1, main text), we saw that it does not abstract the hydrogen geminal to the oxyl group. It plunges instead onto the oxyl oxygen, giving the peroxyl diradical **A** (Scheme S2). This is a simple spin coupling of localized unpaired electrons. In fact, the attraction of the oxyl radical center onto the incoming O atom is such that, even if it approaches in the direction of the geminal hydrogen, it is unavoidably funneled into the well corresponding to **A**. Then $^1\Delta_g$ O$_2$ loss can produces naphthalene again with a barrier of ca. 10 kcal mol^{-1} at T = 400 K. The other dissociation limit presenting the opposite spin situation, $^3\Sigma_g^-$ O$_2$ + triplet naphthalene, is much higher in energy. As an alternative, a singlet hydroperoxide could in principle form by intramolecular H abstraction. But this process in not easy, since the barrier is 33.5 kcal mol^{-1} and is not competitive with dioxygen loss. Actually, this product is not observed experimentally.
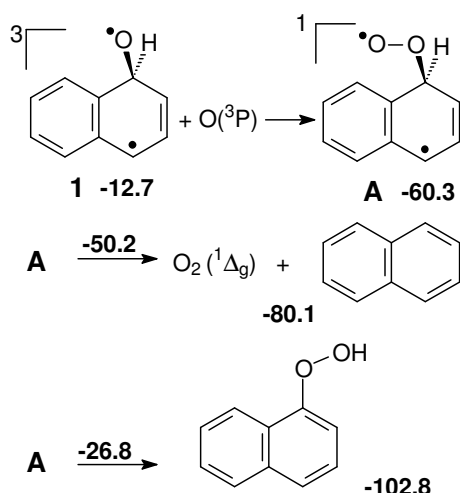
Scheme S2. Further O atom addition to **1** through radical coupling between the two oxygens. ΔG values at the DFT(M06-2X)/cc-pVTZ//DFT(M06-2X)/6-311G(d,p) computational level. Then, fragmentation takes place, while formation of the hydroperoxide is sharply disadvantaged.

Section 5.

Behavior of the rate constant curves over a wider T range.

For X = HO, not only the slopes but also the behavior of $k_{add,eff}$ (see Section 2a for a definition) and k_{abs} lines for each of the X species are different. Figure S2 displays a crossing of the red lines at ca. 850 K. For X = O atom the two blue lines begin at low T more far apart, rise both regularly, and show a crossing at a higher T than HO, ca. 1600 K. Thus, for both species addition is easier at lower temperatures. If both HO and O are present, addition carried out by the former dominates up to 700 K, by the latter in the range 700-1600 K. Then, H abstraction occurs faster at the highest temperatures, initially operated by the oxygen atom beyond 1700 K, then hydroxyl too, more slowly, beyond 2000 and 2300 K.
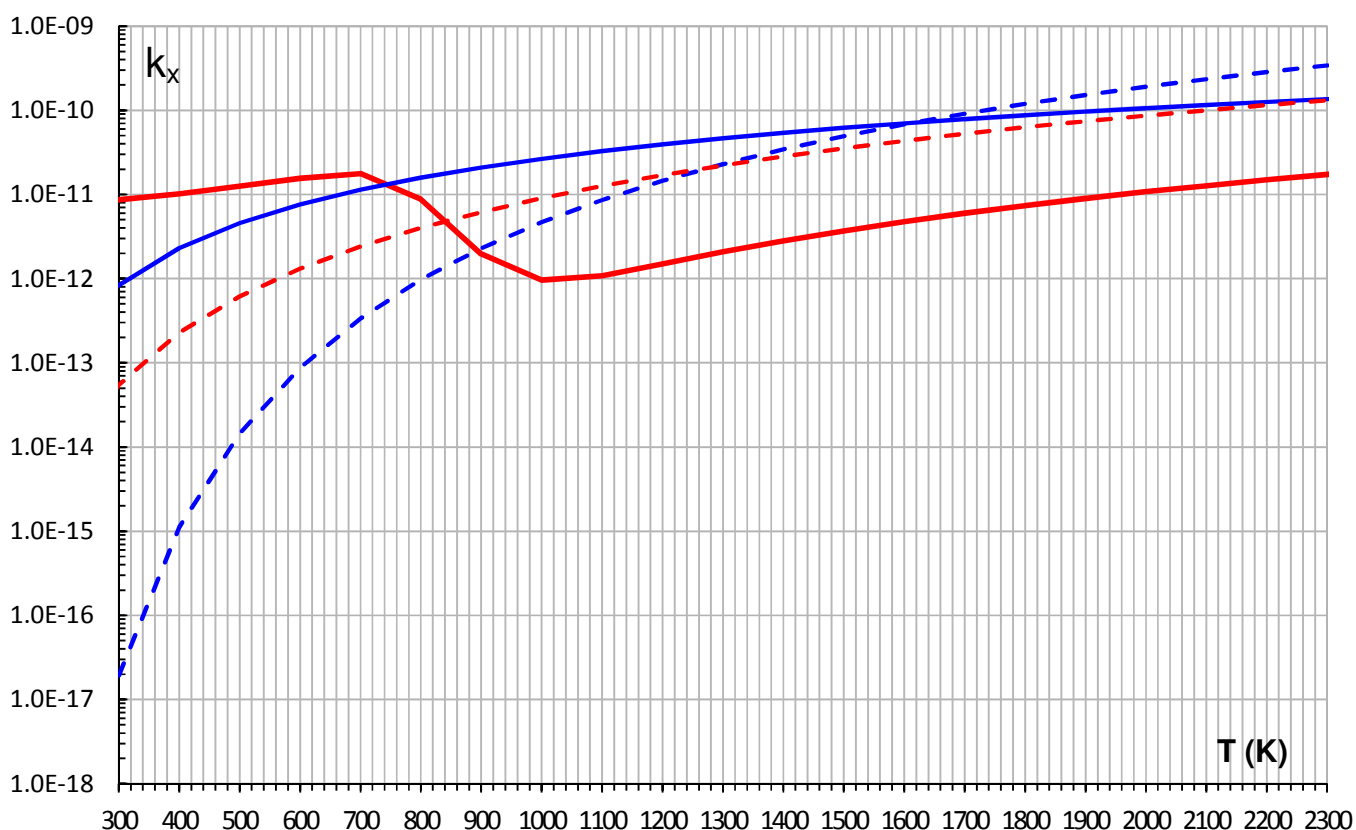
FIGURE S2. Rate constants k_X (molecule^{-1} cm^3 s^{-1}) as a function of T. Red lines: X = HO; blue lines: X = O. k_X "effective" (see main text) for X addition to naphthalene (continuous lines) vs H-abstraction from its position 1 (broken lines). A crossing occurs for HO just around 850 K, and a similar crossing for O at ca. 1600 K. Individual H abstractions can prevail over addition by O above 1640, 2000, or 2300 K.

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We attempt now an analysis of the features exhibited by the four curves.

Addition of HO on naphthalene.

The sum of the exit channels from the adduct (H abstractions: dotted gray curve) is coincident with $k_O[O]$ (blue) in the approximate range 400 – 750 K; then coincident with C–H homolysis (black, k_{-H}) in the range 1060 – 1200 K. Beyond 750 K, k_{-1} (purple) prevails on all other k's.

In the approximate range 400 – 750 K the sum of the exit channels (dotted gray curve) prevails on k_{-1} (purple): as a consequence k_{eff} (plotted as a red continuous line in Figure S2) is dominated by k_1 within that range (less so getting closer to the upper limit), and its ascending behavior is similar to that of the other curves.
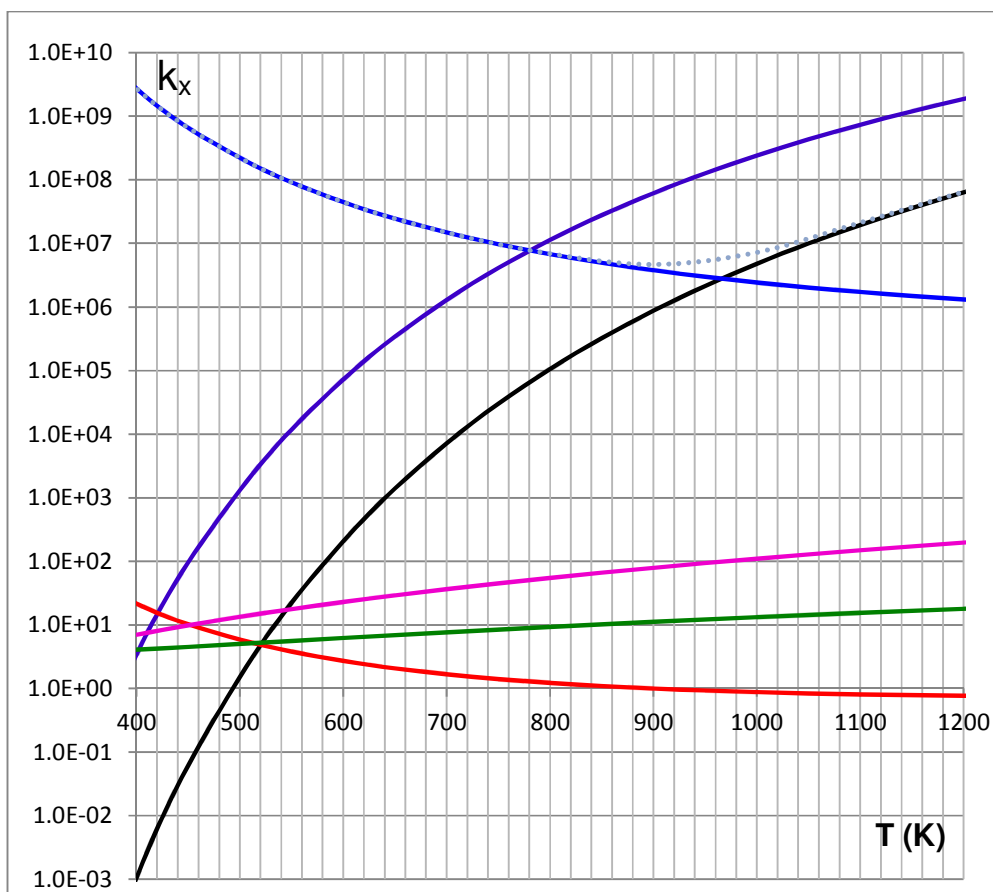
FIGURE S3. Hydroxyl addition to naphthalene. Rate constants as functions of T. Color code:
1. dotted gray: Σk_i for all H-abstraction exit channels 4-7.
2. green: k_1 for adduct formation from the two reactants.
3. purple: k_{-1} for the backwards step from the adduct to reactants.
4. black: k_{-H} for sheer C-H homolysis.
5. red: k_{HO} for H abstraction from the adduct carried out by hydroxyl.
6. blue: k_O for H abstraction from the adduct carried out by the oxygen atom.
7. magenta: k_{O2} for H abstraction from the adduct carried out by dioxygen.

But the importance of k_{-1} grows with T, while, by contrast, the role of the sum of the exit channels declines. Hence the red continuous line of Figure S2 (k_{eff} for addition) does not ascend too steeply, and at ca. 700 K begins to decline.

Within a transition zone, approximately 750-1050 K, the sum of the exit channels sees a minimum. Considering that it damps the effect of k_{-1}, its role goes also through a minimum, and the overall addition rate (red continuous line of Figure S2, k_{eff}) declines.

However, the slope of the sum of the exit channels (dotted gray) becomes again positive. The pure homolysis (k_{-H}) and the backwards step from the adduct to reactants (k_{-1}), black and purple lines, respectively, have a similar dependence on T dictated by their common trait: cleavage of one bond, and consequent entropy effect related to the step from one species to two. However, they show also a somewhat converging behavior: they are separated by more than three orders of magnitude at T=400 K, but only by somewhat more than one at T = 1200 K. Therefore, H loss by sheer homolysis (k_{-H}), chiefly, among the exit channels, thwarts to some extent k_{-1}, and the value of k_{eff} grows again beyond T = 1000 K (Figure S2).

Addition of O on naphthalene.

The main feature is that the sum of exit channels from the adduct (H abstract-ions, gray dotted line in Figure S4) is coincident with C–H homolysis (black line, k_{-H}) in the whole range 400 – 1200 K. It also prevails on k_{-1} (purple line) at all temperatures represented. As a consequence k_{eff} (Figure S2, blue continuous line) is dominated by k_1 within the whole range 400 – 1200 K.
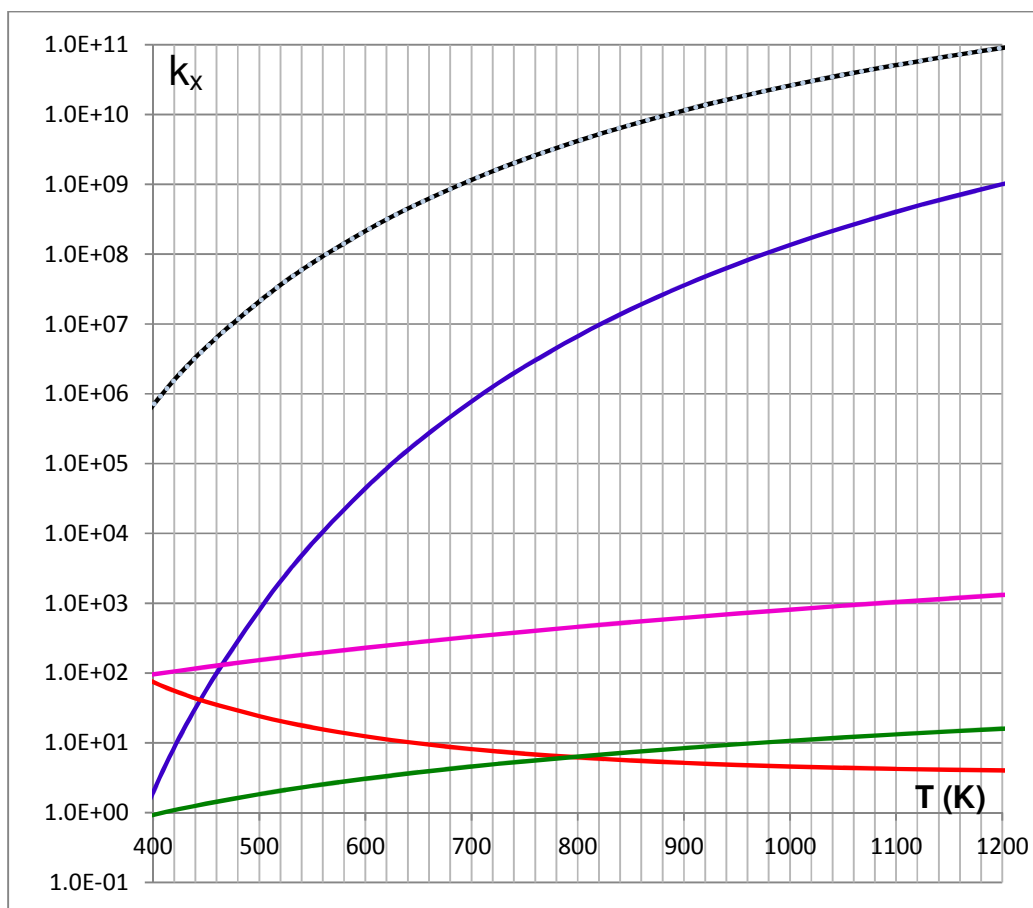
FIGURE S4. Hydroxyl addition to naphthalene. Rate constants k_{HO} as a function of T.
1. dotted gray: Σk_i for all H-abstraction exit channels 4-7.
2. green: k_1 for adduct formation from the two reactants.
3. purple: k_{-1} for the backwards step from the adduct to reactants.
4. black: k_{-H} for sheer C-H homolysis.
5. red: k_{HO} for H abstraction from the adduct carried out by hydroxyl.
6. Magenta: k_{O2} for H abstraction from the adduct carried out by dioxygen.

