New Insights into Thermal Decomposition of PAHs Oxyradicals

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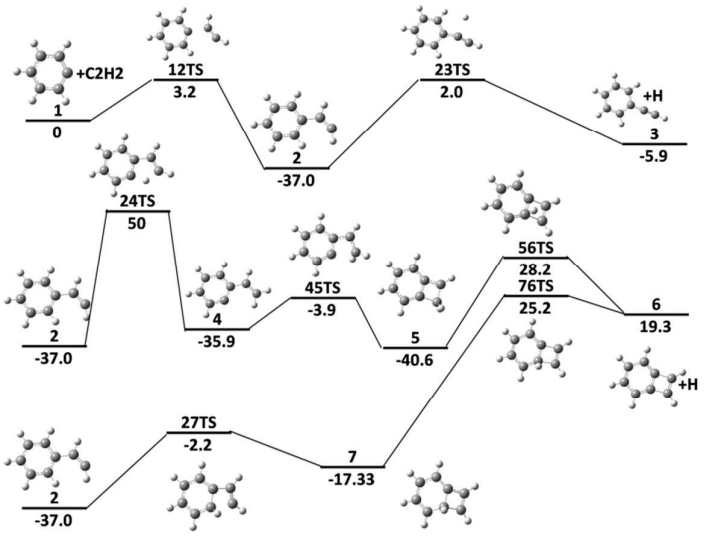
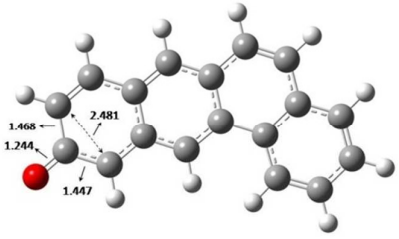
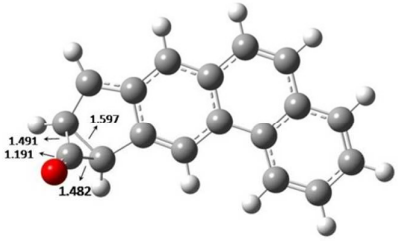


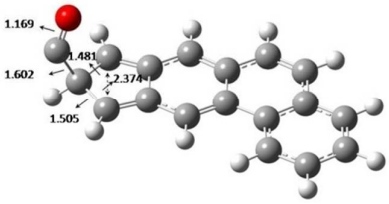
Figure S1. Potential energy surface of reaction C_6H_5+C_2H_2. Energies (in kcal/mol) at 0K relative to reactants are shown for each transition state and local minimum.



1,2-benzanthracene oxyradicals I



S1-CS2



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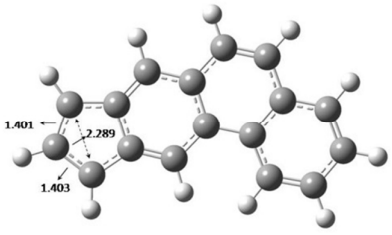

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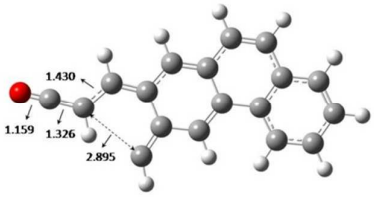

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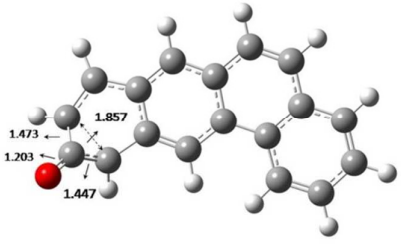

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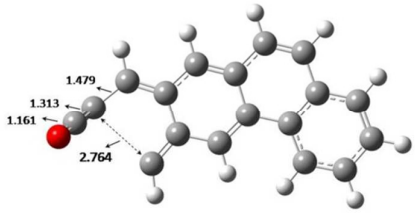

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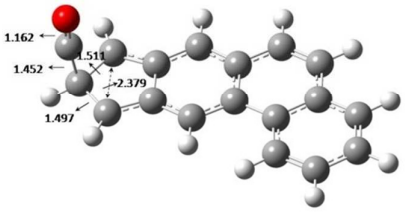
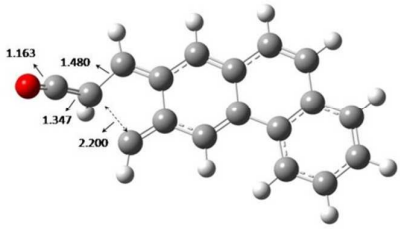
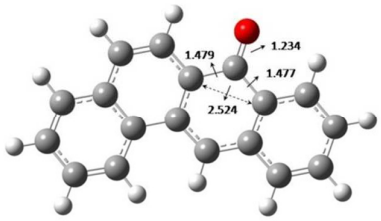


S1-TS23

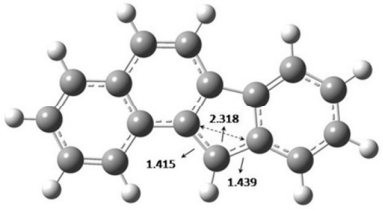


S1-TS53

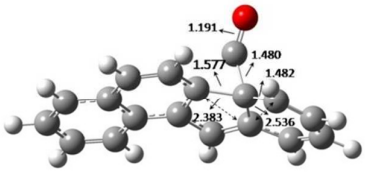
Figure S2. All Structures involving in 1,2-benzanthracene oxyradicals I system



1,2-benzanthracene oxyradicals II

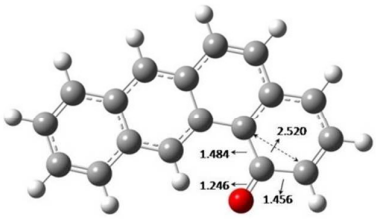


S2-CS2

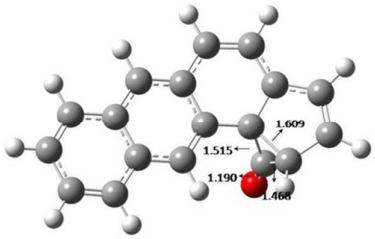


S2-TS12

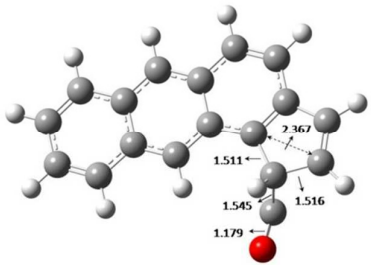
Figure S3. All Structures involving in 1,2-benzanthracene oxyradicals II system



1,2-benzanthracene oxyradicals III



S3-CS2



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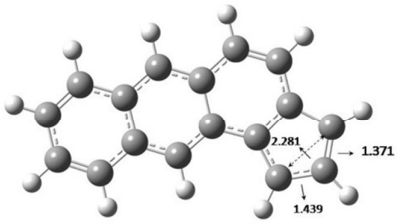

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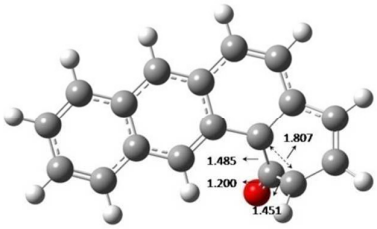
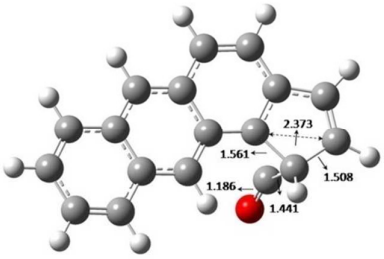
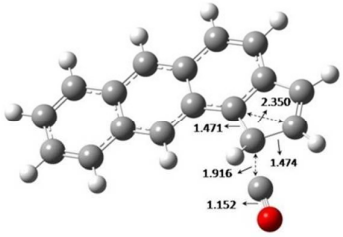


S3-TS12

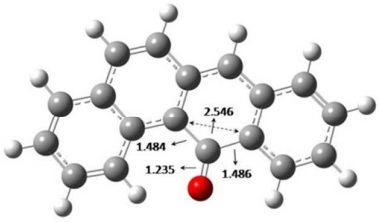


S3-TS23

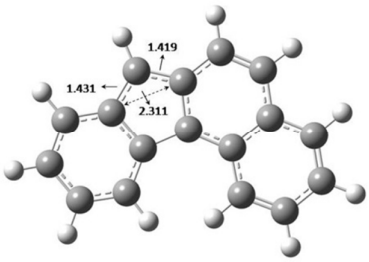


S3-TS34

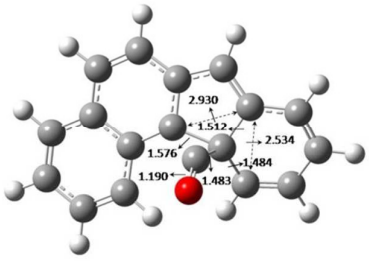
Figure S4. All Structures involving in 1,2-benzanthracene oxyradicals III system



1,2-benzanthracene oxyradicals IV

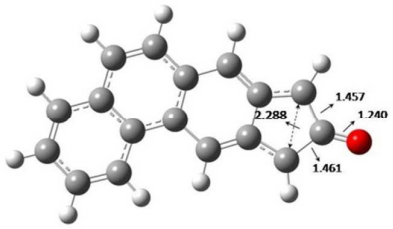


S4-CS2

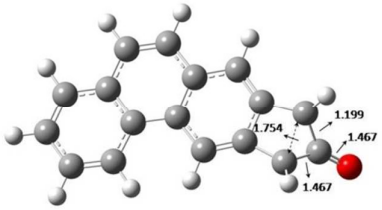


S4-TS12

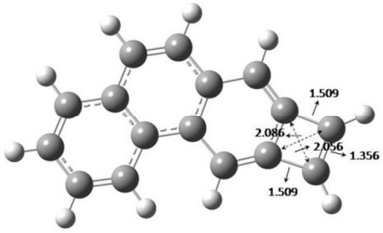
Figure S5. All Structures involving in 1,2-benzanthracene oxyradicals IV system



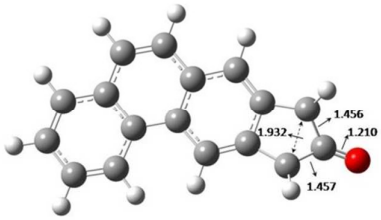
3H-cydopenta[a]anthracene oxyradicals



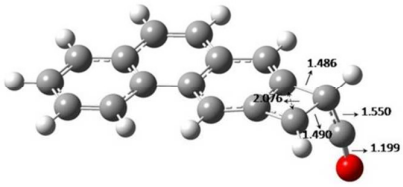
S5-CS2



S5-CS3



S5-TS12



S5-TS23

Figure S6. All Structures involving in 3H-cydopenta[a]anthracene oxyradicals system

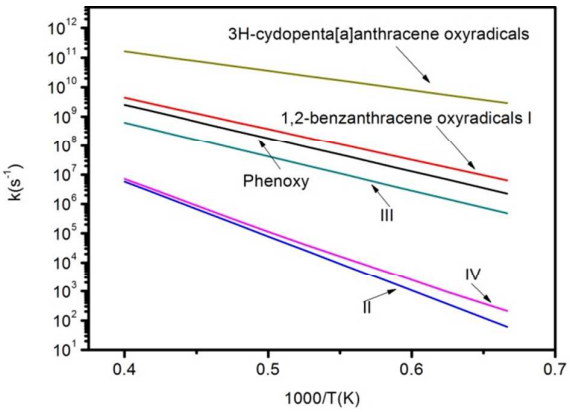


Figure S7. High-pressure limiting rate coefficients of the rate limiting steps in PAHs oxyradicals decomposition

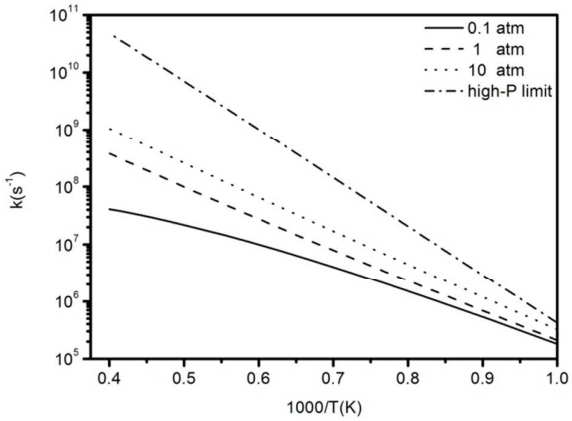


Figure S8. Rate coefficients of decomposition reaction of 3H-cydopenta[a]anthracene oxyradical in pressure range from 0.1 to 10 atm.

1. Details of Computational Methodology

In this study, the geometries of transition states and local minima structures in PAHs oxyradicals decomposition were optimized using the density functional theory (DFT) B3LYP hybrid functional [1, 2] with the 6-311+G(d,p) [3] basis set.[4-7] The same method was applied to calculate zero-point energies (ZPE) and vibrational frequencies, which were scaled by a factor of 0.967.[5, 8] Restricted wave function calculations were employed for singlet, and unrestricted wave function calculations were employed for doublet, triplets and quartets. All transition states were carefully confirmed by examining the motions corresponding to imaginary modes. The minimum-energy path from each transition state was monitored by intrinsic reaction coordinate (IRC) calculations [9] to ensure that the transition states correctly connect with the corresponding energy minima structures. In addition, all of the structures are optimized in their ground states. All calculations were performed using the Gaussian 09 [10] program package.

The rate coefficients of thermal decomposition of PAH oxyradicals were evaluated in temperatures range from 1500 to 2500 K and pressures from 0.1 to 10 atm, using the MultiWell suite of codes (MultiWell-2013.1) [11, 12]. By using Monte Carlo stochastic method, MultiWell can solve the time-dependent energy-transfer master equations for multiwell and multichannel reaction system. Microcanonical rate coefficients were calculated by employing Rice-Ramsperger-Kassel-Marcus (RRKM) theory. The input parameters including vibrational frequencies, reaction

barriers and moments of inertia were obtained from the quantum-chemical results at the B3LYP/6-311+G(d,p) level and presented in Table S19 in supporting information.

The sums and densities of states of local minima structures and transition states were determined by exact count with an energy grain size of 10 cm^{-1}. The maximum energy was 500000 cm^{-1}. The exponential-down model with $<\Delta E_{down}>$=260 cm^{-1} was employed to describe the collisional energy transfer.[13] In addition, detail discussions on temperature-dependent exponential-down model with $<\Delta E_{down}>=200\times(T/300\ K)^{0.85} cm^{-11}$ [14, 15] were presented in the supporting information. In calculation, argon was chosen as the bath gas collider.[16] The Lennard-Jones parameters of PAHs were calculated by the method proposed by Wang et al [17] and presented in the supporting information. The Lennard-Jones parameters σ and ε/k_B of argon were equals to 3.47 Å and 114 K respectively [13]. Symmetry number corrections were carried out according to the study of Duncan.[18, 19] In this study, the real frequencies below 150 cm^{-1} were paid great attention, and internal rotation modes were distinguished by graphically visualizing the normal mode vibrations. All internal rotations were treated as 1-D hindered rotations [20], and the translational and vibrational temperatures were set equal. Tunneling correction was ignored because it almost has no influence on the rate coefficient at high temperatures (> 1000 K) [21] and the calculation of rate coefficients in this study were done in temperature range from 1500 to 2500 K. The number of stochastic trials was changed from 5×10^4 to 1×10^7 to keep the statistical fluctuations below 3%. Besides, the uncertainty of MultiWell for determining rate coefficients of the multiwall and multichannel reactions was estimated to be within one order of magnitude.[5, 22-24]

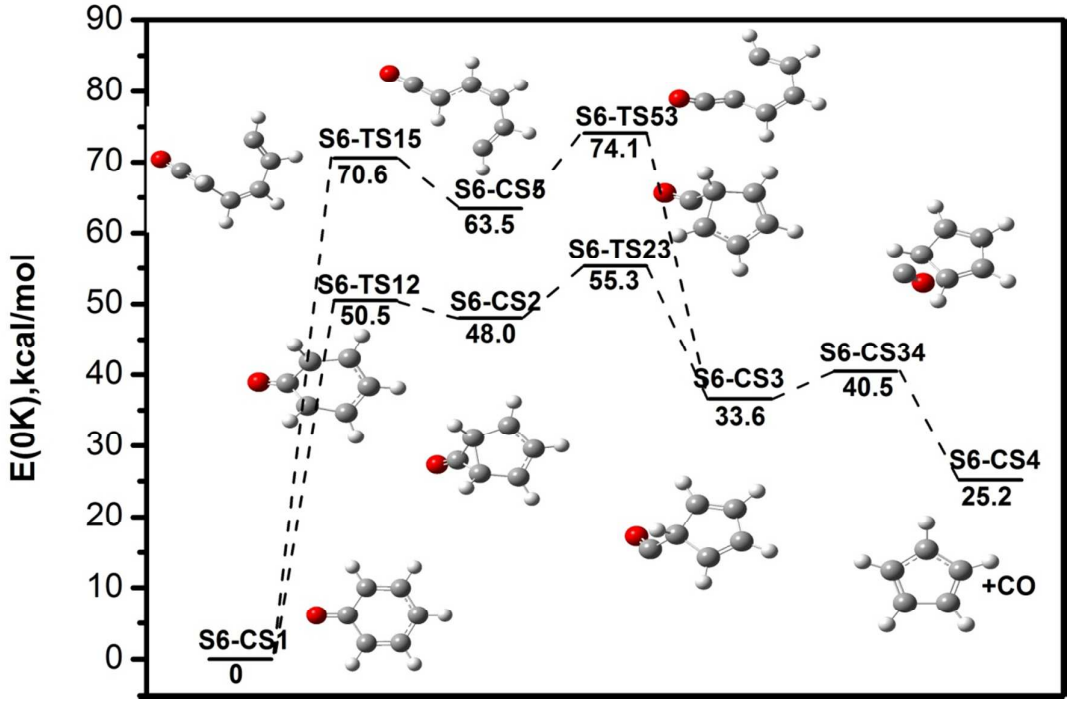
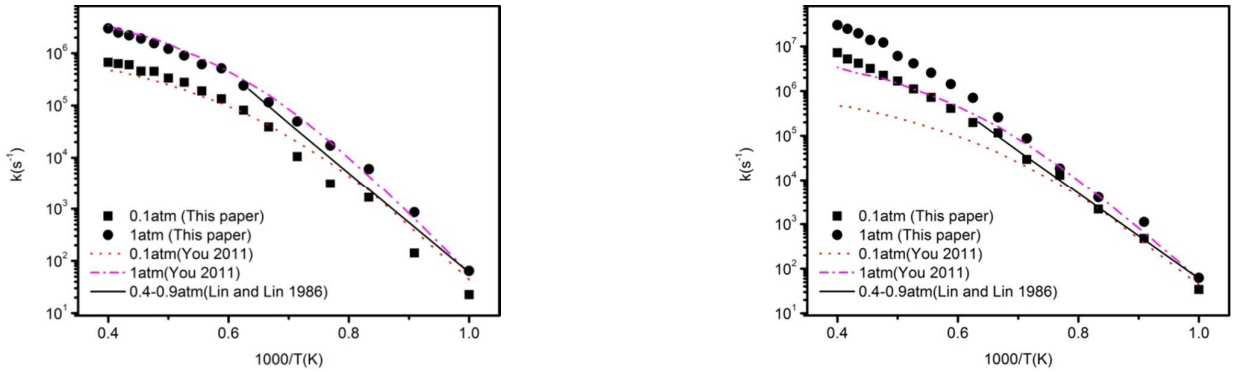