Section 6.

Kinetic simulations.

Hypothesizing three O concentrations, 10^{12} (Figure S5), 10^{14} (Figure S6), and 10^{16} (Figure S7) atoms cm^{-3}, we carried out three kinetic simulations. Other species concentrations were kept constant: [OH] = $1 \cdot 10^{12}$ molec. cm^{-3}, [H] = $1 \cdot 10^{12}$ molec. cm^{-3}, [O$_2$] = $1 \cdot 10^{17}$ molec. cm^{-3}. The amount of naphthol **2** produced by pathways **0**-**1**-**3**-**2** and **0**-**4**-**2**, as a function of time is plotted.
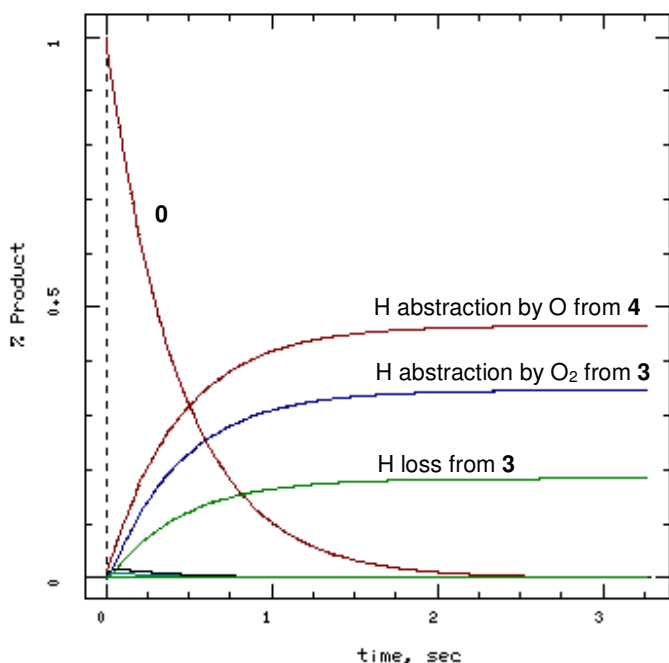
Figure S5. Kinetic simulation of reactions in Scheme 1. Yield vs time, by using [OH] = $1 \cdot 10^{12}$ molec. cm^{-3}, [H] = $1 \cdot 10^{12}$ molec. cm^{-3}, [O$_2$] = $1 \cdot 10^{17}$ molec. cm^{-3}, and [O] = $1 \cdot 10^{12}$ molec. cm^{-3}.

13
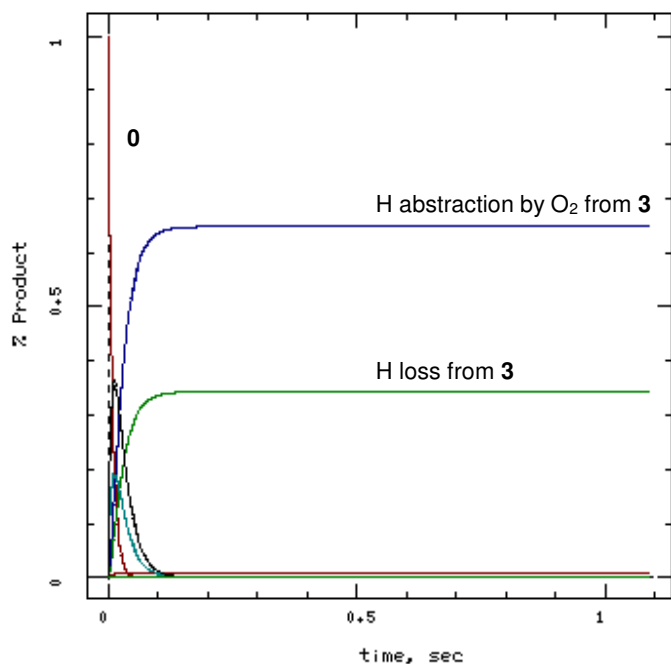
Figure S6. Kinetic simulation of reactions in Scheme 1. Yield vs time, by using $[OH] = 1 \cdot 10^{12}$ molec. cm^{-3}, $[H] = 1 \cdot 10^{12}$ molec. cm^{-3}, $[O_2] = 1 \cdot 10^{17}$ molec. cm^{-3}, and $[O] = 1 \cdot 10^{14}$ molec. cm^{-3}.
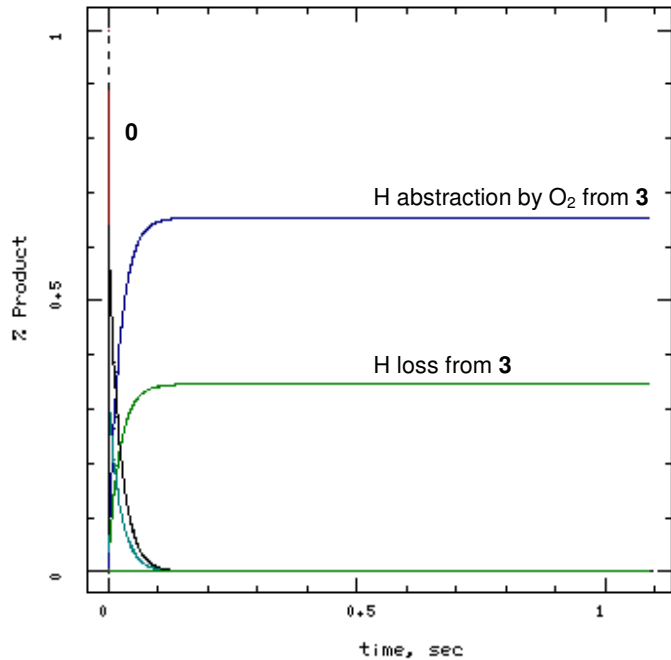
Figure S7. Kinetic simulation of reactions in Scheme 1. Yield vs time, by using $[OH] = 1 \cdot 10^{12}$ molec. cm^{-3}, $[H] = 1 \cdot 10^{12}$ molec. cm^{-3}, $[O_2] = 1 \cdot 10^{17}$ molec. cm^{-3}, and $[O] = 1 \cdot 10^{16}$ molec. cm^{-3}.

Section 7

Table of energies.

Table S3. Energies and Free Energies contribution at 400 K, in Hartrees.

	M06-2X/6-311G(d,p)		M06-2X/cc-pvTz//M06-2X/6-311G(d,p)	
	E /h	dG (400 K)[a]	E /h	E (Yamaguchi)[b]
Naphthalene	-385.811857	0.104490	-385.8551335	
O(^{3}P)	-75.057682	-0.020991	-75.06424175	
$^3O_2$	-150.303973	-0.023998	-75.06424175	
HO	-75.720592	-0.015421	-75.73046559	
H_2O	-76.412327	-0.003485	-76.42524901	
HOO	-150.884668	-0.016524	-150.9041754	
H	0.498134	-0.015224	-0.498134772	
TS 0-1	-460.866971	0.098132	-460.9177528	
1	-460.904033	0.098336	-460.9545195	
TS 1-^{3}2	-460.854989	0.093470	-460.9079429	
^{3}2	-460.926181	0.097028	-460.9794962	
TS 1-3 (H loss)	-460.876666	0.092101	-460.9276107	
TS 1-3 (H-abstraction by $^3O_2$)	-611.206572	0.095830	-611.2739212	
TS 1-3 (H-abstraction by OH)	-536.63526*	0.103609	-536.693962*	-536.695606
3	-460.395224	0.091088	-460.4462003	
TS 3-^{1}2	-460.89287*	0.091743	-460.943960*	-460.948501
^{1}2	-461.034247	0.105028	-461.086946	
TS 3-ketone	-460.892905*	0.087598	-460.943787*	-460.944649
ketone	-461.019251	0.103344	-461.0698945	
TS 0-4	-461.535824	0.108202	-461.5883389	

4	-461.574403	0.110883	-461.6271275	
TS 4-^{1}2 (H loss)	-461.522561	0.105244	-461.5751692	
TS 4-^{1}2 (H-abstraction by O_2)	-611.863862*	0.106954	-611.932787*	-611.944344
TS 4-^{1}2 (H-abstraction by O)	-536.643729*	0.107441	-536.701624*	-536.708359
TS 4-^{1}2 (H-abstraction by OH)	-537.309045*	0.118616	-537.369220*	-537.373684
10	-535.555026	0.091930	-535.6133388	
TS 10-11 (H loss)	-685.849536*	0.086205	-685.924618*	-685.938806
TS 10-11 (H-abstraction by O_2)	-535.518936	0.083265	-535.5783187	
TS 10-11 (H-abstraction by OH)	-611.284329*	0.083265	-611.351425*	-611.355754
11	-535.032520	0.084143	-535.0913612	
TS 1-6	-846.695906	0.229926	-846.7858503	
6	-846.713381	0.233170	-846.8021786	
TS 1-7	-846.712281	0.229640	-846.8040739	
7	-846.739614	0.229469	-846.8325525	
TS 7-8 (H loss)	-846.683606	0.224357	-846.776843	
TS 7-8 (H-abstraction by O_2)	-997.035742*	0.233335	-997.145005*	-997.164564
TS 7-8 (H-abstraction by OH)	-922.470442*	0.237763	-922.571268*	-922.572549
"TS" 1-8 (Maximum of the Free Energy)	-846.033988*	0.210561	-846.126466*	-846.126625
TS 2-8	-846.175383	0.220736	-846.2685643	
5	-385.125532	0.089007	-385.1686143	
TS 2-9	-845.528741*	0.207049	-845.620976*	-845.626459
8	-846.194466	0.223744	-846.2877467	
TS 8-9 (H-abstraction by O)	-921.244568*	0.241213	-921.364426*	-921.370661
TS 8-9 (H loss)	-846.118979	0.216167	-846.2330438	
TS 8-9 (H-abstraction by O_2)	-996.460101*	0.218529	-996.592702*	-996.603752
TS 8-9 (H-abstraction by OH)	-921.904942*	0.230980	-922.033474*	-922.044186
9	-845.650593	0.216222	-845.7444963	
TS naphthalene+O (H-abstraction by O)	-460.847796	0.089706	-460.8987116	

TS naphthalene+OH (H-abstraction by OH)	-461.526073	0.102401	-461.5786021

*Without Yamaguchi's correction

[a] Free energy correction at 400K: G(T) = E + dG(T). [b] Energy values were spin-corrected by Yamaguchi's formula. For singlet diradicaloid structures, the wavefunctions were spin-mixed for better description of the electron distribution, but the energy had to be refined by Yamaguchi's formula. See the Theoretical Method section for details.