Figure S9. Potential energy diagram showing energies of the chemical species (CS) and transition states (TS) involved in the Phenoxy thermal decomposition from S6-CS1 to S6-CS4 at 0K

1.1 Discussion of $<\triangle E>_{down}$

Taking the suggestion of a reviewer, sensitive analysis of collisional energy model were executed. Collisional energy transfer was assumed to be temperature-dependent with the form $200\times(T/300\ K)^{0.85}cm^{-1}$[14], which indicates the $<\triangle E>_{down}$ values of 785 to 1212 cm^{-1} for the temperature range of 1500 to 2500 K. On the other hand, temperature-independent exponential-down model with $<\triangle E>_{down}=260\ cm^{-1}$ was used to describe the collisional energy transfer in this study. As shown in Figure S4, comparisons of computed rate coefficients of Phenoxy thermal decomposition with the experimental [25] and theoretical rates [5], indicating that the temperature-independent exponential-down model with $<\triangle E>_{down}=260\ cm^{-1}$ is more suitable in this system. Generally, it was found that the rate coefficients calculated with temperature-dependent $<\triangle E>_{down}=200\times(T/300\ K)^{0.85}cm^{-1}$ is larger than that of $<\triangle E>_{down}=260\ cm^{-1}$ by an order of magnitude at 2500 K, and the gaps are reduced in low temperature. So, the temperature-independent exponential-down model with $<\triangle E>_{down}=260\ cm^{-1}$ was used in this paper. By the way, the

rate coefficients of Phenoxy thermal decomposition using $<\triangle E>_{down}=200\times(T/300\ K)^{0.85}cm^{-1}$ were presented in Table S5.



(a) (b)

Figure S10. Comparison of computed rate coefficients of Phenoxy thermal decomposition with the experimental [25] and theoretical rates [5], (a) was calculated with $<\triangle E>_{down}=260\ cm^{-1}$, (b) was calculated with $<\triangle E>_{down}=200\times(T/300\ K)^{0.85}cm^{-1}$.

1.2 Discussion of external symmetry number

The sensitive analysis of external symmetry number were presented in Table S1. As a whole, the fluctuation is within 2 times. The determination of external symmetry number is based on group point analysis. Then, we can obtain a accurate external symmetry number accounting to study of Vincent [18, 19]. The external symmetry numbers of investigated structure are all listed in Table S19.

Table S1. Sensitive analysis about external symmetry number ($<\triangle E>_{down}=260\ cm^{-1}$).

External symmetry number	Rate coefficient
1	1.44E+07
2	1.63E+07
3	1.86E+07
4	2.18E+07

Note: Other input parameters required for MultiWell program keep constants. Only the external symmetry number of Phenoxy (S6-CS1) is changed. T=2500K, P=10atm.

1.3 Discussion of optical isomers

The influence of optical isomers on rate coefficients is presented in Table S2. The optical isomers is used as a multipier in MultiWell soft. The value optical isomers were determined as suggested by Baker et al.[26] The number of optical isomers is equal to the number of wells. The optical isomers of investigated structure are all listed in Table S19.

Table S2. Sensitive analysis about optical isomers ($<\triangle E>_{down}$=260 cm^{-1}).

Optical isomers	Rate coefficient
1	1.63E+007
2	1.43E+007
3	1.25E+007
4	1.19E+007

Note: Other input parameters required for MultiWell program keep constants. Only the optical isomers of Phenoxy (S6-CS1) is changed. T=2500K, P=10atm.

1.4 Discussion of maximum energy

Generally, a larger maximum energy will produce a more accurate rate coefficient. But, the computation time is proportion to the maximum energy of 2nd segment of double arrays. As shown in Table S3, rate coefficient reaches has a steady value with maximum energy equals to 500000 cm^{-1}. So maximum energy=500000 cm^{-1} is used in this paper.

Table S3. Sensitive analysis about maximum energy of 2nd segment of double arrays ($<\triangle E>_{down}$=260 cm^{-1}).

Maximum energy (cm^{-1})	Rate coefficient
200000	2.44E+07
300000	2.56E+07

400000	2.35E+07
500000	2.54E+07
600000	2.55E+07

Note: Other input parameters required for MultiWell program keep constants. T=2500K, P=10atm. Rate of thermal decomposition of 1,2-benzanthracene oxyradicals I

Table S4. Parameters of double-arrays for the case that maximum energy equals to 500000 cm^{-1}

Grain (cm^{-1})	Maximum energy	Number of grains
10.000	99990.000	10000
125.031	500000.000	4000

1.5 Calculation procedures

The thermal decomposition rate coefficients were derived from the exponential decay of the reactant molecule after a period of initial relaxation. After a period of initial relaxation, the average vibrational energy reached a constant value, as showed in Fig. S5, and the fraction of the reactant molecule began to decompose exponentially. The rate coefficients equals to the slope of logarithmic reactant fraction against time.

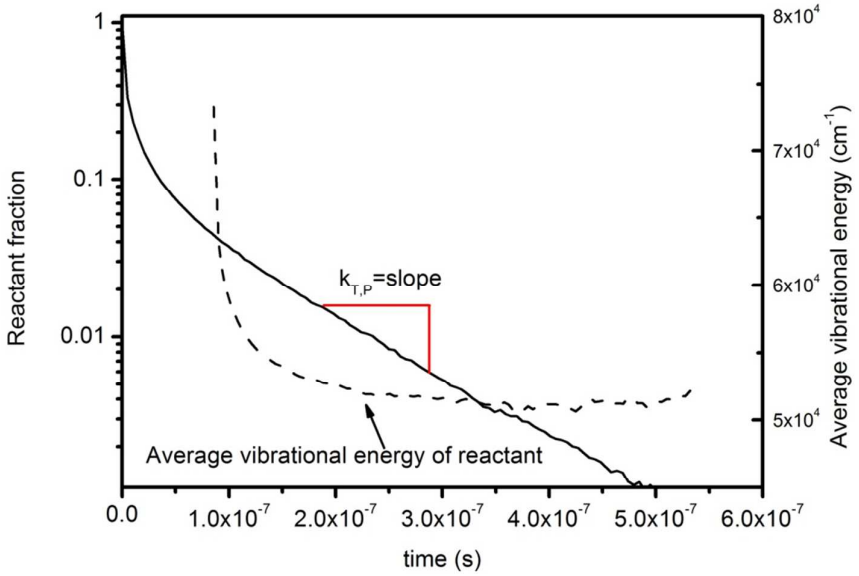


Figure S11. Example of calculation of rate coefficient in MultiWell.

Table S5. The procedure of rate coefficient calculation in MultiWell.

Step 1	To obtain vibrational frequencies, reaction barriers and moments of inertia via quantum-chemical calculation.
Step 2	To determine suitable calculation parameters, such as external symmetry number, optical isomers, maximum energy and collisional energy model.
Step 3	To run the MultiWell soft to obtain simulated data.
Step 4	To extract rate coefficient via mole fraction and time after system had reached steady-state, which is judged by fluctuation of vibrational energy.

Table S6. Rate coefficient (units: s^{-1}) of thermal decomposition of Phenoxy ($<\triangle E>_{down}$=260 cm^{-1})

	P(atm)			
T(K)	0.1	1	10	k_∞
1000	2.26 E+01	6.43E+01	1.06E+02	7.08E+02
1100	1.42 E+02	8.63E+02	1.46E+03	2.37E+03
1200	1.66 E+03	6.04E+03	8.82E+03	4.59E+03
1300	3.11 E+03	1.71E+04	2.05E+04	2.82E+04
1400	1.05E+04	4.95E+04	8.40E+04	1.34E+05
1500	3.88E+04	1.15E+05	2.93E+05	5.21E+05
1600	8.12E+04	2.42E+05	6.44E+05	1.71E+06
1700	1.34E+05	5.15E+05	1.36E+06	4.92E+06
1800	1.90E+05	6.15E+05	2.40E+06	1.27E+07

1900	2.78E+05	9.04E+05	4.04E+06	3.00E+07
2000	3.35E+05	1.21E+06	5.48E+06	6.55E+07
2100	4.49E+05	1.55E+06	8.06E+06	1.34E+08
2200	4.53E+05	1.91E+06	9.87E+06	2.58E+08
2300	6.02E+05	2.20E+06	1.27E+07	4.77E+08
2400	6.33E+05	2.48E+06	1.47E+07	8.39E+08
2500	6.68E+05	2.99E+06	1.63E+07	1.42E+09

Table S7. Rate coefficient (units: s^{-1}) of thermal decomposition of Phenoxy ($<\triangle E>_{down}=200\times(T/300\ K)^{0.85}cm^{-1}$)

	P(atm)		
T(K)	0.1	1	k_∞
1000	3.42E+01	6.24E+01	7.08E+02
1100	4.75E+02	1.12E+03	2.37E+03
1200	2.17E+03	4.04E+03	4.59E+03
1300	1.29E+04	1.84E+04	2.82E+04
1400	2.93E+04	8.73E+04	1.34E+05
1500	1.15E+05	2.58E+05	5.21E+05
1600	1.98E+05	7.05E+05	1.71E+06
1700	4.11E+05	1.43E+06	4.92E+06
1800	7.23E+05	2.57E+06	1.27E+07
1900	1.12E+06	4.17E+06	3.00E+07
2000	1.68E+06	6.09E+06	6.55E+07
2100	2.25E+06	1.22E+07	1.34E+08
2200	3.21E+06	1.40E+07	2.58E+08
2300	4.20E+06	1.96E+07	4.77E+08
2400	5.22E+06	2.49E+07	8.39E+08
2500	7.23E+06	3.01E+07	1.42E+09

Table S8. Rate coefficient (units: s^{-1}) of the elementary steps for the thermal decomposition of Phenoxy (High-pressure limiting rate)

T(K)	$k_{1\to2}$	$k_{1\to5}$	$k_{2\to1}$	$k_{2\to3}$	$k_{3\to2}$	$k_{3\to4}$	$k_{3\to5}$	$k_{5\to1}$	$k_{5\to3}$

500	1.79E-09	6.05E-17	4.34E+11	4.78E+09	2.18E+02	4.15E+09	1.02E-05	2.64E+09	4.03E+07
600	1.02E-05	1.26E-11	7.06E+11	1.76E+10	8.73E+03	1.54E+10	1.14E-02	9.11E+09	2.40E+08
700	4.99E-03	8.18E-08	1.00E+12	4.48E+10	1.23E+05	3.98E+10	1.75E+00	2.21E+10	8.62E+08
800	5.25E-01	5.99E-05	1.30E+12	9.00E+10	8.93E+05	8.14E+10	7.70E+01	4.30E+10	2.25E+09
900	1.97E+01	1.02E-02	1.60E+12	1.55E+11	4.19E+06	1.42E+11	1.47E+03	7.23E+10	4.76E+09
1000	3.61E+02	6.25E-01	1.88E+12	2.39E+11	1.45E+07	2.23E+11	1.56E+04	1.10E+11	8.66E+09
1100	3.91E+03	1.82E+01	2.15E+12	3.41E+11	4.00E+07	3.23E+11	1.08E+05	1.54E+11	1.42E+10
1200	2.85E+04	3.02E+02	2.40E+12	4.58E+11	9.34E+07	4.39E+11	5.43E+05	2.05E+11	2.13E+10
1300	1.53E+05	3.27E+03	2.64E+12	5.88E+11	1.92E+08	5.70E+11	2.13E+06	2.60E+11	3.02E+10
1400	6.48E+05	2.52E+04	2.87E+12	7.28E+11	3.55E+08	7.13E+11	6.89E+06	3.20E+11	4.07E+10
1500	2.27E+06	1.48E+05	3.08E+12	8.77E+11	6.05E+08	8.66E+11	1.91E+07	3.83E+11	5.26E+10
1600	6.78E+06	6.96E+05	3.27E+12	1.03E+12	9.66E+08	1.03E+12	4.64E+07	4.48E+11	6.60E+10
1700	1.78E+07	2.73E+06	3.46E+12	1.19E+12	1.46E+09	1.19E+12	1.02E+08	5.14E+11	8.06E+10
1800	4.22E+07	9.22E+06	3.63E+12	1.35E+12	2.11E+09	1.36E+12	2.05E+08	5.81E+11	9.63E+10
1900	9.11E+07	2.74E+07	3.79E+12	1.51E+12	2.93E+09	1.54E+12	3.84E+08	6.49E+11	1.13E+11
2000	1.82E+08	7.29E+07	3.94E+12	1.68E+12	3.94E+09	1.71E+12	6.74E+08	7.16E+11	1.30E+11

2100	3.41E+08	1.77E+08	4.08E+12	1.84E+12	5.15E+09	1.89E+12	1.12E+09	7.84E+11	1.48E+11
2200	6.04E+08	3.96E+08	4.22E+12	2.00E+12	6.57E+09	2.06E+12	1.78E+09	8.50E+11	1.67E+11
2300	1.02E+09	8.27E+08	4.34E+12	2.16E+12	8.21E+09	2.24E+12	2.73E+09	9.16E+11	1.86E+11
2400	1.64E+09	1.63E+09	4.46E+12	2.32E+12	1.01E+10	2.41E+12	4.02E+09	9.81E+11	2.05E+11
2500	2.55E+09	3.02E+09	4.57E+12	2.47E+12	1.22E+10	2.58E+12	5.75E+09	1.04E+12	2.25E+11

Table S9. Rate coefficient (units: s^{-1}) of thermal decomposition of 1,2-benzanthracene oxyradicals I ($<\triangle E>_{down}$=260 cm^{-1})

	P(atm)			
T(K)	0.1	1	10	k_∞
1500	3.94E+04	7.82E+04	1.13E+05	1.19E+05
1600	6.86E+04	1.57E+05	2.59E+05	4.57E+05
1700	1.11E+05	2.89E+05	5.41E+05	1.50E+06
1800	1.69E+05	4.98E+05	1.04E+06	4.29E+06
1900	2.46E+05	8.09E+05	1.89E+06	1.10E+07
2000	3.42E+05	1.25E+06	3.22E+06	2.55E+07
2100	4.60E+05	1.86E+06	5.24E+06	5.47E+07
2200	5.99E+05	2.67E+06	8.17E+06	1.09E+08
2300	7.60E+05	3.71E+06	1.23E+07	2.05E+08
2400	9.41E+05	5.01E+06	1.79E+07	3.65E+08
2500	1.14E+06	6.61E+06	2.54E+07	6.20E+08

Table S10. Rate coefficient (units: s^{-1}) of the elementary steps for the thermal decomposition of 1,2-benzanthracene oxyradicals I (High-pressure limiting rate)

T(K)	$k_{1\to2}$	$k_{1\to5}$	$k_{2\to1}$	$k_{2\to3}$	$k_{3\to2}$	$k_{3\to4}$	$k_{3\to5}$	$k_{5\to1}$	$k_{5\to3}$
500	5.12E-08	7.76E-27	3.09E+11	1.42E+05	4.96E+06	6.28E+10	6.21E-07	3.04E+08	1.16E+08
600	1.64E-04	7.34E-20	5.46E+11	3.56E+06	3.19E+07	1.07E+11	8.97E-04	1.30E+09	5.35E+08
700	5.33E-02	7.29E-15	8.21E+11	3.58E+07	1.21E+08	1.57E+11	1.64E-01	3.70E+09	1.60E+09

800	4.10E+00	4.15E-11	1.12E+12	2.02E+08	3.29E+08	2.11E+11	8.26E+00	8.10E+09	3.64E+09
900	1.21E+02	3.50E-08	1.41E+12	7.80E+08	7.18E+08	2.65E+11	1.75E+02	1.49E+10	6.90E+09
1000	1.82E+03	7.73E-06	1.71E+12	2.30E+09	1.34E+09	3.19E+11	2.01E+03	2.43E+10	1.15E+10
1100	1.68E+04	6.43E-04	2.00E+12	5.56E+09	2.24E+09	3.71E+11	1.49E+04	3.63E+10	1.75E+10
1200	1.07E+05	2.57E-02	2.27E+12	1.16E+10	3.43E+09	4.22E+11	7.92E+04	5.06E+10	2.48E+10
1300	5.12E+05	5.84E-01	2.54E+12	2.17E+10	4.92E+09	4.70E+11	3.26E+05	6.71E+10	3.34E+10
1400	1.97E+06	8.50E+00	2.79E+12	3.71E+10	6.70E+09	5.15E+11	1.10E+06	8.55E+10	4.30E+10
1500	6.32E+06	8.67E+01	3.02E+12	5.89E+10	8.77E+09	5.58E+11	3.14E+06	1.05E+11	5.36E+10
1600	1.75E+07	6.62E+02	3.24E+12	8.85E+10	1.11E+10	5.99E+11	7.88E+06	1.27E+11	6.50E+10
1700	4.32E+07	3.99E+03	3.45E+12	1.27E+11	1.37E+10	6.37E+11	1.78E+07	1.49E+11	7.70E+10
1800	9.64E+07	1.97E+04	3.65E+12	1.74E+11	1.64E+10	6.74E+11	3.66E+07	1.72E+11	8.96E+10
1900	1.98E+08	8.21E+04	3.84E+12	2.31E+11	1.94E+10	7.08E+11	7.00E+07	1.96E+11	1.03E+11
2000	3.77E+08	2.97E+05	4.01E+12	2.99E+11	2.25E+10	7.40E+11	1.25E+08	2.20E+11	1.16E+11
2100	6.77E+08	9.52E+05	4.18E+12	3.77E+11	2.58E+10	7.71E+11	2.12E+08	2.44E+11	1.29E+11
2200	1.15E+09	2.74E+06	4.33E+12	4.66E+11	2.91E+10	7.99E+11	3.43E+08	2.69E+11	1.43E+11
2300	1.87E+09	7.21E+06	4.48E+12	5.65E+11	3.26E+10	8.27E+11	5.31E+08	2.93E+11	1.57E+11
2400	2.93E+09	1.75E+07	4.62E+12	6.74E+11	3.61E+10	8.52E+11	7.94E+08	3.17E+11	1.70E+11
2500	4.41E+09	3.96E+07	4.75E+12	7.93E+11	3.97E+10	8.77E+11	1.15E+09	3.42E+11	1.84E+11