Section 8

Emission spectra for the discharge in He with residual traces of H$_2$O
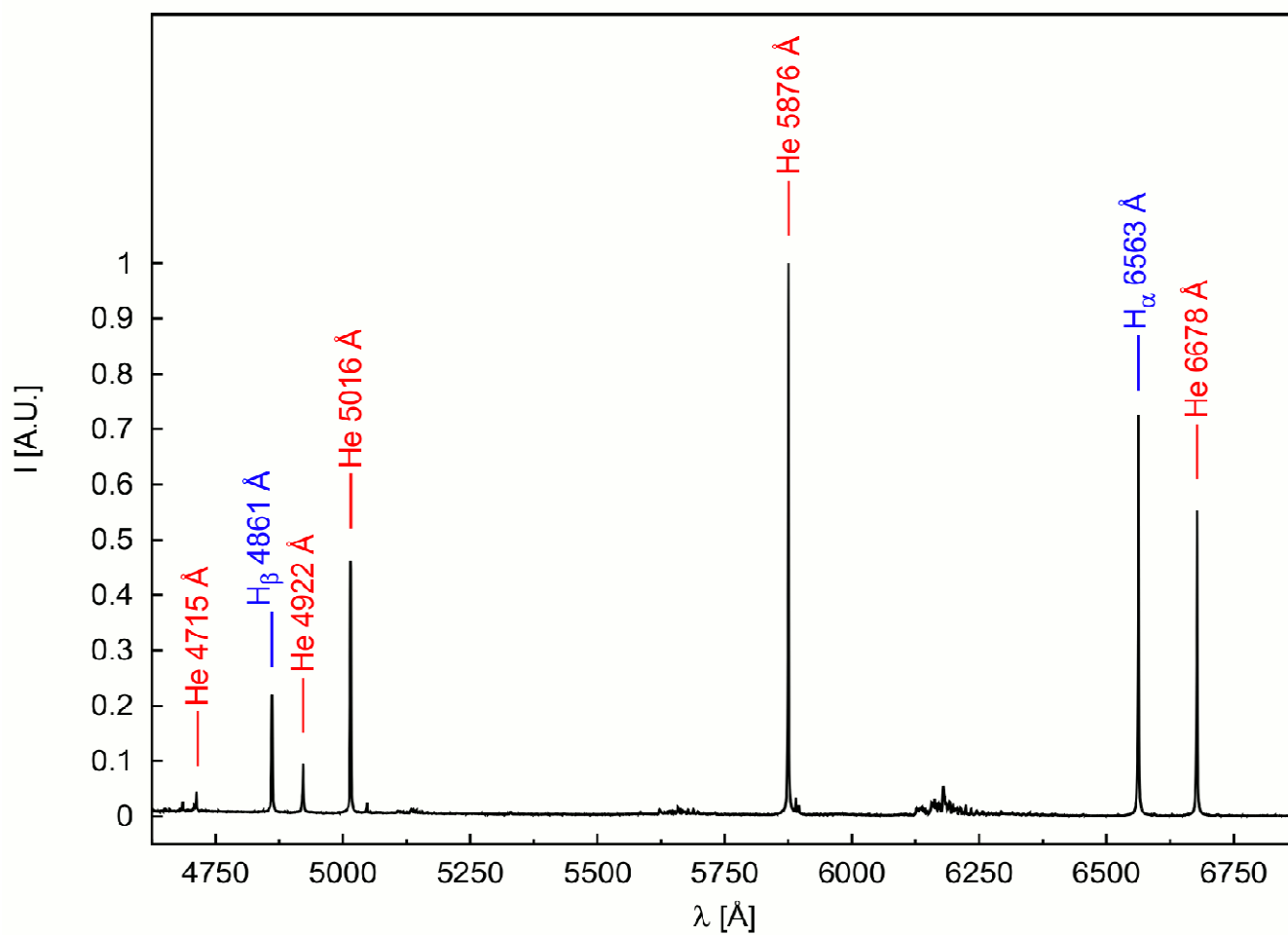
Figure S8. emission from H
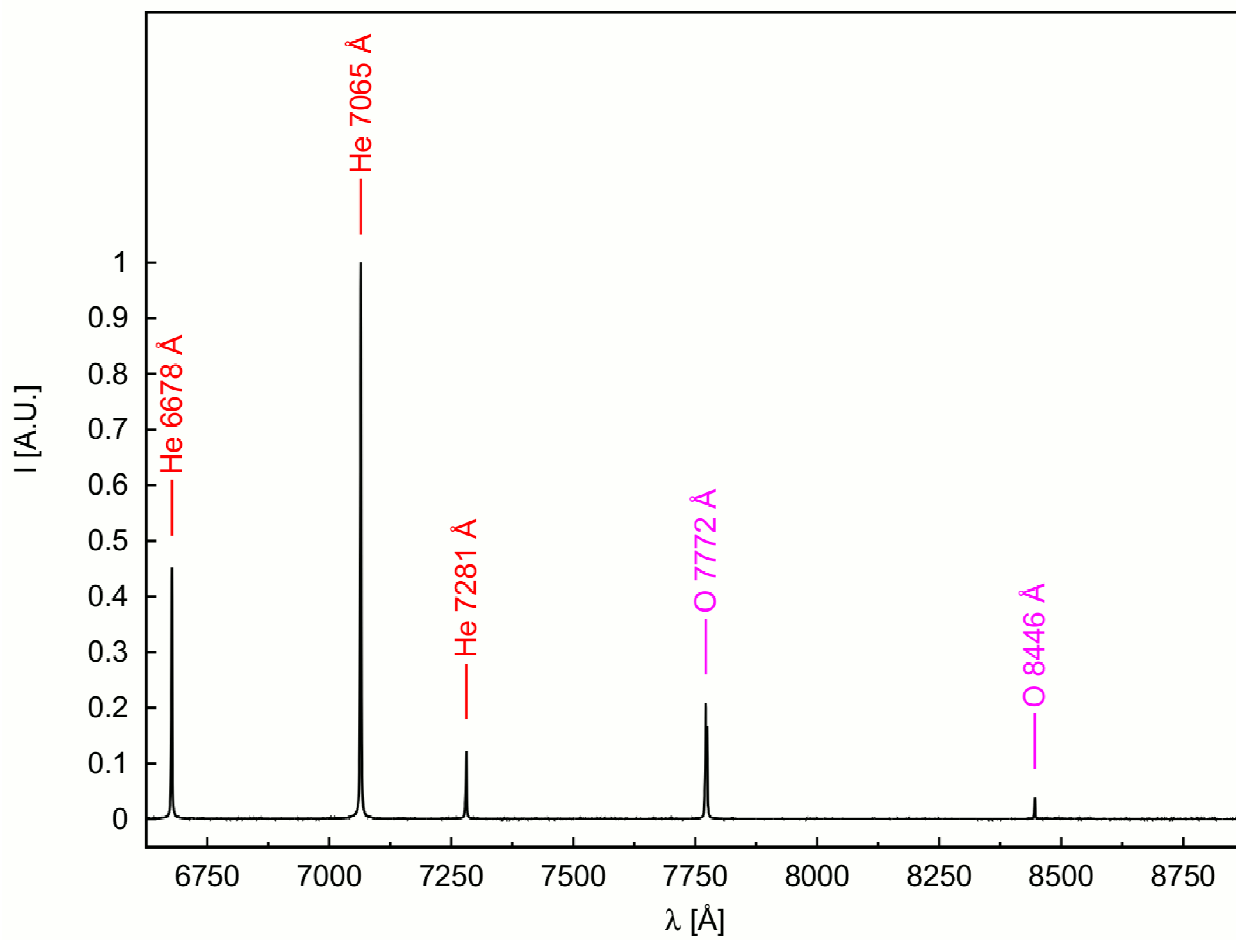
Figure S9. Emission from O
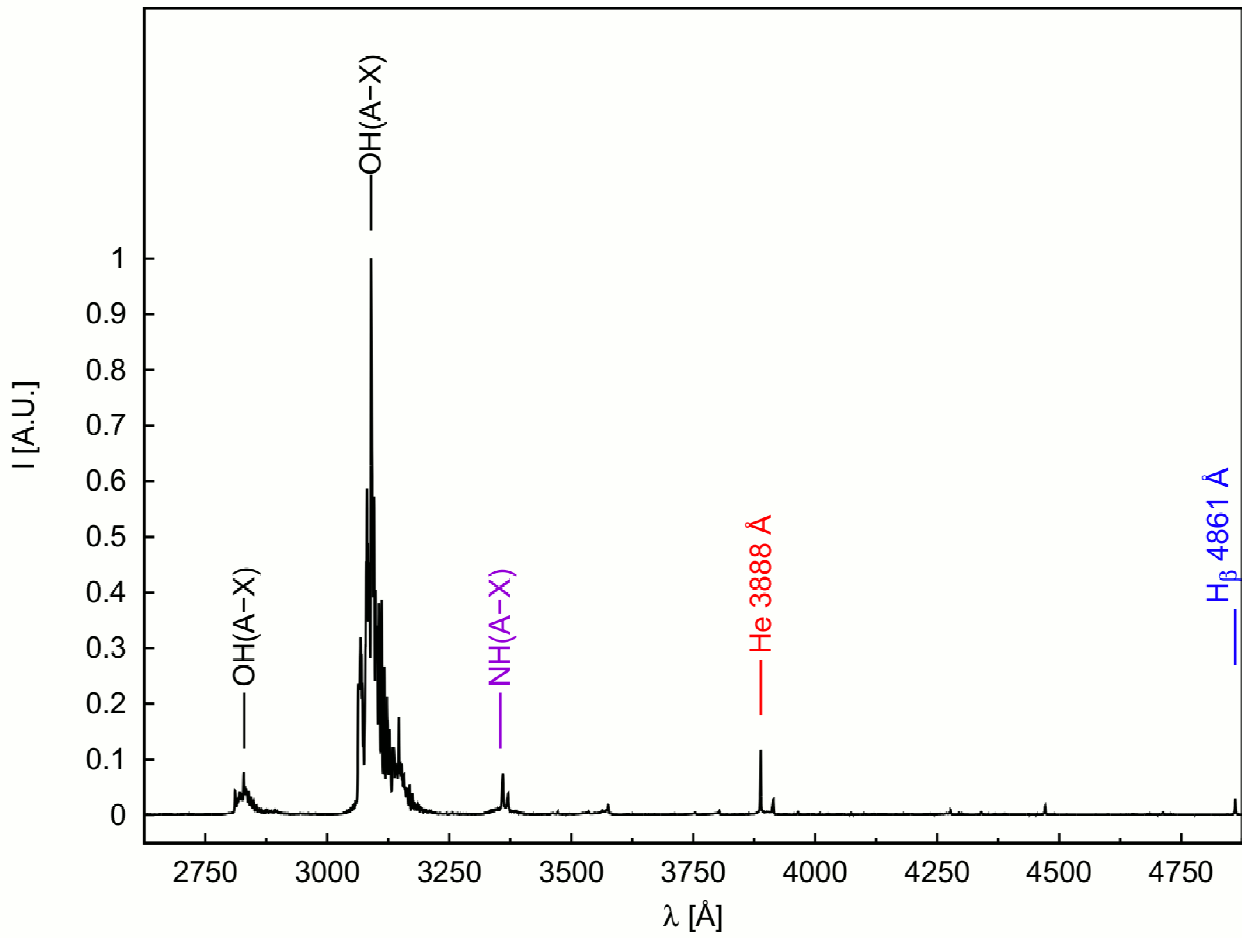
Figure S10. Emission from OH

Section 9.
Geometries

Naphthalene

Atom	X	Y	X	(Angstrom)
6	−0.00920	0.00000	0.00531	
6	0.01644	0.00000	1.42321	
6	1.20490	0.00000	2.10175	
6	2.43016	0.00000	1.39435	
6	2.43675	0.00000	0.02584	
1	−0.92545	0.00000	1.96106	
1	1.21203	0.00000	3.18502	
1	3.36473	0.00000	1.94216	
1	3.37349	0.00000	−0.52093	
6	−1.22431	0.00000	−0.72584	
6	−1.21772	0.00000	−2.09435	
6	0.00754	0.00000	−2.80175	
6	1.19600	0.00000	−2.12321	
6	1.22164	0.00000	−0.70531	
1	−2.16106	0.00000	−0.17907	
1	−2.15230	0.00000	−2.64216	
1	0.00040	0.00000	−3.88502	
1	2.13788	0.00000	−2.66106	

E= −385.811857 (Hartree)

O(^{3}P)

Atom	X	Y	X	(Angstrom)
8	0.00000	0.00000	0.00000	

E= −75.057682 (Hartree)

TS 0−1

Atom	X	Y	X	(Angstrom)
6	0.01043	0.01030	0.01874	
6	0.00717	−0.00504	1.43393	
6	1.24357	0.00295	2.11984	
6	2.42838	0.01628	1.42573	
6	2.42610	0.01779	0.01709	
6	1.23609	0.00999	−0.67269	
6	−1.24805	−0.04917	−0.68577	
6	−2.44197	0.05614	0.03911	
6	−2.42861	0.03422	1.44044	
6	−1.23792	−0.00271	2.12590	
1	1.24068	−0.00464	3.20435	
1	3.37048	0.02114	1.96064	
1	3.36605	0.01926	−0.52142	
1	1.22467	−0.00458	−1.75690	
1	−1.22804	−0.01681	3.21019	
1	−3.36514	0.06168	1.98392	
1	−3.38374	0.10319	−0.49330	
1	−1.24563	0.16332	−1.74741	
8	−1.18687	−1.96382	−0.94924	

E= -460.866971 (Hartree)

1

Atom	X	Y	X	(Angstrom)
6	0.01645	0.01501	0.01426	
6	0.01050	0.05841	1.42330	
6	1.24373	0.05335	2.10212	
6	2.43603	-0.00053	1.40570	
6	2.42823	-0.05872	0.01052	
6	1.22027	-0.05291	-0.67468	
6	-1.28776	0.04151	-0.76451	
6	-2.51729	-0.06933	0.08917	
6	-2.45541	-0.03581	1.45271	
6	-1.23457	0.06440	2.13637	
8	-1.30817	-0.83149	-1.82959	
1	1.24329	0.08262	3.18641	
1	3.37650	-0.00504	1.94348	
1	3.36174	-0.11111	-0.53627	
1	1.20000	-0.11569	-1.75701	
1	-1.21561	0.09471	3.21866	
1	-3.37394	-0.10167	2.02510	
1	-3.45629	-0.17320	-0.44003	
1	-1.33596	1.02243	-1.30036	

E= -460.904033 (Hartree)

TS 1–³2

Atom	X	Y	X	(Angstrom)
6	0.01300	0.03638	0.00188	
6	0.00535	0.01184	1.43803	
6	1.23432	-0.06363	2.14448	
6	2.50351	-0.03718	1.37824	
6	2.42605	-0.16200	-0.10089	
6	1.23250	-0.11468	-0.72932	
6	-1.18601	0.01026	2.16891	
6	-1.17221	-0.06857	3.56176	
6	0.03178	-0.16237	4.23888	
6	1.23684	-0.16276	3.52283	
8	3.65781	-0.46797	1.99699	
1	-2.12977	0.05411	1.63602	
1	-2.10729	-0.06609	4.10893	
1	0.04726	-0.23605	5.31926	
1	2.18675	-0.24249	4.03804	
1	-0.92968	0.10729	-0.52543	
1	1.18707	-0.19295	-1.80938	
1	3.36281	-0.27983	-0.63030	
1	3.44047	0.71729	1.81526	

E= -460.854989 (Hartree)

³2

Atom	X	Y	X	(Angstrom)
6	-0.00524	0.00000	0.01830	
6	0.01806	0.00000	1.41177	
6	1.25229	0.00000	2.13005	

```
6      2.43144      0.00000      1.44843
6      2.44317      0.00000      0.01738
1     -0.92140      0.00000      1.95238
1      1.23820      0.00000      3.21279
1      3.37473      0.00000      1.98127
1      3.38204      0.00000     -0.51981
6     -1.21387      0.00000     -0.71979
6     -1.22017      0.00000     -2.16773
6     -0.05262      0.00000     -2.84239
6      1.19993      0.00000     -2.11370
6      1.25074      0.00000     -0.69432
1     -2.15463      0.00000     -0.18351
1     -2.16514      0.00000     -2.69529
1     -0.02735      0.00000     -3.92770
8      2.37961      0.00000     -2.77482
1      2.22275      0.00000     -3.72283
```
E= −460.926181 (Hartree)

TS 1−3 (H loss)
```
Atom       X            Y            X          (Angstrom)
6      0.00321      0.04898      0.01484
6      0.00283      0.03760      1.42579
6      1.23786      0.00074      2.10234
6      2.42296     -0.02782      1.39590
6      2.40899     -0.02290     -0.00449
6      1.20500      0.01759     -0.68771
6     -1.29104      0.11479     -0.72232
6     -2.50481     -0.02548      0.07656
6     -2.45684     -0.04063      1.45267
6     -1.24184      0.02664      2.13244
8     -1.33116     -0.09080     -1.97221
1      1.24335     -0.01141      3.18689
1      3.36722     -0.05727      1.92635
1      3.34281     -0.05003     -0.55275
1      1.16902      0.02658     -1.77061
1     -1.22378      0.02483      3.21603
1     -3.37752     -0.11944      2.01896
1     -3.43560     -0.08555     -0.47288
1     -1.26423      1.73356     -0.95850
```
E= −460.876666 (Hartree)

TS 1−3 (H-abstraction by $^3O_2$)
```
Atom       X            Y            X          (Angstrom)
6     -0.05940      0.07478      0.09745
6     -0.03685      0.16642      1.48108
6      1.18049      0.13888      2.16756
6      2.36658      0.03302      1.46758
6      2.36367     -0.05523      0.06387
6      1.12944     -0.04217     -0.61485
6      1.10510     -0.19684     -2.11300
6      2.41222     -0.07635     -2.79211
6      3.59554     -0.05644     -2.06927
6      3.58973     -0.09438     -0.68741
```

```
8         0.06217        0.32928       -2.76002
1         2.39350        0.04591       -3.86691
1         4.53857        0.00332       -2.59937
1         4.52566       -0.09189       -0.14055
1         3.31554        0.02554        1.99273
1         1.19378        0.20748        3.24854
1        -0.96520        0.25906        2.03159
1        -0.99419        0.09986       -0.44996
1         0.86319       -1.36837       -2.26620
8         1.29141       -2.80138       -2.82619
8         2.34360       -2.55729       -3.37918
E= -611.206572 (Hartree)
```

TS 1-3 (H-abstraction by OH)
```
Atom        X              Y              X         (Angstrom)
6         0.06747        0.09332        0.02363
6         0.09386        0.08307        1.45947
6         1.32446       -0.02338        2.13971
6         2.63221       -0.00400        1.36666
6         2.47103       -0.14716       -0.11657
6         1.24649       -0.06686       -0.71734
6         1.35388       -0.08923        3.52761
6         0.17520       -0.02812        4.26217
6        -1.04947        0.09350        3.60099
6        -1.08971        0.14211        2.21929
8         3.59692       -0.82176        1.88261
8         2.23495        2.72746        2.41991
1         3.38213       -0.29205       -0.68302
1         1.18190       -0.13913       -1.79718
1        -0.88864        0.16975       -0.47919
1        -2.03992        0.22137        1.70202
1        -1.97010        0.14144        4.17023
1         0.20727       -0.07685        5.34373
1         2.31333       -0.18729        4.02294
1         3.08924        1.01261        1.55099
1         1.39944        2.45256        2.83605
E= -536.635260 (Hartree)
```

³O₂

$^3O_2$
```
Atom        X              Y              X         (Angstrom)
8         0.00000        0.00000        0.00000
8         0.00000        0.00000        1.18851
E= -150.303973 (Hartree)
```

OH
```
Atom        X              Y              X         (Angstrom)
8         0.00000        0.00000        0.01431
1         0.00000        0.00000        0.98569
E=  -75.720592 (Hartree)
```

HOO
```
Atom        X              Y              X         (Angstrom)
8         0.00000        0.00000        0.00000
```

```
8       0.00000         0.00000         1.30728
1       0.93406         0.00000         1.57577
```
E= -150.884668 (Hartree)

H₂O
```
Atom        X               Y               X               (Angstrom)
8       0.01031         0.00000         0.00791
1       0.01740         0.00000         0.96665
1       0.93821         0.00000        -0.23338
```
E= -76.412327 (Hartree)

H
E=   0.498134 (Hartree)

3
```
Atom        X               Y               X               (Angstrom)
6       0.00929         0.00000         0.01337
6       0.01874         0.00000         1.42336
6       1.21284         0.00000         2.11277
6       2.43009         0.00000         1.41695
6       2.44138         0.00000         0.03331
1      -0.92499         0.00000         1.95793
1       1.21220         0.00000         3.19613
1       3.36396         0.00000         1.96596
1       3.36722         0.00000        -0.52929
6      -1.21180         0.00000        -0.72697
6      -1.21248         0.00000        -2.11993
6      -0.02831         0.00000        -2.82815
6       1.26099         0.00000        -2.15920
6       1.24102         0.00000        -0.67787
1      -2.14909         0.00000        -0.18216
1      -2.15766         0.00000        -2.64983
1      -0.00789         0.00000        -3.91104
8       2.31574         0.00000        -2.79083
```
E= -460.395224 (Hartree)

TS 3–¹2
```
Atom        X               Y               X               (Angstrom)
6      -0.12228         0.01654         0.00502
6      -0.05372         0.01338         1.41666
6       1.21151        -0.03410         2.03792
6       2.35984        -0.08310         1.27722
6       2.28081        -0.08360        -0.12355
6       1.05040        -0.03111        -0.75275
6      -1.43094         0.05027        -0.66645
6      -2.60238         0.05819         0.17216
6      -2.50327         0.07556         1.55287
6      -1.26149         0.05167         2.17558
8      -1.51886         0.06397        -1.90546
1       1.26754        -0.03526         3.12110
1       3.32803        -0.12187         1.76194
1       3.18940        -0.12230        -0.71221
1       0.96470        -0.01911        -1.83287
```

```
1        -1.19528        0.05751        3.25783
1        -3.40268        0.09920        2.15656
1        -3.56006        0.06803       -0.33371
1        -0.72829       -1.65687       -2.67706
E= -460.892870 (Hartree)
```

¹2

```
Atom        X               Y               X              (Angstrom)
6        -0.03578        0.00000        0.01133
6        -0.02370        0.00000        1.43008
6         1.23053        0.00000        2.09264
6         2.40115        0.00000        1.38249
6         2.37945        0.00000       -0.03117
6         1.18641        0.00000       -0.70408
6        -1.29377        0.00000       -0.65841
6        -2.46594        0.00000        0.05208
6        -2.43805        0.00000        1.46576
6        -1.25123        0.00000        2.14383
8        -1.24708        0.00000       -2.01753
1         1.24388        0.00000        3.17720
1         3.35156        0.00000        1.90287
1         3.31223        0.00000       -0.58199
1         1.15387        0.00000       -1.78596
1        -1.22911        0.00000        3.22735
1        -3.37620        0.00000        2.00749
1        -3.41707        0.00000       -0.47034
1        -2.14325        0.00000       -2.36367
E= -461.034247 (Hartree)
```

TS 3-ketone

```
Atom        X               Y               X              (Angstrom)
6         0.09186        0.15441        0.10063
6         0.04209        0.11329        1.52738
6         1.24656        0.04658        2.26208
6         2.54874        0.01968        1.55516
6         2.50262        0.06597        0.10365
6         1.30748        0.13037       -0.58130
6        -1.18253        0.13945        2.22530
6        -1.20020        0.10023        3.60352
6         0.00108        0.03390        4.32350
6         1.21295        0.00744        3.65632
8         3.61382       -0.03776        2.16570
1        -2.10894        0.19017        1.66373
1        -2.14524        0.12028        4.13274
1        -0.02216        0.00346        5.40613
1         2.15528       -0.04334        4.18837
1        -0.83958        0.21284       -0.45060
1         1.30818        0.16455       -1.66442
1         3.45694        0.04749       -0.40799
1        -0.85338       -2.97799       -1.14005
E= -460.892905 (Hartree)
```

ketone

```
Atom        X              Y              X          (Angstrom)
6        0.01112       -0.00014        0.01139
6        0.01738       -0.00028        1.40824
6        1.24394       -0.00026        2.07610
6        2.43443       -0.00011        1.36691
6        2.42182        0.00002       -0.02915
6        1.21326        0.00001       -0.70097
6       -1.27019       -0.00007       -0.75533
6       -2.51758       -0.00020        0.03761
6       -2.51127       -0.00034        1.37051
6       -1.26560       -0.00050        2.19569
8       -1.29067       -0.00006       -1.96708
1        1.25810       -0.00036        3.16131
1        3.37787       -0.00010        1.90010
1        3.35398        0.00013       -0.58062
1        1.16221        0.00012       -1.78323
1       -1.28435        0.87028        2.86312
1       -3.45194       -0.00038        1.91332
1       -3.43745       -0.00014       -0.53515
1       -1.28432       -0.87163        2.86266
E= -461.019251 (Hartree)
```

TS 0-4
```
Atom        X              Y              X          (Angstrom)
6       -0.00549        0.04032       -0.00681
6       -0.01807       -0.01123        1.40920
6        1.21439       -0.04663        2.10591
6        2.40323       -0.03529        1.42233
6        2.41130        0.00738        0.01172
6        1.22979        0.03987       -0.68696
6       -1.25209        0.04443       -0.71838
6       -2.44900        0.10833       -0.00952
6       -2.45142        0.04567        1.39580
6       -1.26800       -0.01128        2.09053
1        1.20141       -0.08288        3.18997
1        3.34150       -0.06272        1.96322
1        3.35585        0.00869       -0.51876
1        1.22670        0.05358       -1.77106
1       -1.26847       -0.05053        3.17455
1       -3.39394        0.05603        1.92945
1       -3.38291        0.15833       -0.55395
1       -1.23839        0.24962       -1.78036
8       -1.46304       -1.92502       -1.25688
1       -1.43010       -2.28386       -0.35735
E= -461.535824 (Hartree)
```

4
```
Atom        X              Y              X          (Angstrom)
6       -0.01489       -0.02519        0.00514
6       -0.01123       -0.02532        1.43885
6        1.21458        0.04146        2.13331
6        2.53903        0.00308        1.39932
6        2.39755        0.09560       -0.08676
```

```
6        1.18684         0.05614        -0.71440
6       -1.20892        -0.05449         2.17697
6       -1.19462        -0.00956         3.55882
6        0.01957         0.07951         4.24065
6        1.20941         0.10694         3.52263
8        3.24728        -1.21520         1.65475
1       -2.15132        -0.10816         1.64227
1       -2.12637        -0.03284         4.11099
1        0.03595         0.13337         5.32229
1        2.15324         0.19349         4.05564
1       -0.96385        -0.07304        -0.51483
1        1.14912         0.08253        -1.79753
1        3.31988         0.12586        -0.65353
1        3.15402         0.84375         1.75700
1        3.24495        -1.36001         2.60504
```
E= −461.574403 (Hartree)

TS 4–^{1}2 (H loss)
```
 Atom        X               Y               X            (Angstrom)
6       -0.02042         0.08940         0.04211
6        0.00457         0.01296         1.41326
6        1.23420        -0.07367         2.09863
6        2.41653        -0.07412         1.40352
6        2.42695         0.01358        -0.00977
6        1.18531         0.09165        -0.68633
6        1.19518         0.12912        -2.12777
6        2.39799         0.32177        -2.80710
6        3.61530         0.22723        -2.11442
6        3.63884         0.05278        -0.75378
8       -0.01640         0.33852        -2.71652
1        2.38446         0.45916        -3.88299
1        4.54303         0.30412        -2.66835
1        4.58073        -0.01868        -0.22240
1        3.36400        -0.13717         1.92773
1        1.24118        -0.13877         3.18028
1       -0.92299         0.01713         1.97282
1       -0.95634         0.14681        -0.49850
1        1.27109        -1.62084        -2.25639
1        0.08427         0.28987        -3.67078
```
E= −461.522561 (Hartree)

TS 4–^{1}2 (H-abstraction by O_2)
```
Atom        X               Y               X            (Angstrom)
6        0.02817         0.02662        -0.00117
6        0.04137         0.04176         1.42480
6        1.28030        -0.00551         2.10924
6        2.52690         0.13228         1.31954
6        2.42838        -0.14985        -0.09236
6        1.20097        -0.10947        -0.73016
6        1.30414        -0.08488         3.50407
6        0.12157        -0.10450         4.21928
6       -1.11156        -0.03323         3.55332
6       -1.15234         0.03405         2.17957
```

```
8        3.70881       -0.29151        1.92113
8        3.09554        2.61319        1.98885
8        3.63313        2.28133        3.05144
1        3.35590       -0.28336       -0.63528
1        1.15514       -0.20972       -1.80768
1       -0.92836        0.06087       -0.50997
1       -2.10177        0.07332        1.65697
1       -2.03233       -0.04249        4.12397
1        0.14610       -0.17767        5.29978
1        2.25564       -0.14680        4.01671
1        2.62764        1.34937        1.30217
1        3.95619        0.36337        2.58803
E= -611.863862 (Hartree)
```

TS 4-^{1}2 (H-abstraction by O)

Atom	X	Y	X	(Angstrom)
6	-0.01275	0.05985	-0.01259	
6	-0.01778	-0.01527	1.39441	
6	1.21404	-0.12665	2.07386	
6	2.40534	-0.16337	1.35246	
6	2.39013	-0.08141	-0.03164	
6	1.17455	0.02958	-0.71529	
6	1.24982	-0.26488	3.57116	
6	-0.04036	0.01903	4.23574	
6	-1.21955	0.10929	3.53699	
6	-1.23729	0.06447	2.14212	
8	2.34549	0.40319	4.17343	
8	3.04832	-2.21892	3.91560	
1	-0.01793	0.08593	5.31715	
1	-2.15078	0.24517	4.07470	
1	-2.17422	0.14169	1.60342	
1	-0.95881	0.14530	-0.53633	
1	1.16592	0.08948	-1.79700	
1	3.32121	-0.11032	-0.58493	
1	3.33564	-0.26691	1.89797	
1	1.49588	-1.34636	3.78586	
1	2.23580	1.34289	3.99426	

E= -536.643729 (Hartree)

TS 4-^{1}2 (H-abstraction by OH)

Atom	X	Y	X	(Angstrom)
6	0.08477	-0.25508	-0.16218	
6	0.02622	-0.25679	1.22585	
6	1.19943	-0.12775	1.97341	
6	2.41599	0.01032	1.33259	
6	2.49471	0.01808	-0.07304	
6	1.30635	-0.12473	-0.81961	
6	1.34553	-0.19195	-2.32842	
6	2.64871	0.22633	-2.90639	
6	3.78130	0.35761	-2.14376	
6	3.74239	0.21921	-0.75337	
8	0.23953	0.45623	-2.93428	
1	2.67375	0.35583	-3.98194	

```
1       4.72321         0.59605         -2.62444
1       4.64596         0.32419         -0.16525
1       3.32836         0.12098          1.90877
1       1.15541        -0.13056          3.05593
1      -0.92919        -0.35640          1.72677
1      -0.81435        -0.35252         -0.76072
1       1.19140        -1.26389         -2.61777
8       0.17718        -2.76084         -2.18931
1       0.38087        -2.58961         -1.25385
1       0.31284         1.39175         -2.71940
E= -537.309045 (Hartree)
```

A (see Scheme S2)

Atom	X	Y	X	(Angstrom)
6	-0.03615	0.22287	0.09390	
6	-0.03846	-0.01227	1.47658	
6	1.10115	-0.35048	2.14773	
6	2.41952	-0.44928	1.46378	
6	2.37051	-0.28066	-0.03139	
8	3.26192	0.62781	2.04313	
8	4.51555	0.30642	2.05833	
1	2.95594	-1.36283	1.73595	
1	1.09176	-0.52017	3.21699	
1	-0.97021	0.07341	2.02368	
1	-0.95013	0.50117	-0.41586	
6	3.52925	-0.45451	-0.78068	
6	3.51662	-0.26263	-2.15656	
6	2.33180	0.10196	-2.79845	
6	1.17169	0.26846	-2.06602	
6	1.16694	0.08048	-0.67187	
1	4.44816	-0.72651	-0.27364	
1	4.42612	-0.39764	-2.72878	
1	2.32001	0.25135	-3.87134	
1	0.24661	0.54457	-2.56033	

E= -536.060064 (Hartree)