Table S11. Rate coefficient (units: s^{-1}) of thermal decomposition of 1,2-benzanthracene oxyradicals II ($<\triangle E>_{down}$=260 cm^{-1})

	P(atm)			
T(K)	0.1	1	10	k_∞
1500	3.72E+01	3.83E+01	5.99E+01	6.05E+01
1600	1.35E+02	2.01E+02	2.79E+02	3.63E+02
1700	3.99E+02	8.25E+02	1.09E+03	1.77E+03
1800	1.00E+03	2.75E+03	3.69E+03	7.21E+03
1900	2.21E+03	7.73E+03	1.10E+04	2.54E+04
2000	4.33E+03	1.88E+04	2.95E+04	7.87E+04
2100	7.72E+03	4.07E+04	7.23E+04	2.19E+05
2200	1.27E+04	7.93E+04	1.64E+05	5.57E+05
2300	1.95E+04	1.42E+05	3.46E+05	1.31E+06
2400	2.82E+04	2.35E+05	6.90E+05	2.86E+06
2500	3.88E+04	3.64E+05	1.30E+06	5.85E+06

Table S12. Rate coefficient (units: s^{-1}) of the elementary steps for the thermal decomposition of 1,2-benzanthracene oxyradicals II (High-pressure limiting rate)

T(K)	k_∞

500	1.10E-23
600	1.60E-17
700	4.08E-13
800	8.39E-10
900	3.19E-07
1000	3.71E-05
1100	1.84E-03
1200	4.72E-02
1300	7.39E-01
1400	7.82E+00
1500	6.05E+01
1600	3.63E+02
1700	1.77E+03
1800	7.21E+03
1900	2.54E+04
2000	7.87E+04
2100	2.19E+05
2200	5.57E+05
2300	1.31E+06
2400	2.86E+06
2500	5.85E+06

Table S13. Rate coefficient (units: s^{-1}) of thermal decomposition of 1,2-benzanthracene oxyradicals III ($<\triangle E>_{down}$=260 cm^{-1})

	P(atm)			
T(K)	0.1	1	10	k_∞
1500	3.46E+04	3.58E+04	6.93E+04	8.25E+04
1600	6.25E+04	7.72E+04	1.69E+05	2.54E+05
1700	1.03E+05	1.50E+05	3.68E+05	6.88E+05
1800	1.58E+05	2.68E+05	7.28E+05	1.66E+06
1900	2.28E+05	4.45E+05	1.33E+06	3.65E+06
2000	3.12E+05	6.97E+05	2.28E+06	7.41E+06
2100	4.09E+05	1.04E+06	3.69E+06	1.40E+07
2200	5.16E+05	1.47E+06	5.68E+06	2.51E+07
2300	6.30E+05	2.01E+06	8.38E+06	4.25E+07
2400	7.50E+05	2.67E+06	1.19E+07	6.88E+07
2500	8.72E+05	3.44E+06	1.64E+07	1.07E+08

Table S14. Rate coefficient (units: s^{-1}) of the elementary steps for the thermal decomposition of 1,2-benzanthracene

oxyradicals III (High-pressure limiting rate)

T(K)	$k_{1\rightarrow2}$	$k_{2\rightarrow1}$	$k_{2\rightarrow3}$	$k_{3\rightarrow2}$	$k_{3\rightarrow4}$
500	1.74E-10	1.53E+12	8.81E+10	6.45E+01	2.32E+11
600	1.21E-06	1.93E+12	1.68E+11	2.68E+03	4.91E+11
700	6.79E-04	2.28E+12	2.61E+11	3.78E+04	8.48E+11
800	7.91E-02	2.59E+12	3.56E+11	2.72E+05	1.29E+12
900	3.23E+00	2.86E+12	4.48E+11	1.25E+06	1.79E+12
1000	6.29E+01	3.09E+12	5.32E+11	4.22E+06	2.33E+12
1100	7.17E+02	3.30E+12	6.07E+11	1.13E+07	2.89E+12
1200	5.45E+03	3.49E+12	6.73E+11	2.56E+07	3.47E+12
1300	3.04E+04	3.65E+12	7.30E+11	5.08E+07	4.06E+12
1400	1.33E+05	3.80E+12	7.79E+11	9.11E+07	4.64E+12
1500	4.78E+05	3.93E+12	8.20E+11	1.50E+08	5.21E+12
1600	1.46E+06	4.05E+12	8.54E+11	2.33E+08	5.77E+12
1700	3.93E+06	4.16E+12	8.83E+11	3.41E+08	6.32E+12
1800	9.47E+06	4.26E+12	9.07E+11	4.78E+08	6.84E+12
1900	2.08E+07	4.35E+12	9.27E+11	6.45E+08	7.35E+12
2000	4.22E+07	4.43E+12	9.43E+11	8.43E+08	7.85E+12
2100	8.02E+07	4.51E+12	9.56E+11	1.07E+09	8.32E+12
2200	1.44E+08	4.58E+12	9.67E+11	1.33E+09	8.78E+12
2300	2.45E+08	4.64E+12	9.75E+11	1.62E+09	9.22E+12
2400	3.99E+08	4.71E+12	9.82E+11	1.94E+09	9.64E+12
2500	6.25E+08	4.76E+12	9.87E+11	2.29E+09	1.00E+13

Table S15. Rate coefficient (units: s^{-1}) of thermal decomposition of 1,2-benzanthracene oxyradicals IV ($<\triangle E>_{down}$=260 cm^{-1})

	P(atm)			
T(K)	0.1	1	10	k∞
1500	1.21E+02	1.54E+02	1.76E+02	2.12E+02
1600	3.45E+02	5.31E+02	8.02E+02	9.29E+02
1700	8.71E+02	1.58E+03	3.05E+03	3.89E+03
1800	1.98E+03	4.18E+03	1.00E+04	1.32E+04
1900	4.13E+03	9.97E+03	2.90E+04	3.98E+04
2000	8.01E+03	2.18E+04	7.54E+04	1.13E+05
2100	1.46E+04	4.42E+04	1.79E+05	3.03E+05
2200	2.51E+04	8.40E+04	3.94E+05	7.44E+05
2300	4.12E+04	1.51E+05	8.07E+05	1.69E+06
2400	6.49E+04	2.58E+05	1.56E+06	3.59E+06
2500	9.85E+04	4.23E+05	2.86E+06	7.17E+06

Table S16. Rate coefficient (units: s^{-1}) of the elementary steps for the thermal decomposition of 1,2-benzanthracene oxyradicals IV (High-pressure limiting rate)

T(K)	k_∞
500	1.52E-22
600	1.33E-16
700	2.39E-12
800	3.75E-09
900	1.16E-06
1000	1.14E-04
1100	4.88E-03
1200	1.12E-01
1300	1.59E+00
1400	1.55E+01
1500	2.12E+02
1600	9.29E+02
1700	3.89E+03
1800	1.32E+04
1900	3.98E+04
2000	1.13E+05
2100	3.03E+05
2200	7.44E+05
2300	1.69E+06
2400	3.59E+06
2500	7.17E+06

Table S17. Rate coefficient (units: s^{-1}) of thermal decomposition of 3H-cydopenta[a]anthracene oxyradicals ($<\triangle E>_{down}$=260 cm^{-1})

	P(atm)			
T(K)	0.1	1	10	k∞
1500	5.52E+06	1.20E+07	2.67E+07	2.76E+08
1600	8.03E+06	2.02E+07	4.68E+07	6.23E+08
1700	1.10E+07	3.21E+07	7.71E+07	1.27E+09
1800	1.44E+07	4.87E+07	1.20E+08	2.40E+09
1900	1.80E+07	7.10E+07	1.80E+08	4.24E+09
2000	2.19E+07	1.00E+08	2.59E+08	7.04E+09
2100	2.59E+07	1.37E+08	3.60E+08	1.12E+10
2200	2.99E+07	1.82E+08	4.87E+08	1.69E+10
2300	3.38E+07	2.37E+08	6.42E+08	2.47E+10

2400	3.75E+07	3.02E+08	8.29E+08	3.48E+10
2500	4.11E+07	3.78E+08	1.05E+09	4.78E+10

Table S18. Rate coefficient (units: s^{-1}) of the elementary steps for the thermal decomposition of 3H-cydopenta[a]anthracene oxyradicals (High-pressure limiting rate)

T(K)	$k_{1\rightarrow2}$	$k_{2\rightarrow1}$	$k_{2\rightarrow3}$
500	3.78E+08	1.55E+12	6.62E+00
600	2.00E+09	1.83E+12	9.32E+02
700	6.56E+09	2.06E+12	3.23E+04
800	1.60E+10	2.26E+12	4.63E+05
900	3.19E+10	2.42E+12	3.70E+06
1000	5.55E+10	2.57E+12	1.95E+07
1100	8.71E+10	2.69E+12	7.62E+07
1200	1.27E+11	2.80E+12	2.38E+08
1300	1.75E+11	2.89E+12	6.22E+08
1400	2.29E+11	2.98E+12	1.42E+09
1500	2.90E+11	3.05E+12	2.91E+09
1600	3.57E+11	3.12E+12	5.45E+09
1700	4.29E+11	3.19E+12	9.47E+09
1800	5.04E+11	3.24E+12	1.55E+10
1900	5.83E+11	3.29E+12	2.41E+10
2000	6.64E+11	3.34E+12	3.58E+10
2100	7.47E+11	3.38E+12	5.13E+10
2200	8.32E+11	3.42E+12	7.11E+10
2300	9.17E+11	3.46E+12	9.58E+10
2400	1.00E+12	3.49E+12	1.26E+11
2500	1.09E+12	3.53E+12	1.62E+11

Table S19. Relative zero-point energies, expectation values of S^2 operator (projected values are in parentheses), vibrational frequencies, rotational constants for all optimized structures at B3LYP/6-311+G(d,p) level in this work.