TS 1-A

Atom	X	Y	X	(Angstrom)
6	0.26816	2.09891	-0.37357	
6	1.59531	2.02461	0.03018	
6	2.09908	0.87328	0.60870	
6	1.29428	-0.31115	0.68753	
6	-0.13502	-0.17874	0.43855	
8	1.86126	-1.27413	-0.71299	
8	1.32251	-2.40241	-0.72489	
1	1.58350	-1.06641	1.41241	
1	3.13008	0.82715	0.93532	
1	2.23963	2.88706	-0.09188	
1	-0.11578	3.00422	-0.82956	
6	-1.01191	-1.23680	0.70021	
6	-2.35318	-1.12944	0.37665	
6	-2.84453	0.04292	-0.21444	
6	-1.99574	1.09765	-0.47285	

```
6      -0.62521       1.01057      -0.15245
1      -0.62420      -2.14405       1.14698
1      -3.02650      -1.95305       0.58022
1      -3.89565       0.11991      -0.46494
1      -2.37260       2.00919      -0.92405
E= -536.051044 (Hartree)
```

O₂ (¹Δg)
```
Atom        X              Y              X            (Angstrom)
8       0.00000       0.00000       0.00000
8       0.00000       0.00000       1.18815
E= -150.281225 (Hartree)
```

TS A-hydroperoxide
```
Atom        X              Y              X            (Angstrom)
6       0.06251       0.01221       0.03292
6       0.01388       0.01700       1.46263
6       1.21740       0.00176       2.19960
6       2.50152       0.16205       1.45938
6       2.46817      -0.12232       0.02962
6       1.26797      -0.09131      -0.65295
6      -1.20829      -0.03592       2.16446
6      -1.22096      -0.11244       3.54033
6      -0.01530      -0.13681       4.25552
6       1.19668      -0.07111       3.58980
8       3.62963      -0.28243       2.13882
8       4.12279       1.02212       2.45466
1      -0.87295       0.02243      -0.51467
1      -2.13667      -0.02006       1.60407
1      -2.16365      -0.15603       4.07202
1      -0.03256      -0.20502       5.33660
1       2.13888      -0.07438       4.12453
1       1.26104      -0.19608      -1.73119
1       3.41881      -0.26134      -0.46936
1       2.70878       1.31626       1.53425
E= -536.013801 (Hartree)
```

Hydroperoxide
```
Atom        X              Y              X            (Angstrom)
6       0.06821       0.00383       0.03886
6       0.00795      -0.01610       1.45843
6       1.21289      -0.03082       2.20866
6       2.44023      -0.01084       1.49042
6       2.47841       0.00605       0.12470
6       1.27082       0.00425      -0.61178
6      -1.22722      -0.03915       2.15495
6      -1.25637      -0.08756       3.52250
6      -0.05143      -0.11805       4.26201
6       1.15935      -0.08945       3.62317
8       3.64017      -0.08880       2.17166
8       3.79435       1.09015       2.97284
1      -0.86113       0.01045      -0.51973
1      -2.14843      -0.02269       1.58289
```

```
1    -2.20505    -0.10699    4.04544
1    -0.09011    -0.16639    5.34368
1     2.08686    -0.10317    4.18020
1     1.30803     0.01175   -1.69411
1     3.44075     0.00747   -0.37235
1     4.31426     1.65178    2.38368
E= -536.147797 (Hartree)
```

10

Atom	X	Y	X	(Angstrom)
6	0.00017	-0.01451	-0.00534	
6	0.00149	-0.03190	1.38660	
6	1.21392	-0.03202	2.07815	
6	2.41892	0.00431	1.37454	
6	2.41386	0.03146	-0.00980	
6	1.20117	0.01555	-0.69928	
6	-1.31599	-0.01754	2.13855	
6	-1.20378	-0.30528	3.61246	
6	-0.04168	-0.32487	4.26067	
6	1.25356	-0.11887	3.56858	
8	2.29210	-0.06052	4.18680	
8	-2.31682	-0.72711	1.53040	
1	3.34165	0.00314	1.94228	
1	3.34854	0.05693	-0.55662	
1	1.19495	0.02534	-1.78279	
1	-0.94647	-0.03846	-0.53200	
1	0.02094	-0.50366	5.32786	
1	-2.14774	-0.47206	4.12115	
1	-1.71175	1.02298	2.06464	

```
E= -535.555026 (Hartree)
```

TS 10-11 (H loss)

Atom	X	Y	X	(Angstrom)
6	0.08074	0.09261	-0.02017	
6	0.06480	0.07691	1.47344	
6	1.25172	-0.01870	2.20720	
6	2.58215	0.00457	1.50057	
6	2.53795	-0.17414	0.01808	
6	1.40031	-0.07927	-0.67753	
6	-1.16111	0.10677	2.13845	
6	-1.20014	0.04208	3.52153	
6	-0.01337	-0.05778	4.25018	
6	1.20982	-0.08246	3.59822	
8	3.65324	-0.31481	2.13897	
8	-0.93229	0.20703	-0.67183	
1	-2.06468	0.17475	1.54448	
1	-2.15180	0.06378	4.03844	
1	-0.04669	-0.11721	5.33148	
1	2.14252	-0.15903	4.14379	
1	1.37620	-0.16585	-1.75788	
1	3.50178	-0.32064	-0.45821	
1	2.71282	1.26154	1.45642	
8	2.36453	2.66185	1.18992	

```
8        1.40182         2.74887         0.47133
E= -685.849536 (Hartree)


TS 10-11 (H-abstraction by O₂)
Atom       X               Y               X            (Angstrom)
6        0.00000         0.00054         0.00012
6        0.00001         0.00061         1.39197
6        1.20925         0.00016         2.09462
6        2.41560         0.01005         1.39829
6        2.41269         0.01949         0.01111
6        1.20510         0.01173        -0.68715
6       -1.31070        -0.02259         2.12685
6       -1.24010        -0.05612         3.62366
6       -0.08020        -0.08314         4.28444
6        1.23026        -0.03290         3.58753
8        2.26499        -0.02096         4.21433
8       -2.37074        -0.22992         1.54863
1        3.33808         0.00556         1.96620
1        3.35064         0.02811        -0.53072
1        1.20757         0.01286        -1.77051
1       -0.95109        -0.01077        -0.51837
1       -0.03079        -0.13383         5.36620
1       -2.20182        -0.09008         4.12372
1       -1.31556         1.68183         2.26447
E= -535.518936 (Hartree)


TS 10-11 (H-abstraction by OH)
Atom       X               Y               X            (Angstrom)
6        0.07790         0.20436         0.03290
6        0.04546         0.11027         1.52072
6        1.22404         0.02383         2.26426
6        2.56944         0.13986         1.57615
6        2.53232        -0.03940         0.08025
6        1.40045         0.02328        -0.62034
6       -1.19103         0.06497         2.16609
6       -1.24971        -0.07678         3.54239
6       -0.07062        -0.17816         4.28029
6        1.16265        -0.12391         3.64573
8        3.59278        -0.49840         2.18127
8       -0.92118         0.38252        -0.62695
1       -2.08753         0.13679         1.56211
1       -2.20878        -0.11420         4.04441
1       -0.11460        -0.29999         5.35606
1        2.08496        -0.20306         4.20823
1        1.38144        -0.07110        -1.70033
1        3.49892        -0.18564        -0.39130
1        2.87741         1.22432         1.72133
8        2.18499         2.86247         0.98825
1        1.93659         2.60242         0.08394
E= -611.284329 (Hartree)


11
Atom       X               Y               X            (Angstrom)
```

6	-0.04854	-0.04544	-0.02828
6	-0.01269	-0.05484	1.46463
6	1.20768	-0.05250	2.14749
6	2.49874	-0.04072	1.39700
6	2.42209	-0.03142	-0.08914
6	1.25809	-0.03381	-0.74046
6	-1.20891	-0.06596	2.17588
6	-1.18486	-0.07467	3.56377
6	0.03187	-0.07232	4.24459
6	1.22729	-0.06128	3.53906
8	3.56894	-0.03865	1.95904
1	-2.14025	-0.06757	1.62271
1	-2.11484	-0.08333	4.11924
1	0.04499	-0.07910	5.32777
1	2.18592	-0.05929	4.04345
1	1.19421	-0.02726	-1.82284
1	3.37797	-0.02281	-0.60091
8	-1.08743	-0.04713	-0.64628

E= -535.032520 (Hartree)

TS 1-6

Atom	X	Y	X	(Angstrom)
6	-0.55090	-0.58462	0.29616	
6	-0.20611	-0.14645	1.58604	
6	1.14215	0.18741	1.86609	
6	2.09623	0.11050	0.82495	
6	1.73314	-0.30796	-0.43320	
6	0.40024	-0.67025	-0.69842	
6	-1.20381	0.02850	2.62888	
6	-0.74300	0.11935	3.96716	
6	0.58830	0.44115	4.22713	
6	1.50902	0.53362	3.20002	
6	-1.88485	1.93303	2.26372	
6	-2.91873	2.18160	3.27291	
6	-4.26959	1.94642	2.97616	
6	-4.67063	1.45115	1.59443	
6	-3.60927	1.67942	0.54902	
6	-2.33213	1.91150	0.87964	
6	-2.58366	2.65920	4.54764	
6	-3.56325	2.88832	5.50055	
6	-4.90219	2.65041	5.19482	
6	-5.24962	2.18760	3.93250	
8	-5.91166	1.87667	1.19386	
1	-1.54127	2.85643	4.77558	
1	-3.28723	3.26208	6.47951	
1	-5.67148	2.83526	5.93468	
1	-6.28798	2.02505	3.66826	
1	-1.58979	2.04981	0.10140	
1	-3.94498	1.64555	-0.48090	
1	-4.84094	0.34887	1.66532	
1	-0.92352	2.40445	2.44985	
1	-1.45453	0.04691	4.77996	
1	0.90709	0.60823	5.24964	

```
1        2.54091         0.79414         3.40658
1       -2.17413        -0.42878         2.45383
1        3.12620         0.37363         1.04117
1        2.47505        -0.36922        -1.22042
1        0.12188        -1.01703        -1.68629
1       -1.58252        -0.85077         0.09211
E= -846.695906 (Hartree)


6
Atom       X              Y               X              (Angstrom)
6       -0.41415        -0.58848         0.24618
6       -0.10057        -0.14278         1.52625
6        1.24857         0.12269         1.85294
6        2.23016        -0.00036         0.85250
6        1.89546        -0.41458        -0.42353
6        0.57003        -0.72842        -0.72642
6       -1.17914         0.12271         2.55130
6       -0.66280         0.01648         3.95309
6        0.65518         0.24874         4.23647
6        1.60219         0.40947         3.21445
6       -1.77679         1.58454         2.33225
6       -2.85180         1.88728         3.35225
6       -4.19133         1.61055         3.07077
6       -4.57263         1.07306         1.69909
6       -3.57924         1.47735         0.63459
6       -2.31022         1.72897         0.93136
6       -2.52666         2.44509         4.59027
6       -3.51001         2.69973         5.53640
6       -4.84026         2.40534         5.25160
6       -5.17897         1.86962         4.01681
8       -5.87118         1.31576         1.34421
1       -1.48958         2.67994         4.80638
1       -3.24033         3.13553         6.49113
1       -5.61233         2.60719         5.98432
1       -6.21216         1.66466         3.76399
1       -1.61066         2.00646         0.15080
1       -3.97036         1.54868        -0.37416
1       -4.57037        -0.04149         1.75345
1       -0.93677         2.27009         2.48036
1       -1.37832        -0.14116         4.75025
1        0.98221         0.28499         5.26985
1        2.63734         0.62423         3.45120
1       -2.01385        -0.57062         2.39656
1        3.26356         0.21337         1.10452
1        2.66355        -0.51066        -1.18148
1        0.30561        -1.07810        -1.71694
1       -1.44692        -0.81833         0.00601
E= -846.713381 (Hartree)


TS 1-7
Atom       X              Y               X              (Angstrom)
6       -0.24480        -0.89508         0.20617
6       -0.31173        -0.31572         1.48593
```

```
6       0.86520        0.19679        2.07942
6       2.08260        0.12423        1.36362
6       2.12610       -0.44538        0.11473
6       0.95278       -0.96354       -0.46813
6       0.79533        0.74189        3.39358
6      -0.38358        0.73599        4.10509
6      -1.55423        0.22718        3.53163
6      -1.55927       -0.19552        2.19480
8      -2.21075        1.52156        1.38778
6      -3.51964        1.34260        0.91947
6      -4.48656        0.99151        2.03681
6      -5.23493       -0.20354        2.01042
6      -5.14919       -1.07660        0.87382
6      -4.33348       -0.75241       -0.22181
6      -3.57770        0.38695       -0.23754
6      -6.05476       -0.51481        3.11384
6      -6.13645        0.33633        4.19899
6      -5.39780        1.52294        4.21300
6      -4.57688        1.83688        3.13766
1      -6.62530       -1.43746        3.09849
1      -6.77453        0.08458        5.03788
1      -5.46312        2.19363        5.06124
1      -3.97273        2.73831        3.15025
1      -5.73282       -1.98915        0.87129
1      -4.30297       -1.42694       -1.07089
1      -2.93479        0.62159       -1.07830
1      -3.78650        2.35209        0.55220
1       1.70210        1.13719        3.83890
1      -0.40494        1.11872        5.11837
1      -2.48207        0.21293        4.09092
1      -2.40484       -0.76675        1.82719
1       2.98335        0.52072        1.81996
1       3.06342       -0.49885       -0.42580
1       0.99745       -1.41412       -1.45248
1      -1.15573       -1.28037       -0.23925
E= -846.712281 (Hartree)
```

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```
Atom        X               Y               X              (Angstrom)
6       0.18266       -0.37547        0.00090
6       0.06718       -0.11804        1.36210
6       1.22638        0.10293        2.13453
6       2.47908        0.09415        1.49369
6       2.57954       -0.14292        0.13572
6       1.42845       -0.38755       -0.61461
6       1.12011        0.27542        3.55510
6      -0.12032        0.14893        4.19761
6      -1.27289       -0.04652        3.49235
6      -1.30484       -0.04006        1.99270
8      -2.09458       -1.09233        1.44733
6      -3.50542       -0.97171        1.64078
6      -4.20409       -0.90726        0.29755
6      -5.30943       -1.73416        0.01145
```

```
6      -5.75304      -2.69700       0.97796
6      -5.06123      -2.86729       2.18651
6      -3.98713      -2.09057       2.51118
6      -5.93845      -1.61476      -1.24252
6      -5.48662      -0.70708      -2.18099
6      -4.38877       0.10580      -1.89114
6      -3.75830      -0.00072      -0.65832
1       3.37094       0.26431       2.08746
1       3.55164      -0.15059      -0.34272
1       1.50394      -0.59108      -1.67585
1      -0.71481      -0.58861      -0.56820
1       2.02282       0.43895       4.13077
1      -0.15982       0.19507       5.28020
1      -2.22207      -0.14808       4.00728
1      -1.76225       0.91702       1.67484
1      -6.60226      -3.32489       0.73836
1      -5.37608      -3.65021       2.86718
1      -3.42753      -2.25961       3.42380
1      -3.69973      -0.01672       2.15886
1      -6.78598      -2.25465      -1.46421
1      -5.98217      -0.62754      -3.14114
1      -4.02973       0.81788      -2.62415
1      -2.90222       0.62757      -0.43358
E= -846.739614 (Hartree)
```

TS 7-8 (H loss)
```
Atom       X              Y              X              (Angstrom)
6       0.04821      -0.10853      -0.04833
6      -0.01371      -0.00671       1.33591
6       1.18013       0.07869       2.08583
6       2.40716       0.13108       1.40061
6       2.45331       0.06559       0.02019
6       1.27240      -0.07226      -0.70805
6       1.13020       0.01102       3.51870
6      -0.07590      -0.28636       4.17159
6      -1.25685      -0.34862       3.48967
6      -1.34384       0.06186       2.05225
8      -2.29297      -0.73271       1.32367
6      -3.62495      -0.40782       1.38768
6      -4.13788       0.68315       0.59080
6      -5.54320       0.87716       0.56141
6      -6.39560      -0.05097       1.22074
6      -5.88064      -1.16873       1.82725
6      -4.49357      -1.37691       1.87808
6      -6.06325       1.97538      -0.16534
6      -5.23043       2.82891      -0.84202
6      -3.83686       2.61710      -0.82615
6      -3.30016       1.56621      -0.12186
1       3.32389       0.20068       1.97622
1       3.40715       0.10041      -0.49242
1       1.30526      -0.15734      -1.78736
1      -0.86846      -0.24531      -0.60860
1       2.05560       0.07977       4.07693
```

```
1      -0.06406       -0.48967        5.23632
1      -2.18656       -0.59741        3.98734
1      -1.69407        1.10809        2.02515
1      -7.46640        0.11610        1.19098
1      -6.54317       -1.90021        2.27349
1      -4.06389       -2.25192        2.34907
1      -3.72741        0.61056        2.86666
1      -7.13753        2.12367       -0.18265
1      -5.64104        3.66347       -1.39732
1      -3.18557        3.28602       -1.37562
1      -2.22890        1.41009       -0.12042
E= -846.683606 (Hartree)
```

TS 7-8 (H-abstraction by O$_2$)

Atom	X	Y	X	(Angstrom)
6	-0.18677	0.45159	0.02367	
6	-0.12233	0.16514	1.39100	
6	1.08495	-0.30228	1.94508	
6	2.20007	-0.48777	1.11025	
6	2.12306	-0.20716	-0.23808	
6	0.92483	0.27116	-0.77990	
6	1.17412	-0.51301	3.37052	
6	0.14073	-0.25318	4.20453	
6	-1.12731	0.15773	3.68016	
6	-1.31663	0.26290	2.26418	
8	-2.28851	1.19512	1.86761	
6	-3.41855	0.68480	1.16074	
6	-3.96986	1.77672	0.26979	
6	-5.34449	1.77056	-0.05439	
6	-6.23665	0.88252	0.63631	
6	-5.78301	0.13989	1.73610	
6	-4.45845	0.09598	2.06733	
6	-5.82488	2.70894	-0.98413	
6	-4.97885	3.64697	-1.54803	
6	-3.63435	3.67880	-1.18034	
6	-3.13695	2.74598	-0.27576	
1	-6.87941	2.70003	-1.23781	
1	-5.36483	4.36683	-2.25974	
1	-2.97430	4.43065	-1.59605	
1	-2.09913	2.78024	0.03084	
1	-7.28685	0.88872	0.37230	
1	-6.50329	-0.38898	2.34973	
1	-4.11768	-0.44841	2.93820	
1	-3.06118	-0.12734	0.49850	
1	2.12679	-0.84061	3.77378	
1	0.25397	-0.35642	5.27630	
1	-1.84779	0.65038	4.32053	
1	-1.78317	-0.90011	2.14745	
1	3.12601	-0.84892	1.54474	
1	2.98740	-0.35051	-0.87467	
1	0.86510	0.50030	-1.83711	
1	-1.11156	0.81886	-0.40452	
8	-2.27841	-2.06174	2.77866	

```
8        -2.11498        -1.66114        3.95034
E= -997.035742 (Hartree)
```

TS 7-8 (H-abstraction by OH)
```
Atom        X               Y               X               (Angstrom)
6        -0.22452        -0.21163        0.10464
6        -0.08664        -0.04559        1.48044
6         1.19550         0.18510        2.02229
6         2.30009         0.26530        1.15158
6         2.14255         0.11415        -0.21181
6         0.87335        -0.13031        -0.74129
6         1.35851         0.32785        3.43887
6         0.25373         0.25307        4.29798
6        -1.00924         0.05036        3.81996
6        -1.31239        -0.10478        2.36704
8        -2.24061         0.93357        2.00320
6        -3.39461         0.51478        1.29395
6        -3.85832         1.63672        0.39417
6        -5.23642         1.85035        0.17937
6        -6.20261         1.10658        0.93605
6        -5.79357         0.24923        1.97052
6        -4.47058         0.00105        2.20659
6        -5.63226         2.84207        -0.73710
6        -4.69216         3.60430        -1.40489
6        -3.33216         3.39872        -1.16729
6        -2.92184         2.41845        -0.27152
1        -6.69117         3.00970        -0.90204
1        -5.01216         4.36714        -2.10453
1        -2.59431         4.00514        -1.67839
1        -1.86928         2.25892        -0.06767
1        -7.25582         1.28556        0.75833
1        -6.54560        -0.19500        2.61340
1        -4.15374        -0.62014        3.03817
1        -3.10134        -0.31697        0.62726
1         2.35120         0.50278        3.83544
1         0.40613         0.37331        5.36459
1        -1.86149         0.03198        4.48919
1        -1.80967        -1.07784        2.20467
1         3.28382         0.44611        1.57186
1         3.00191         0.17766        -0.86865
1         0.74377        -0.26237        -1.80861
1        -1.20443        -0.41184        -0.31528
8        -3.14639        -2.53077        1.12703
1        -4.07893        -2.25546        1.19210
E= -922.470442 (Hartree)
```

"TS" 1-8 Maximum on the Free Energy Surface. (C-O = 3.50 A)
```
Atom        X               Y               X               (Angstrom)
6        -0.41930         0.95956        0.24988
6        -0.31307         0.15218        1.37694
6         0.94803        -0.10597        1.95482
6         2.08379         0.48114        1.36442
6         1.96743         1.28476        0.24613
```

6	0.71192	1.53358	-0.31435
6	1.04489	-0.90280	3.14007
6	-0.10960	-1.39580	3.77395
6	-1.35299	-1.19106	3.25584
6	-1.56927	-0.50682	1.93594
8	-1.86599	-1.41644	0.91953
6	-4.93189	-1.02245	2.56120
6	-5.29620	-0.01056	1.66171
6	-6.36905	0.83351	2.07764
6	-6.98680	0.59998	3.33607
6	-6.57178	-0.41530	4.15545
6	-5.50032	-1.26666	3.76266
6	-6.77930	1.87931	1.21115
6	-6.16035	2.07190	0.00552
6	-5.09901	1.22785	-0.40121
6	-4.67280	0.20603	0.40455
1	3.05692	0.29418	1.80517
1	2.85291	1.72638	-0.19505
1	0.62123	2.16881	-1.18662
1	-1.40065	1.13542	-0.17797
1	2.02420	-1.08988	3.56250
1	-0.00157	-1.94618	4.70169
1	-2.23888	-1.56954	3.75254
1	-2.36975	0.24398	2.00197
1	-7.80176	1.24761	3.63957
1	-7.05563	-0.57931	5.11118
1	-5.16971	-2.07248	4.40755
1	-7.59426	2.52387	1.52248
1	-6.48351	2.87419	-0.64693
1	-4.62589	1.39112	-1.36221
1	-3.86099	-0.44909	0.10675

E= -846.033988 (Hartree)

TS 2-8

Atom	X	Y	X	(Angstrom)
6	0.04540	0.86011	0.13360	
6	-0.08321	0.35001	1.43275	
6	0.98637	-0.37862	2.00274	
6	2.15729	-0.58441	1.24084	
6	2.26229	-0.07799	-0.03406	
6	1.20109	0.65544	-0.59152	
6	0.87032	-0.85163	3.34226	
6	-0.25143	-0.57073	4.09838	
6	-1.31554	0.14125	3.55135	
6	-1.31541	0.49961	2.18071	
8	-2.33059	-0.88632	1.40423	
6	-3.59926	-0.84785	1.75747	
6	-4.50878	0.03857	1.07686	
6	-5.86837	0.08970	1.47899	
6	-6.31163	-0.74619	2.53761	
6	-5.43621	-1.59768	3.16652	
6	-4.08209	-1.64164	2.79118	
6	-6.74512	0.97675	0.80464	

```
6      -6.29381      1.76368      -0.22294
6      -4.94481      1.69112      -0.63483
6      -4.07297      0.84249       0.00032
1       2.97522     -1.14730       1.67767
1       3.16468     -0.24201      -0.61047
1       1.29094      1.05576      -1.59399
1      -0.77795      1.42199      -0.29382
1       1.69357     -1.41454       3.76797
1      -0.30104     -0.89904       5.12973
1      -2.19501      0.35278       4.14724
1      -7.35299     -0.70439       2.83695
1      -5.78616     -2.23668       3.96889
1      -3.38038     -2.29923       3.29088
1      -7.78383      1.01792       1.11454
1      -6.97399      2.43752      -0.73021
1      -4.60474      2.30131      -1.46310
1      -3.04356      0.74418      -0.32277
1      -1.99981      1.27537       1.85117
E= -846.175383 (Hartree)
```

Naphthyl radical 5

```
Atom        X            Y            X          (Angstrom)
6      -0.01112      0.00000       0.00700
6       0.01855      0.00000       1.42502
6       1.20899      0.00000       2.10103
6       2.43628      0.00000       1.39613
6       2.44895      0.00000       0.02762
1      -0.92215      0.00000       1.96510
1       1.21569      0.00000       3.18439
1       3.36911      0.00000       1.94681
1       3.38169      0.00000      -0.52345
6      -1.22474      0.00000      -0.73118
6      -1.22448      0.00000      -2.10071
6       0.00231      0.00000      -2.82194
6       1.14259      0.00000      -2.09590
6       1.23020      0.00000      -0.69752
1      -2.16197      0.00000      -0.18601
1      -2.16096      0.00000      -2.64635
1       0.00744      0.00000      -3.90555
E= -385.125532 (Hartree)
```

TS 2-9

```
Atom        X            Y            X          (Angstrom)
6      -2.28822     -1.11901      -0.94371
6      -2.40319     -0.27360       0.16592
6      -3.46700      0.65379       0.24288
6      -4.40414      0.70520      -0.81133
6      -4.27781     -0.13245      -1.89724
6      -3.21424     -1.04774      -1.96655
6      -3.56117      1.51684       1.37465
6      -2.61986      1.47124       2.39368
6      -1.55605      0.58410       2.33636
6      -1.40868     -0.33744       1.24557
```

```
8      -0.46456      -1.14969       1.19912
6       1.15926      -0.17038      -0.43034
6       2.46000      -0.48431      -0.01982
6       3.51180       0.21467      -0.68307
6       3.18278       1.16613      -1.68676
6       1.88009       1.42508      -2.02166
6       0.81598       0.73758      -1.37089
6       4.84956      -0.06641      -0.30484
6       5.11978      -0.98446       0.67452
6       4.06899      -1.66924       1.33151
6       2.76441      -1.42707       0.99497
1      -5.22328       1.41386      -0.75475
1      -5.00133      -0.08695      -2.70233
1      -3.12336      -1.70126      -2.82587
1      -1.45733      -1.81434      -0.97400
1      -4.38493       2.22010       1.42521
1      -2.71324       2.14450       3.23750
1      -0.80345       0.54371       3.11417
1      -0.21884       0.93933      -1.62783
1       1.64956       2.15634      -2.78821
1       3.99003       1.69142      -2.18537
1       5.65562       0.46018      -0.80482
1       6.14629      -1.18951       0.95488
1       4.30404      -2.38772       2.10781
1       1.93978      -1.92784       1.48704
E= -845.528741 (Hartree)


8
Atom      X              Y              X           (Angstrom)
6       0.04831       0.27203       0.06570
6       0.01923       0.40270       1.47771
6       1.05655      -0.18594       2.25061
6       2.07365      -0.91589       1.58277
6       2.06853      -1.04265       0.22010
6       1.04726      -0.43617      -0.54714
6       1.06107      -0.01677       3.65939
6       0.08214       0.71543       4.27331
6      -0.96303       1.29120       3.51621
6      -1.00139       1.13138       2.15618
8      -2.01342       1.71393       1.43518
6      -3.06246       0.81667       1.00984
6      -3.88482       1.53809      -0.03147
6      -5.28826       1.39383      -0.05403
6      -5.95325       0.68030       0.99794
6      -5.22919       0.19367       2.09569
6      -3.86838       0.29039       2.15526
6      -6.01621       2.00991      -1.08836
6      -5.37717       2.75986      -2.05761
6      -3.99232       2.92392      -2.00844
6      -3.25699       2.31501      -0.99851
1      -7.09496       1.89687      -1.10644
1      -5.95276       3.23020      -2.84577
1      -3.48931       3.52894      -2.75287
```