Species	Energy (hartree):	Relative ZEP Energy (kcal/mol)	Frequencies (unscaled) (cm^{-1})	Rotational Constants (GHz)	$<S^2>$	External symmetry number	Optical isomers	Electronic ground state	σ/ Å	(ε/k_B)/K

1,2-benzanthra cene oxyradicals I	ZPE: -767.721979 Energy: -767.708789	0	55.9646 67.4896 113.6757 143.6810 170.4200 206.4099 281.6100 285.4602 306.8624 322.7089 410.8251 424.1013 425.2969 440.7232 463.8702 501.9397 531.3563 533.4093 551.5389 582.5259 598.0773 622.4025 657.6321 698.0011 728.1783 731.2534 752.5576 758.7762 776.3919 785.6504 807.8230 826.6969 854.0863 855.0619 877.3109 885.5611 887.7370 918.0091 930.6417 967.9404 986.4543 994.0813 998.3120 1000.7454 1060.9349 1120.0690 1139.4659 1173.4912	1.03341 0.21103 0.17524	0.7897(0.75)	1	1	Doublet	7.9497	969.155

			1182.4092 1195.2500 1202.5284 1231.9562 1254.2160 1270.3705 1288.8279 1307.9817 1320.7127 1333.8756 1365.4821 1379.9678 1419.4554 1430.6100 1455.4350 1462.8408 1493.9425 1507.6400 1529.6918 1544.9365 1584.1524 1616.1784 1621.7146 1643.5181 1651.9253 3155.9991 3160.2182 3162.8384 3164.7203 3173.3164 3180.6492 3181.7690 3185.6457 3191.2282 3193.2343 3203.5578							

S1-CS2	ZPE: -767.651310 Energy: -767.637878	44.3	54.4732 58.3764 99.4527 134.3195 171.3646 188.6094 235.7035 288.8730 320.7460 338.9143 369.3850 405.9053 430.5592 454.5430 482.5596 505.4857 527.3164 533.6590 551.9688 567.6851 615.2362 632.6320 659.2589 702.4204 709.5368 715.2853 739.7214 753.6525 766.7439 779.0941 785.9056 814.3587 833.6586 864.7589 877.7692 880.2851 884.1873 892.4355 921.3920 962.1644 973.0153 982.2451 994.1720 1001.1179 1014.2265 1056.5115 1061.3679 1115.8146	0.96411 0.22100 0.18769	0.7795(0.75)	1	1	Doublet	7.9497	969.155

			1148.5200 1174.0848 1176.3355 1188.3234 1211.7048 1213.6367 1235.3506 1248.7500 1260.0122 1287.4456 1311.5427 1322.3779 1364.6990 1393.4700 1427.6247 1455.3135 1461.5776 1464.9120 1510.0877 1548.8102 1585.9794 1614.5912 1644.3764 1649.1715 1904.2131 3127.7909 3145.5156 3157.9305 3160.7795 3168.9564 3170.4093 3177.6670 3184.2360 3190.8807 3204.6852 3215.0519							
S1-CS3	ZPE: -767.634816 Energy: -767.620521	51.7	11.6978 47.7916 63.1922 113.0828 142.7454 179.7908 195.9889 237.1989 298.2819 311.6648 335.7938 372.4238	1.01150 0.20812 0.18201	0.7974(0.75)	1	2	Doublet	7.9497	969.155

			383.0556 420.9144 443.7834 456.3084 504.5117 531.4362 540.5040 551.9684 568.7845 623.8153 654.8249 677.8486 689.0939 708.9431 726.2444 752.1447 757.9420 772.4567 778.8316 781.9050 806.4207 817.2577 846.2494 875.4390 883.3936 884.4782 891.5375 945.6629 961.5286 985.4876 986.6790 995.2745 1026.9702 1066.6072 1123.8078 1141.7710 1152.5158 1165.8641 1189.3012 1196.8877 1203.1271 1233.9461 1255.1794 1271.8362 1274.7171 1290.6714 1317.6700 1346.6557							

			1375.9144 1403.4526 1434.7470 1445.2457 1483.9523 1505.9539 1529.4528 1573.8633 1591.2242 1627.7138 1650.0387 1661.0040 1892.8388 3073.8652 3157.6109 3161.3214 3167.1889 3171.3558 3177.5993 3184.0732 3190.4992 3202.9794 3222.6909 3229.6029							
S1-CS4	ZPE: -654.356350 Energy: -654.344798	13.6	71.2083 81.4409 158.7674 182.3048 206.4423 287.5696 315.6173 326.7999 374.0186 408.5640 434.2724 463.1257 508.9454 527.1495 545.6605 548.6181 566.6220 624.0989 676.5549 706.9580 722.8223 728.0394 733.9133 756.1189	1.29268 0.30367 0.24590	0.7712 （0.75）	1	1	Doublet	7.9497	969.155

			779.1559 782.3109 791.2547 796.6442 823.2394 872.6758 873.6856 891.4183 895.1353 905.1018 913.4501 963.9250 981.6251 981.7995 995.4721 1026.2317 1055.9932 1078.8460 1114.8397 1135.7313 1172.6852 1184.7327 1202.3565 1213.6907 1229.3452 1245.8474 1261.3791 1288.3780 1318.2721 1368.8434 1383.7370 1391.7911 1412.6383 1428.0156 1462.3937 1473.9938 1485.3425 1529.8567 1553.7508 1609.4276 1619.8945 1640.6231 1653.4819 3156.2399 3159.5417 3160.8548 3170.2031 3176.5578							

			3183.3341 3188.8088 3203.4898 3203.8570 3212.8186 3227.1185							
S1-CS5	ZPE: -767.586664 Energy: -767.571526	84.9	25.4872* 60.5047 67.5478 83.9260 111.3209 158.7091 175.6607 228.8047 240.9030 272.6451 291.3208 348.5020 354.9781 418.2049 437.7624 443.4160 454.8453 492.4271 496.6934 509.6576 527.2804 543.6112 552.6322 603.8461 643.8703 646.1052 676.0515 707.0484 721.4464 728.0948 751.4114 774.2707 776.6111 793.1534 803.6670 831.5953 858.4208 861.3354 877.5791 899.6146 915.1394 958.6176	1.25155 0.16948 0.14927	1.0472 （0.75）	1	1	Doublet	7.9497	969.155

			981.6189 991.7604 993.1739 1065.3859 1082.4655 1127.8054 1142.7783 1156.4219 1176.6825 1188.8496 1211.2166 1225.3375 1251.0718 1260.3244 1281.9468 1320.4946 1343.4491 1348.6890 1392.1052 1417.7239 1438.7489 1449.2398 1485.6637 1495.9380 1509.8259 1571.5411 1587.5767 1612.2468 1645.0559 1651.1266 2185.9467 3059.7001 3154.0384 3157.3622 3159.9735 3162.9479 3169.6058 3176.8051 3182.0102 3189.9889 3200.4341 3235.8542							
S1-TS12	ZPE: -767.646745	47.2	-442.9643 56.7512 62.0494 113.3630 142.8705 176.2519	0.97760 0.21706	0.8119 (0.75)	1	1	Doublet	-	-

	Energy: -767.633597		199.0864 253.8846 307.7189 317.3409 342.2809 384.6504 414.2643 431.5970 436.2597 470.0543 508.0714 532.9691 538.5860 558.0762 601.5167 608.7118 650.2736 663.1128 688.4888 719.1907 736.6296 754.3701 760.3842 779.2252 790.2986 817.1885 826.5937 854.8232 870.9551 885.7435 886.4676 892.7581 905.8268 963.7263 974.9736 983.0340 996.0749 996.9182 1057.8534 1074.7440 1095.7659 1121.3363 1161.9123 1175.6309 1183.4620 1191.6134 1219.6763 1241.2597	0.18235						

			1248.0716 1265.4475 1282.4362 1303.4478 1317.6885 1337.2521 1365.7161 1396.4300 1432.6059 1458.0468 1468.5175 1470.0414 1516.4712 1547.3811 1591.9998 1611.8134 1644.8935 1650.6831 1838.5845 3129.4599 3131.6071 3158.9973 3161.7544 3167.6451 3171.4517 3178.5458 3184.7403 3191.4092 3197.4618 3204.8686							
S1-TS15	ZPE: -767.573361 Energy: -767.558831	93.3	-168.5649 31.2129 51.3855 84.5212 103.2359 136.5375 161.6219 207.9331 238.8323 265.1182 307.2465 316.4872 353.6831 402.8065 417.6560 432.3664 455.0765 478.0449	1.07723 0.18841 0.16540	1.0550 （0.75）	1	1	Doublet	-	-