```
1      -2.18512         2.46249        -0.94102
1      -7.03138         0.58371         0.96342
1      -5.76624        -0.26061         2.92069
1      -3.31807        -0.09050         3.00717
1      -2.57129        -0.04451         0.52496
1       1.86077        -0.46751         4.23624
1       0.09628         0.85468         5.34753
1      -1.74830         1.86871         3.98907
1       2.86202        -1.36752         2.17508
1       2.85290        -1.60073        -0.27710
1       1.06185        -0.52911        -1.62635
1      -0.72482         0.75055        -0.52267
E= -846.194466 (Hartree)
```

TS 8-9 (H-abstraction by O)

Atom	X	Y	X	(Angstrom)
6	2.14913	1.55512	-0.83520	
6	2.32104	0.26289	-0.28142	
6	3.61863	-0.17615	0.08530	
6	4.71262	0.70134	-0.11751	
6	4.52508	1.94673	-0.65656	
6	3.22998	2.37779	-1.01940	
6	3.78759	-1.47029	0.64863	
6	2.70727	-2.28503	0.82481	
6	1.40411	-1.86902	0.45634	
6	1.21227	-0.61622	-0.07643	
8	0.01298	-0.09636	-0.44932	
6	-1.18673	-0.77606	-0.10114	
6	-2.28485	0.22857	0.09024	
6	-3.59721	-0.07393	-0.32598	
6	-3.85471	-1.28668	-1.04269	
6	-2.81025	-2.13870	-1.40572	
6	-1.51551	-1.88058	-1.02922	
6	-4.62335	0.85298	-0.05631	
6	-4.35007	2.03564	0.60029	
6	-3.04368	2.32286	1.00946	
6	-2.02040	1.42066	0.75866	
8	-0.21018	-0.82803	2.45465	
1	5.70589	0.36694	0.16431	
1	5.37165	2.60735	-0.80685	
1	3.09282	3.36506	-1.44606	
1	1.15264	1.87438	-1.11362	
1	4.78234	-1.79634	0.93221	
1	2.83258	-3.27296	1.25338	
1	0.57868	-2.55272	0.60467	
1	-4.87045	-1.50436	-1.35282	
1	-3.02237	-3.00201	-2.02689	
1	-0.69925	-2.50739	-1.36927	
1	-5.63480	0.62435	-0.37684	
1	-5.14805	2.74174	0.79971	
1	-2.83018	3.25046	1.52784	
1	-1.00667	1.62590	1.08371	
1	-1.01294	-1.21689	0.92711	

E= -921.244568 (Hartree)

TS 8-9 (H loss)

Atom	X	Y	X	(Angstrom)
6	0.10329	-0.11503	-0.06250	
6	0.01717	-0.02578	1.34193	
6	1.19622	0.10402	2.11605	
6	2.44347	0.14025	1.44656	
6	2.50941	0.05885	0.07952	
6	1.32834	-0.06847	-0.68158	
6	1.09788	0.22056	3.52942	
6	-0.12904	0.27607	4.14038	
6	-1.31624	0.16788	3.39706	
6	-1.24623	-0.10481	2.03424	
8	-2.33886	-0.04673	1.20687	
6	-3.59758	-0.41358	1.61447	
6	-4.65489	0.27485	0.95144	
6	-5.99339	-0.08406	1.26032	
6	-6.24032	-1.10528	2.21432	
6	-5.19731	-1.74050	2.82759	
6	-3.85698	-1.39898	2.53084	
6	-7.04793	0.59775	0.60092	
6	-6.78491	1.58173	-0.31352	
6	-5.44967	1.93649	-0.61412	
6	-4.40648	1.29906	0.00318	
1	-8.07119	0.32352	0.83727	
1	-7.60101	2.09437	-0.81044	
1	-5.25278	2.72016	-1.33696	
1	-3.38160	1.56831	-0.21945	
1	-7.26588	-1.37128	2.44733	
1	-5.38593	-2.52360	3.55310	
1	-3.04668	-1.92329	3.02045	
1	2.00835	0.30837	4.11235	
1	-0.19503	0.42240	5.21240	
1	-2.28005	0.24763	3.88266	
1	3.34851	0.23960	2.03727	
1	3.47062	0.08987	-0.42084	
1	1.39008	-0.13406	-1.76183	
1	-0.80703	-0.22802	-0.63792	
1	-1.08778	-1.88458	2.15361	

E= -846.118979 (Hartree)

TS 8-9 (H-abstraction by O$_2$)

Atom	X	Y	X	(Angstrom)
6	0.17473	0.09930	0.00555	
6	0.11327	0.01755	1.41866	
6	1.31435	-0.07398	2.16780	
6	2.54915	-0.07446	1.47085	
6	2.58599	0.00845	0.10466	
6	1.38579	0.09410	-0.63571	
6	1.25099	-0.16127	3.58396	
6	0.04077	-0.15703	4.21549	
6	-1.16976	-0.06534	3.48629	

```
6        -1.13251         0.02438          2.11833
8        -2.22314         0.14392          1.30358
6        -3.51973         0.04414          1.82758
6        -4.50382         0.80634          1.05235
6        -5.87594         0.50164          1.24196
6        -6.24103        -0.62701          2.01663
6        -5.27918        -1.49302          2.52790
6        -3.93378        -1.22713          2.36467
6        -6.84178         1.31893          0.60550
6        -6.45589         2.35672         -0.20456
6        -5.08883         2.62483         -0.41216
6        -4.12569         1.86868          0.21669
1         3.46827        -0.14263          2.04389
1         3.53808         0.00818         -0.41421
1         1.42574         0.15535         -1.71744
1        -0.74942         0.15851         -0.55533
1         2.17336        -0.23121          4.15013
1        -0.01144        -0.22115          5.29643
1        -2.10546        -0.06182          4.03000
1        -7.29461        -0.84386          2.15549
1        -5.58829        -2.40128          3.03208
1        -3.17238        -1.91417          2.71484
1        -7.89339         1.10105          0.76033
1        -7.20420         2.97139         -0.69174
1        -4.79477         3.44032         -1.06277
1        -3.07239         2.08149          0.08190
1        -3.55380         0.79094          2.84705
8        -3.85148         1.81901          3.76059
8        -4.71940         2.51693          3.22705
E= -996.460101 (Hartree)
```

TS 8-9 (H-abstraction by OH)

```
Atom        X                Y                X           (Angstrom)
6        -0.09520         0.16560          0.07732
6        -0.06972         0.02673          1.48639
6         1.17429        -0.01252          2.16602
6         2.36532         0.08767          1.40432
6         2.31880         0.21984          0.04164
6         1.07612         0.25900         -0.62850
6         1.19669        -0.14088          3.58191
6         0.02615        -0.23155          4.27802
6        -1.22821        -0.19812          3.61738
6        -1.27907        -0.06812          2.24786
8        -2.40920        -0.00090          1.50648
6        -3.68300         0.11420          2.15135
6        -4.62280         0.80862          1.20524
6        -5.94452         0.34752          1.04274
6        -6.37262        -0.84096          1.71682
6        -5.47384        -1.59303          2.47866
6        -4.17499        -1.19318          2.65489
6        -6.80971         1.05728          0.18659
6        -6.37279         2.18207         -0.48317
6        -5.06093         2.63335         -0.30819
```

```
6      -4.19626        1.95088        0.53492
1       3.31817        0.05846        1.92303
1       3.23780        0.29475       -0.52881
1       1.05178        0.36254       -1.70735
1      -1.05367        0.19130       -0.42573
1       2.15211       -0.16781        4.09442
1       0.03869       -0.33186        5.35750
1      -2.13182       -0.27676        4.20788
1      -7.39357       -1.17978        1.58271
1      -5.80361       -2.53131        2.91147
1      -3.47223       -1.82105        3.19013
1      -7.82724        0.70223        0.05672
1      -7.04719        2.71776       -1.14158
1      -4.71909        3.52122       -0.82752
1      -3.18572        2.30597        0.69906
1      -3.54067        0.82550        3.00877
8      -2.72647        2.42791        3.41051
1      -1.79715        2.15104        3.50265
E= -921.904942 (Hartree)
```

9

```
Atom      X                Y                X              (Angstrom)
6      -2.58553       -0.21856       -1.57413
6      -2.23314       -0.26913       -0.20277
6      -3.20494        0.03541        0.78576
6      -4.51405        0.37849        0.36290
6      -4.83474        0.42032       -0.96766
6      -3.85981        0.12051       -1.94631
6      -2.84303       -0.00337        2.15833
6      -1.56669       -0.32806        2.52258
6      -0.58339       -0.63482        1.55209
6      -0.91759       -0.61096        0.22441
8      -0.04123       -0.90705       -0.79089
6       1.30475       -0.96325       -0.49263
6       2.02289        0.25525       -0.34841
6       3.41447        0.18045       -0.07728
6       4.03619       -1.09141        0.03268
6       3.30858       -2.23895       -0.12382
6       1.91978       -2.17785       -0.38582
6       4.14342        1.38871        0.06928
6       3.52036        2.60104       -0.05427
6       2.13541        2.66755       -0.33402
6       1.40002        1.52213       -0.47909
1       5.20614        1.33201        0.27818
1       4.08723        3.51733        0.06010
1       1.65640        3.63397       -0.43409
1       0.34011        1.57009       -0.69838
1       5.10012       -1.13600        0.23658
1       3.78929       -3.20643       -0.04567
1       1.32919       -3.07735       -0.50836
1      -3.59237        0.23065        2.90573
1      -1.28918       -0.35456        3.56950
1       0.42356       -0.88766        1.85803
```

```
1       -5.25851        0.60973         1.11707
1       -5.83906        0.68500        -1.27626
1       -4.12470        0.15992        -2.99613
1       -1.83125       -0.45301        -2.31402
E= -845.650593 (Hartree)
```

TS naphalene+H   (H addition)

Atom	X	Y	X	(Angstrom)
6	0.00445	0.03635	0.02016	
6	0.00550	0.01129	1.43783	
6	1.24666	-0.01829	2.12156	
6	2.42779	-0.02536	1.42755	
6	2.42332	-0.00055	0.01473	
6	1.23680	0.03291	-0.67144	
6	-1.24903	0.09528	-0.67037	
6	-2.43572	-0.00347	0.03651	
6	-2.42344	-0.02032	1.44404	
6	-1.23534	-0.00025	2.12997	
1	1.24378	-0.03651	3.20605	
1	3.37102	-0.04859	1.95995	
1	3.36309	-0.00465	-0.52417	
1	1.22731	0.06338	-1.75577	
1	-1.22578	-0.01437	3.21435	
1	-3.36110	-0.05745	1.98542	
1	-3.37885	-0.02952	-0.49536	
1	-1.24784	-0.00691	-1.75014	
1	-1.23338	1.92701	-1.02638	

```
E= -386.303601 (Hartree)
```

TS naphalene+H   (H-abstraction by H)

Atom	X	Y	X	(Angstrom)
6	0.00000	0.00000	0.00000	
6	0.00000	0.00000	1.42125	
6	1.24075	0.00000	2.10799	
6	2.42262	0.00000	1.41803	
6	2.42262	0.00000	0.00322	
6	1.24075	0.00000	-0.68675	
6	-1.24075	0.00000	-0.68674	
6	-2.42262	0.00000	0.00322	
6	-2.42262	0.00000	1.41803	
6	-1.24075	0.00000	2.10799	
1	1.23560	0.00000	3.19262	
1	3.36433	0.00000	1.95349	
1	3.36433	0.00000	-0.53224	
1	1.23560	0.00000	-1.77137	
1	-1.23560	0.00000	3.19262	
1	-3.36433	0.00000	1.95349	
1	-3.36433	0.00000	-0.53224	
1	-1.23458	0.00000	-1.98673	
1	-1.34485	-0.71088	-2.97668	

```
E= -386.282836 (Hartree)
```

TS naphthalene+O (H-abstraction by O)

Atom	X	Y	X	(Angstrom)
6	0.02506	−0.05964	0.00540	
6	0.02442	−0.05509	1.42311	
6	1.25842	−0.00228	2.13529	
6	2.46397	0.04499	1.38974	
6	2.43996	0.03973	0.02110	
6	1.21015	−0.01312	−0.67708	
6	−1.14165	−0.10063	2.20764	
6	−1.18172	−0.09858	3.56259	
6	0.06047	−0.04558	4.25192	
6	1.23803	0.00094	3.55543	
8	−3.21518	−0.19093	0.81756	
1	3.40623	0.08543	1.92534	
1	3.36783	0.07620	−0.53673	
1	1.21092	−0.01668	−1.76029	
1	−0.92767	−0.10057	−0.50919	
1	2.18354	0.04137	4.08487	
1	0.06317	−0.04245	5.33541	
1	−2.11677	−0.13553	4.10783	
1	−2.33028	−0.15260	1.50623	

E= −460.847796 (Hartree)

TS naphthalene+OH (H-abstraction by OH)

Atom	X	Y	X	(Angstrom)
6	0.02478	0.00545	−0.03509	
6	0.04946	0.01530	1.38412	
6	1.29839	0.15847	2.05185	
6	2.45260	0.28692	1.25002	
6	2.42911	0.26525	−0.11073	
6	1.17692	0.12709	−0.76442	
6	−1.12645	−0.11562	2.16644	
6	−1.06027	−0.10699	3.53373	
6	0.18527	0.03482	4.19150	
6	1.34031	0.16536	3.46924	
1	−2.07972	−0.22209	1.65987	
1	−1.96525	−0.20777	4.12084	
1	0.21894	0.04255	5.27425	
1	2.30401	0.27905	3.95276	
1	−0.93106	−0.10268	−0.53630	
1	1.14253	0.11726	−1.84729	
1	3.34176	0.35807	−0.68663	
1	3.50851	0.44656	1.83335	
8	4.52433	0.22070	2.57560	
1	4.47215	−0.74728	2.59965	

E= −461.526073 (Hartree)

TS naphthalene+OH (OH addition)

Atom	X	Y	X	(Angstrom)
6	−0.00549	0.04032	−0.00681	
6	−0.01807	−0.01123	1.40920	
6	1.21439	−0.04663	2.10591	
6	2.40323	−0.03529	1.42233	

6	2.41130	0.00738	0.01172
6	1.22979	0.03987	−0.68696
6	−1.25209	0.04443	−0.71838
6	−2.44900	0.10833	−0.00952
6	−2.45142	0.04567	1.39580
6	−1.26800	−0.01128	2.09053
1	1.20141	−0.08288	3.18997
1	3.34150	−0.06272	1.96322
1	3.35585	0.00869	−0.51876
1	1.22670	0.05358	−1.77106
1	−1.26847	−0.05053	3.17455
1	−3.39394	0.05603	1.92945
1	−3.38291	0.15833	−0.55395
1	−1.23839	0.24962	−1.78036
8	−1.46304	−1.92502	−1.25688
1	−1.43010	−2.28386	−0.35735

E= −461.535824 (Hartree)

TS 1+0 → 3+14

Atom	X	Y	X	(Angstrom)
6	0.73419	0.50970	0.27211	
6	−0.20612	0.23353	1.25699	
6	0.08764	0.48778	2.61426	
6	1.34220	1.03541	2.93863	
6	2.26804	1.31691	1.95005	
6	1.96961	1.04841	0.61185	
6	−0.88246	0.17662	3.62221	
6	−2.09053	−0.45836	3.29752	
6	−2.43122	−0.70799	1.99543	
6	−1.57771	−0.25087	0.87378	
8	−1.74689	−0.80419	−0.28686	
6	−2.62406	2.39379	0.52989	
6	−1.42592	3.11836	0.57424	
6	−0.94149	3.60755	1.79388	
6	−1.67281	3.44964	2.95076	
6	−2.94671	2.81955	2.93281	
1	0.01938	4.10707	1.82388	
1	1.57631	1.23155	3.97979	
1	3.23069	1.73778	2.21553	
1	2.70026	1.25871	−0.16000	
1	0.47786	0.29038	−0.75835	
1	−0.64031	0.38696	4.65753	
1	−2.76175	−0.75766	4.09453	
1	−3.34726	−1.21777	1.72402	
1	−2.08378	0.95562	0.63434	
1	−3.07765	2.16647	−0.43181	
1	−0.84576	3.25077	−0.33080	
6	−3.72178	2.66001	4.10678	
6	−4.94608	2.04086	4.06135	
6	−5.45194	1.55599	2.83799	
6	−4.71465	1.69008	1.68506	
6	−3.45480	2.32169	1.70699	
1	−3.32938	3.03616	5.04581	