			497.9992 528.5139 537.8919 546.7022 550.3835 631.3405 640.7498 660.7097 669.6022 704.5672 711.3680 723.9447 752.2005 767.3045 773.8179 778.9162 798.4856 816.9013 856.6864 871.3818 879.1083 893.4492 908.9021 960.8386 973.9027 986.1890 994.8029 1035.6373 1066.1802 1121.9295 1134.0574 1148.1361 1173.4372 1190.2204 1208.0877 1224.8039 1249.3531 1260.5254 1277.1322 1320.0459 1346.2574 1349.1587 1376.7603 1418.5750 1430.9225 1440.4088 1485.5257 1498.9798							

			1509.1576 1563.6932 1588.2013 1611.2293 1645.1915 1651.8636 2197.6013 3119.5503 3130.5522 3156.1935 3159.4114 3161.4894 3171.2866 3176.9439 3184.2509 3190.4640 3201.9003 3207.7147							
*Vibration frequency replaced by unsymmetrical 1-D hindered rotor (hrd 8 14 1)			(Vhrd2) 1 0 187.22 -33.57 110.42 -28.59 87.54 -16.36 5.19 -1.03	(Ihrd1) 1 0 124.31 -28.21 -16.57 6.67 3.99 -4.87 -1.08 3.03 -0.87 -0.59 1.02 0.08 -2.31 -0.17						
S1-TS23	ZPE: -767.622865 Energy: -767.609322	62.2	-392.6568 49.2539 56.1960 87.8204 140.9012 166.5238 186.4892 232.8466 301.7166 318.8253 326.5065 361.9480 387.2210 405.4031 427.7645 461.2590 478.0471 506.8413 536.6231 544.9319 556.0223	1.02767 0.21299 0.18782	0.7567 （0.75）	1	1	Doublet	-	-

			622.7461 629.3967 681.8198 687.7368 713.4333 724.6230 742.8038 753.0514 770.8229 775.4398 780.8582 811.5792 841.5642 854.1523 862.3408 877.0261 881.9143 890.8119 959.7907 976.1100 977.8074 980.0439 991.0572 1015.2282 1061.5356 1121.1165 1146.7912 1162.8508 1172.1402 1177.4659 1187.2127 1202.8278 1233.8070 1250.6457 1261.7281 1278.0291 1292.9459 1315.6258 1355.6611 1359.7356 1391.2086 1434.1805 1463.6231 1468.3359 1481.2966 1512.6462 1541.8535 1584.5842							

			1594.3643 1641.8137 1647.9134 2029.2670 3001.2174 3154.4628 3158.4796 3168.4699 3164.6007 3174.6083 3183.0929 3188.9221 3203.0515 3230.9844 3238.5482							
S1-TS34	ZPE: -767.635466 Energy: -767.621526	54.3	-401.6309 43.508* 48.8374 74.2371 120.6718 150.4959 180.0125 199.7310 243.7781 303.1542 329.1730 348.7673 369.3708 401.8483 424.2448 447.3506 463.7902 502.9922 530.5066 544.4393 554.1682 577.3692 624.8860 655.2485 689.5985 710.8479 724.0340 749.6573 756.2513 759.4744 776.9313 779.7906 801.7704	0.98954 0.21349 0.18793	0.7695 （0.75）	1	1	Doublet	-	-

			813.4044 840.8189 872.8736 879.9574 885.8331 888.5709 961.8885 965.5545 974.3726 983.7903 994.5410 1001.4769 1064.3911 1108.3575 1123.8470 1142.4437 1165.2541 1189.7057 1192.8547 1214.3864 1234.8078 1253.6736 1276.2770 1287.7332 1305.0926 1316.0754 1350.4747 1366.7571 1385.3395 1431.8668 1441.9270 1479.6956 1492.0995 1521.0268 1550.3079 1586.8492 1609.5414 1644.3819 1654.6476 1923.2937 3142.2158 3157.2260 3160.9500 3165.8959 3171.2881 3177.2186 3184.3594 3190.3660							

			3204.4073 3223.8361 3228.5940							
*Vibration frequency replaced by unsymmetrical 1-D hindered rotor (hrd 5 8 1)			(Vhrd2) 1 0 203.45 -23.57 140.12 21.71 -3.03	(Ihrd1) 1 0 68.32 11.25 -7.54 -9.54 6.19 1.06 -0.91 -4.67						
S1-TS53	ZPE: -767.572381 Energy: -767.558003	93.9	-471.6114 33.2011 55.8188 81.6749 101.8649 154.2279 162.5186 191.1145 247.6324 277.7535 304.6940 335.0323 367.7119 415.2114 421.7598 436.2460 457.4843 486.6952 501.4433 527.6554 547.3742 549.9374 599.3111 627.3247 633.3254 662.5707 673.7879 707.7347 717.1955 729.7399 753.0146 769.2598 775.2282 778.5866 798.9857 815.7408	1.14971 0.18233 0.16030	0.9507 (0.75)	1	1	Doublet	-	-

			866.4813 876.4060 883.0327 893.3499 918.8773 960.8752 984.7439 987.2085 994.8937 1023.2211 1066.7509 1107.4115 1129.3707 1168.4843 1177.6453 1192.5990 1220.6953 1224.6425 1246.5690 1258.1975 1275.7967 1309.1505 1322.0115 1345.5703 1354.6379 1417.9052 1433.6575 1440.9684 1485.2210 1502.6170 1513.4467 1576.2268 1590.5573 1620.7406 1647.7610 1657.6164 2137.0827 3055.4168 3155.8667 3159.6292 3161.2007 3170.8658 3176.4006 3183.8404 3185.5602 3187.0076 3190.1699 3202.3841							

1,2-benzanthrace ne oxyradicals II	ZPE: -767.734738 Energy: -767.721600	0	54.0864 63.4747 113.6690 155.0381 162.3826 205.6402 274.5025 292.5753 293.6123 322.4664 370.7401 423.1286 433.0921 444.6735 511.0608 514.1134 518.3605 533.5176 542.6478 595.5813 611.4661 640.7751 665.2717 687.2687 704.3874 753.6691 757.3940 773.0293 775.8356 803.8563 829.8612 841.2373 848.8913 880.1619 890.3791 892.3117 916.1485 967.7748 974.2798 985.5331 997.8176 1004.7171 1009.2567 1049.9332 1056.2018 1104.3642 1123.4835 1165.7214	0.91601 0.24911 0.19585	0.7907 (0.75)	1	1	Doublet	7.9497	969.155

			1176.0317 1183.3421 1198.5808 1214.9466 1230.9418 1252.2540 1273.2730 1300.0273 1309.5792 1333.9989 1359.7479 1367.8528 1394.3687 1445.7489 1458.5420 1469.7619 1495.1253 1520.0443 1532.0545 1576.4372 1588.6350 1602.9851 1613.7671 1642.0507 1648.0471 3162.4292 3163.0926 3168.7271 3173.3975 3174.6717 3185.9065 3187.7640 3192.1508 3199.9552 3202.3056 3205.2421							
S2-CS2	ZPE: -654.365601 Energy: -654.354065	15.8	65.9107 93.8036 157.2309 166.9767 195.8265 292.6622 297.3821 320.4238 387.1273 418.4142 432.3122 497.2490	1.46086 0.28982 0.24184	0.7783 (0.75)	1	1	Doublet	7.9497	969.155

			516.5472 534.4638 541.2428 562.3444 567.3234 583.6505 660.1719 682.7173 705.3375 729.0348 746.5813 759.8593 763.7567 778.6460 802.8131 825.3285 850.5846 875.2629 880.8437 887.6146 916.4152 949.6120 958.0139 968.9220 983.2841 993.9422 1030.7055 1040.8944 1053.5632 1095.7613 1106.8946 1157.3819 1167.0264 1180.5200 1184.0559 1217.7329 1225.4543 1231.9497 1271.5957 1304.5387 1330.6419 1359.0402 1370.8807 1388.8629 1424.7552 1455.8382 1475.8588 1485.6472							

			1495.5044 1549.8031 1575.2075 1588.7575 1609.6234 1619.8227 1647.8297 3158.8077 3160.7364 3162.0925 3166.7062 3167.4076 3176.8623 3178.7271 3180.1713 3189.4305 3190.0544 3213.3975							
S2-TS12	ZPE: -767.602349 Energy: -767.588810	83.1	-794.5031 57.6684* 85.1655 108.2554 136.1967 152.9422 185.1590 200.7292 258.5483 275.2696 331.9892 368.3403 384.7734 423.8845 467.6962 491.5834 511.4762 515.5704 533.3068 554.9047 563.2546 570.1886 607.7636 654.1790 664.0171 689.9323 713.6966 743.6719 752.4465 772.5823	0.93850 0.26105 0.22628	0.7872 (0.75)	1	1	Doublet	-	-

			786.1673 804.4993 810.8219 855.0720 872.3181 880.4182 887.4239 900.1194 959.8188 967.4375 974.6460 975.5389 986.4850 992.1638 996.6110 1050.6372 1078.4790 1115.8170 1164.0485 1169.4391 1173.5736 1185.8996 1198.4624 1206.1465 1230.0907 1233.6564 1291.7185 1343.6972 1353.2150 1368.0048 1384.3983 1420.1233 1434.4427 1448.3500 1462.4767 1507.7988 1535.2527 1545.0412 1568.5854 1615.7074 1635.3576 1647.0673 1831.6190 3160.3796 3162.7688 3164.1399 3168.2090 3168.8678							