```
1      -5.52990        1.92518        4.96684
1      -6.42027        1.07126        2.81056
1      -5.09130        1.30545        0.74273
1      -1.29046        3.82084        3.89554
E=    -846.712852 (Hartree)
```

TS 4+0 → 2+14

Atom	X	Y	X	(Angstrom)
6	0.15862	0.12775	0.21506	
6	-0.16922	0.10981	1.57763	
6	0.80515	0.46351	2.54552	
6	2.09551	0.82218	2.09678	
6	2.40434	0.82521	0.75459	
6	1.43339	0.47051	-0.19521	
6	0.46125	0.45028	3.92710	
6	-0.79437	0.04023	4.33966	
6	-1.76958	-0.31639	3.41195	
6	-1.53931	-0.12049	2.02551	
8	-2.43669	-0.68759	1.11047	
6	-2.34154	2.51932	1.70039	
6	-2.45182	2.82306	3.11944	
6	-1.33965	3.39999	3.78328	
6	-0.19462	3.77484	3.02607	
6	-0.17477	3.63469	1.64961	
6	-1.25450	3.07020	0.97434	
6	-1.40245	3.57436	5.18457	
6	-2.51926	3.19676	5.89479	
6	-3.62062	2.63065	5.23129	
6	-3.57823	2.44142	3.86404	
1	0.68994	3.96850	1.08801	
1	2.84418	1.09770	2.83209	
1	3.40032	1.10144	0.42896	
1	1.68102	0.47343	-1.24988	
1	-0.60817	-0.12697	-0.50725	
1	1.21324	0.73452	4.65431	
1	-1.02572	-0.00607	5.39736	
1	-2.75299	-0.64524	3.72605	
1	-1.94003	1.19813	1.86311	
1	-3.26306	2.29656	1.16591	
1	-1.23265	2.97881	-0.10460	
1	-0.55027	4.01193	5.69395	
1	-2.55218	3.33812	6.96869	
1	-4.49922	2.33818	5.79359	
1	-4.42005	1.99224	3.34651	
1	0.65424	4.20503	3.54573	
1	-2.22258	-1.62351	1.03767	

```
E=    -847.362625 (Hartree)
```

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Atom	X	Y	X	(Angstrom)
6	-0.02122	0.00015	-0.00164	
6	-0.00692	0.00017	1.43405	
6	1.22294	0.00032	2.12684	

```
6        2.53490         0.00057         1.37573
6        2.39469         0.00036        -0.11331
6        1.17738         0.00021        -0.73079
6       -1.20375        -0.00000         2.17450
6       -1.18777        -0.00003         3.55650
6        0.03089         0.00011         4.23635
6        1.21986         0.00028         3.51792
1       -2.14714        -0.00012         1.63900
1       -2.11931        -0.00016         4.10967
1        0.05138         0.00009         5.31939
1        2.16828         0.00039         4.04652
1       -0.97559         0.00003        -0.51312
1        1.13275         0.00011        -1.81433
1        3.30454         0.00038        -0.70191
1        3.13023        -0.86907         1.68914
1        3.12978         0.87061         1.68894
E=   -386.364079 (Hartree)
```

TS 5-13

```
Atom       X               Y               X            (Angstrom)
6       -0.02204        -0.01176        -0.10528
6       -0.15902         0.28428         1.24781
6        0.97607         0.37843         2.07064
6        2.23717         0.25123         1.54096
6        2.42191         0.05570         0.14482
6        1.28470        -0.03876        -0.69617
6        1.46482        -0.22238        -2.08468
6        2.72404        -0.30778        -2.62295
6        3.85987        -0.21889        -1.78773
6        3.71143        -0.04089        -0.43653
6       -0.39568        -2.26121        -0.05799
6        0.69729        -3.05248        -0.19187
6        0.53179        -4.45546        -0.03304
6       -0.69956        -4.98177         0.25019
6       -1.83794        -4.14487         0.39122
6       -1.68893        -2.73284         0.23693
6       -2.83093        -1.90165         0.37877
6       -4.05783        -2.44123         0.65824
6       -4.20675        -3.83971         0.81095
6       -3.12452        -4.66748         0.68015
1        1.67461        -2.63851        -0.42022
1        1.39227        -5.10634        -0.13978
1       -0.82556        -6.05221         0.37143
1       -3.23510        -5.74079         0.79507
1       -5.18394        -4.25245         1.03119
1       -4.92263        -1.79711         0.76324
1       -2.72025        -0.83047         0.25787
1       -1.14648         0.39230         1.68033
1        0.85098         0.55967         3.13144
1        3.11200         0.32034         2.17805
1        4.58072         0.02825         0.20883
1        4.85032        -0.29189        -2.22084
1        2.85147        -0.44999        -3.68925
```

```
1        0.58740      -0.31155      -2.71653
1       -0.87553       0.06323      -0.77053
E=   -770.936110 (Hartree)
```

13

Atom	X	Y	X	(Angstrom)
6	0.11126	-0.30123	-0.23381	
6	-0.05194	-0.12568	1.16420	
6	1.09931	0.01237	1.99190	
6	2.37635	-0.01691	1.36699	
6	2.50085	-0.18418	0.01277	
6	1.35571	-0.33160	-0.80082	
6	0.92138	0.17713	3.40266	
6	-0.34909	0.22543	3.92019	
6	-1.48730	0.09626	3.09371	
6	-1.34380	-0.08126	1.74674	
6	2.13843	0.37153	4.31578	
6	2.56334	1.81183	4.21590	
6	2.53672	2.66106	5.28443	
6	2.17921	2.22282	6.56744	
6	1.87537	0.84147	6.80919	
6	1.87943	-0.07819	5.74012	
6	1.62672	-1.42288	5.99513	
6	1.35764	-1.87278	7.28091	
6	1.33407	-0.96415	8.34108	
6	1.59120	0.37284	8.10693	
1	-0.48314	0.35631	4.98803	
1	-2.47401	0.13400	3.53955	
1	-2.21045	-0.18802	1.10359	
1	-0.77715	-0.41027	-0.84684	
1	1.46768	-0.46459	-1.87010	
1	3.48556	-0.20216	-0.43890	
1	3.27267	0.10147	1.96303	
1	2.82944	2.17765	3.23049	
1	2.80038	3.70260	5.13848	
1	2.15883	2.91547	7.39979	
1	1.58356	1.08248	8.92753	
1	1.11986	-1.30715	9.34629	
1	1.16458	-2.92362	7.45882	
1	1.62865	-2.12274	5.16487	
1	2.94099	-0.26682	3.92522	

```
E=   -770.988975 (Hartree)
```

TS 13-14 (H loss)

Atom	X	Y	X	(Angstrom)
6	0.03402	-0.68093	0.09334	
6	-0.03123	-0.33911	1.46765	
6	1.04506	0.37235	2.05878	
6	2.17846	0.66318	1.26189	
6	2.21702	0.31427	-0.06426	
6	1.12806	-0.35446	-0.66196	
6	0.98410	0.68619	3.47627	
6	-0.18187	0.37558	4.17470	

```
6      −1.22475       −0.35197        3.57848
6      −1.15366       −0.70735        2.25738
6       1.91686        1.68395        4.09414
6       2.51401        1.48049        5.38253
6       3.33041        2.51307        5.92809
6       3.52701        3.71582        5.20450
6       2.93303        3.89538        3.98740
6       2.12630        2.87672        3.43915
6       2.33757        0.29779        6.15457
6       2.93586        0.15400        7.37835
6       3.74771        1.17969        7.91051
6       3.93775        2.33049        7.19786
1       1.64753        3.04031        2.48039
1       3.07041        4.81874        3.43770
1       4.14948        4.48983        5.63999
1       4.55768        3.12912        7.59088
1       4.21570        1.05045        8.87897
1       2.78672       −0.75836        7.94355
1       1.72370       −0.50584        5.77148
1      −0.27755        0.70645        5.20228
1      −2.09917       −0.60545        4.16590
1      −1.96183       −1.25632        1.78700
1      −0.80134       −1.21494       −0.34655
1       1.16874       −0.62271       −1.71077
1       3.09607        0.54230       −0.65514
1       3.03297        1.14775        1.71707
1       2.00575       −0.77804        3.77395
E=   −770.928493 (Hartree)
```

TS 13−14 (H-abstraction by O_2)

```
Atom      X              Y              X              (Angstrom)
6      −0.03120       −0.01214        0.00936
6      −0.01948        0.01376        1.42761
6       1.22623       −0.00855        2.11916
6       2.41931       −0.04925        1.34465
6       2.37305       −0.06780       −0.02398
6       1.13484       −0.05021       −0.70390
6      −1.23039        0.06670        2.16247
6      −1.20960        0.11085        3.52801
6       0.02181        0.09521        4.21854
6       1.22012        0.02134        3.55028
6       2.51758        0.06506        4.33281
6       2.59356       −0.63993        5.63179
6       3.50208       −0.18028        6.62097
6       4.24214        1.00785        6.40430
6       4.07661        1.75635        5.24440
6       3.20620        1.33991        4.25983
6       1.86951       −1.82374        5.87082
6       2.01935       −2.51746        7.04935
6       2.91823       −2.06365        8.03339
6       3.64742       −0.92282        7.81966
8       4.22482       −1.73301        3.41414
8       4.55648       −2.21056        4.50158
```
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                                                                          53
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1	0.02304	0.14144	5.30160
1	−2.13393	0.16341	4.09058
1	−2.16933	0.07955	1.61972
1	−0.98930	0.00231	−0.49903
1	1.11431	−0.06691	−1.78689
1	3.29549	−0.09982	−0.59115
1	3.38567	−0.06398	1.83200
1	3.04409	1.94913	3.37766
1	4.61346	2.68981	5.12505
1	4.92832	1.33966	7.17528
1	4.34995	−0.56875	8.56621
1	3.03740	−2.62240	8.95389
1	1.45597	−3.42782	7.21425
1	1.19710	−2.19184	5.10508
1	3.27673	−0.70099	3.72168

E=   −921.276801 (Hartree)

TS 13+14 (H-abstraction by OH)

Atom	X	Y	X	(Angstrom)
6	0.17589	0.50553	0.06126	
6	0.13438	0.26143	1.44873	
6	1.28587	−0.25029	2.08272	
6	2.42358	−0.51927	1.32251	
6	2.44574	−0.28269	−0.04613	
6	1.31348	0.23897	−0.67626	
6	−1.05722	0.50333	2.21232	
6	−1.10394	0.19212	3.57751	
6	−0.02203	−0.31931	4.23638	
6	1.30757	−0.53395	3.57209	
6	2.35621	0.29004	4.32534	
6	2.91271	−0.20336	5.54804	
6	3.84124	0.61047	6.25812	
6	4.18780	1.88736	5.74793	
6	3.63340	2.33993	4.58410	
6	2.71358	1.53628	3.87473	
6	2.58031	−1.47243	6.09736	
6	3.13798	−1.90372	7.27217	
6	4.06177	−1.09421	7.96926	
6	4.40298	0.13249	7.46963	
1	2.28479	1.91132	2.95222	
1	3.89495	3.31719	4.19594	
1	4.89611	2.49476	6.30065	
1	5.10980	0.76538	7.99566	
1	4.49595	−1.44801	8.89655	
1	2.86982	−2.87562	7.66911	
1	1.87532	−2.11680	5.58690	
1	−0.07880	−0.54053	5.29613	
1	−2.02326	0.36304	4.12623	
1	−1.92563	0.91028	1.70939	
1	−0.70868	0.90319	−0.42455	
1	1.32583	0.43069	−1.74259	
1	3.33875	−0.49911	−0.61968	
1	3.30159	−0.91804	1.82095	

```
1        1.58798        -1.59260         3.68312
8        1.37400        -3.29945         2.30499
1        1.16086        -2.75756         1.52500
E=   -846.719150 (Hartree)
```

TS 13-14 (H-abstraction by O)

```
Atom        X                Y                X            (Angstrom)
6        4.21409        -0.54767        -0.30120
6        2.85461        -0.70707        -0.66957
6        1.86681         0.12940        -0.07569
6        2.30045         1.12604         0.84596
6        3.62654         1.24950         1.18456
6        4.59486         0.39978         0.61193
6        2.46508        -1.68655        -1.61708
6        1.14891        -1.83377        -1.95475
6        0.16346        -1.02761        -1.34412
6        0.49342        -0.07462        -0.41234
6       -0.59335         0.78884         0.23423
6       -1.91936         0.06752         0.36030
6       -3.07882         0.54824        -0.28136
6       -3.02425         1.76087        -1.04662
6       -1.83657         2.49795        -1.13334
6       -0.68573         2.08054        -0.52570
6       -1.99230        -1.09001         1.13084
6       -3.18529        -1.78664         1.26530
6       -4.33407        -1.32613         0.61743
6       -4.28019        -0.17445        -0.14301
8        1.15511        -0.26299         2.64710
1       -0.87897        -1.17827        -1.60156
1        0.84944        -2.58045        -2.68031
1        3.22840        -2.31413        -2.06369
1        4.95169        -1.19901        -0.75800
1        5.63690         0.50708         0.88725
1        3.93067         2.01403         1.88927
1        1.58731         1.82063         1.27041
1        0.22731         2.65686        -0.62611
1       -1.82888         3.42094        -1.70234
1       -3.92301         2.10598        -1.54275
1       -5.17067         0.19390        -0.64126
1       -5.26729        -1.86771         0.71534
1       -3.22280        -2.68506         1.86925
1       -1.09091        -1.45083         1.61828
1       -0.26068         0.99874         1.26274
E=   -846.022841 (Hartree)
```

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```
Atom        X                Y                X            (Angstrom)
6        0.21533        -0.27699         0.16900
6        0.01108        -0.08837         1.56063
6        1.12818        -0.14409         2.43883
6        2.41723        -0.37083         1.88696
6        2.58098        -0.54753         0.53910
6        1.46797        -0.50432        -0.33161
```

```
6        0.91799        0.04042        3.84228
6       -0.34961        0.28803        4.31000
6       -1.45653        0.34979        3.43259
6       -1.28133        0.15997        2.09030
6        2.05980       -0.02124        4.79926
6        2.70678       -1.26461        5.08800
6        3.79904       -1.27897        5.99848
6        4.21518       -0.06760        6.60837
6        3.57190        1.10604        6.33049
6        2.49015        1.12589        5.42036
6        2.29015       -2.49121        4.50531
6        2.93536       -3.66208        4.80116
6        4.02911       -3.67319        5.69692
6        4.44666       -2.50941        6.28230
1        1.99659        2.06404        5.19242
1        3.89003        2.02939        6.79952
1        5.05071       -0.09225        7.29964
1        5.28045       -2.50800        6.97623
1        4.53045       -4.60727        5.92074
1        2.60542       -4.58908        4.34772
1        1.44950       -2.49003        3.82188
1       -0.49999        0.42257        5.37534
1       -2.44422        0.54181        3.83430
1       -2.12505        0.19825        1.40968
1       -0.64442       -0.23513       -0.49116
1        1.61289       -0.64678       -1.39587
1        3.57097       -0.72006        0.13419
1        3.27477       -0.40016        2.54844
E=   -770.441397 (Hartree)
```