			3181.6596 3185.2548 3187.2699 3191.4925 3193.3602 3206.7542							
*Vibration frequency replaced by unsymmetrical 1-D hindered rotor (hrd 5 6 1)			(Vhrd2) 1 0 367.51 -16.55 74.82 -6.31 -2.15	(Ihrd1) 1 0 15.54 3.12 -2.51 -0.34 0.21 -0.15						
1,2-benzanthracene oxyradicals III	ZPE: -767.718098 Energy: -767.704929	0	44.6572 67.2708 107.0580 158.4088 169.7611 205.7197 264.3829 295.2331 303.7628 327.6041 402.8546 413.9078 468.8457 471.5263 477.7813 509.4573 517.3921 537.3668 541.5539 560.4176 615.1000 621.8175 636.9091 690.7057 708.4460 741.6704 750.0187 759.0010 769.8601 796.5194 799.1642 827.4728 836.7042	0.93664 0.24924 0.19686	0.7864 （0.75）	1	1	Doublet	7.9497	969.155

			860.8441 896.0486 904.0149 917.1822 944.1821 963.0191 980.8966 983.4354 989.5405 1000.4087 1030.4673 1058.8166 1097.9971 1140.3365 1158.6395 1169.2561 1183.9236 1194.3008 1218.9381 1223.5219 1254.1798 1287.7830 1302.8002 1332.5566 1351.6657 1375.8049 1376.1097 1412.5699 1417.6382 1445.4088 1454.8705 1479.5153 1507.0329 1530.1197 1553.4584 1564.4048 1581.1842 1623.2359 1637.5949 1660.8095 3155.4445 3160.3603 3161.6468 3166.2444 3167.4969 3178.3434 3179.0888 3181.6827							

			3189.7694 3199.3299 3235.5875							
S3-CS2	ZPE: -767.637078 Energy: -767.623570	50.8	52.0451 61.5969 111.9356 139.5189 155.4171 178.0381 234.6016 275.7643 295.9476 321.5857 365.2439 408.0486 433.3665 474.9144 477.4071 485.0670 515.7604 544.8015 558.6039 596.0022 614.2854 635.3065 641.3177 679.7738 711.7714 743.4007 751.4857 754.1783 764.7350 777.7312 789.0939 796.9518 836.0193 857.0530 892.1860 895.7228 903.4046 915.8419 919.8614 934.8541 941.1037 969.0037 980.7280 993.9537 1014.6908	0.89835 0.25739 0.21674	0.7877 (0.75)	1	1	Doublet	7.9497	969.155

			1039.9646 1053.4374 1097.5716 1108.2847 1154.6980 1174.8987 1193.2409 1206.6870 1222.6999 1243.7041 1273.0221 1292.5691 1294.7082 1328.0687 1340.5962 1385.9079 1393.7472 1403.6884 1408.1799 1460.6132 1490.8386 1520.6755 1523.0287 1544.4236 1594.8369 1632.7790 1652.9012 1895.2850 3112.1205 3155.4219 3157.7529 3159.3758 3163.2416 3164.2631 3176.4485 3181.8183 3188.8581 3198.2963 3218.8169							
S3-CS3	ZPE: -767.666681 Energy:	32.3	28.0134 53.7037 69.3561 108.6712 151.3362 173.7523 215.1338 267.1577 292.4332	0.74514 0.26835 0.20145	0.7542 (0.75)	1	1	Doublet	7.9497	969.155

	-767.652776		309.2763 355.6742 382.9842 409.8785 419.6009 468.8553 475.2803 493.3565 519.1832 543.0171 560.2726 604.1707 623.5639 640.1996 656.3238 717.4518 728.6569 754.2595 761.8726 777.2805 787.5452 819.7644 828.7325 850.6428 865.1236 888.6336 900.9526 904.2888 917.1608 956.2890 966.5428 975.7435 979.0545 990.0129 997.4726 1027.8216 1054.4250 1122.2968 1150.4370 1166.0680 1173.2470 1182.1390 1193.0730 1215.2483 1234.2229 1252.6886 1287.5613 1299.7029							

			1336.8987 1363.5120 1377.5536 1397.0290 1417.5020 1424.4226 1466.4612 1479.0635 1514.5301 1559.1914 1584.9187 1602.5187 1621.0774 1653.8083 1664.8494 1888.9535 3020.6566 3156.2403 3160.0449 3163.6908 3164.6242 3169.5435 3177.6714 3182.6524 3189.4399 3198.4096 3228.9974							
S3-CS4	ZPE: -654.344611 Energy: -654.332893	18.5	73.3266 89.2935 163.8052 179.5261 191.8253 273.2699 305.1993 317.7163 366.0078 417.2395 456.0686 473.9967 474.3029 511.5400 535.1159 546.6303 548.7735 603.6894 635.9388 659.0390 695.8558	1.35593 0.29353 0.24129	0.7879 (0.75)	1	1	Doublet	7.9497	969.155

			711.9811 752.5008 753.8085 766.0194 767.5275 792.8720 812.9701 826.7852 840.8901 852.8503 896.6234 902.1526 904.8602 911.0619 944.2247 965.5433 974.1005 982.9892 995.2218 1029.5298 1053.9678 1095.9490 1145.2256 1157.9378 1181.4629 1185.1915 1194.3966 1227.4087 1284.2085 1290.6208 1303.2478 1323.2560 1350.5385 1376.2372 1385.7190 1413.4413 1416.8140 1456.8063 1473.5084 1508.3451 1520.5192 1550.2541 1576.8122 1582.7495 1637.6711 1658.1259 3155.1315 3158.2915							

			3161.8368 3162.4134 3165.7464 3176.1619 3178.6803 3188.3895 3206.2162 3213.7407 3232.3174							
S3-TS12	ZPE: -767.635504 Energy: -767.622413	51.8	-274.9838 60.7416 66.0999 123.8814 141.8217 168.3140 208.2169 243.2534 295.8206 299.0257 341.0203 382.2863 410.7871 463.2810 474.4372 483.9310 513.0674 524.2677 544.5465 563.8923 611.8809 627.3931 635.9354 661.6617 710.5949 728.1933 734.3469 754.1606 757.2298 770.0134 794.5806 802.3382 827.6625 858.2316 876.3000 898.8862 904.8296 912.1466 916.1277	0.89210 0.25970 0.21340	0.7705 (0.75)	1	1	Doublet	-	-

			947.3200 972.4198 979.5619 995.8401 996.7462 1038.9563 1047.7634 1054.4099 1112.0879 1113.7217 1156.9226 1176.0543 1194.5125 1204.7632 1245.1001 1254.6986 1274.4369 1291.2407 1298.5208 1330.1728 1345.1236 1392.2838 1400.4191 1405.1950 1422.1809 1459.1787 1493.7334 1518.8333 1523.6329 1560.3447 1595.0250 1630.4381 1654.1552 1845.3020 3116.2636 3157.2130 3160.3580 3163.6795 3164.7780 3168.8691 3177.4097 3181.9528 3189.4229 3190.4020 3211.1967							
S3-TS23	ZPE:	54.7	-532.4568 60.2210 64.8601	0.87208	0.7656	1	1	Doublet	-	-

	-767.630925 Energy: -767.617643		112.7871 141.7983 160.5878 187.7898 245.3508 290.4471 305.7597 336.5929 374.5799 407.0403 413.050 6454.8853 476.2587 490.4012 496.4214 537.7922 560.1580 592.3329 610.7452 634.9454 649.1112 703.8313 728.7150 753.7026 761.1000 773.6092 779.9020 789.9499 802.7446 835.8800 853.4014 887.5538 894.5447 900.0464 915.6270 937.2668 955.9456 969.9314 971.5890 979.9001 994.1698 1034.6413 1044.3397 1091.2698 1116.5306 1131.9055 1161.2982 1174.5760	0.26313 0.21567	(0.75)					

			1192.4778 1211.2995 1226.8773 1253.8335 1280.4824 1298.4918 1307.0766 1345.9420 1365.8113 1389.2004 1395.3164 1407.2951 1445.0139 1462.0255 1511.9641 1519.8540 1534.3919 1575.5598 1590.0348 1633.3949 1656.4965 1898.0774 3004.1391 3157.0026 3159.2907 3161.6894 3164.5583 3165.7908 3176.6085 3182.2419 3188.7749 3198.7503 3225.5840							
S3-TS34	ZPE: -767.661161 Energy: -767.647039	35.7	-463.3813 37.3926* 55.8907 64.2476 110.6495 113.1827 170.7625 205.2259 224.0035 286.4780 290.7008 312.0935 349.0420 385.5147 419.4418	0.73214 0.25684 0.19694	0.7543 (0.75)	1	1	Doublet	-	-

			465.5977 475.2020 511.9698 520.8337 549.7221 592.5889 605.8573 616.8567 637.4314 656.5066 718.2576 730.8820 753.3335 763.5502 784.1068 790.5285 820.0881 823.9365 851.2301 859.7233 890.3744 904.0565 913.9602 927.4608 938.0905 972.8521 976.3526 985.0066 995.2809 995.5973 1027.7178 1055.3232 1111.1975 1152.0291 1167.2833 1180.7450 1193.3677 1224.2065 1234.9075 1269.6522 1290.6115 1298.2965 1338.5980 1358.6989 1378.2070 1392.4146 1418.7163 1425.7479							

			1468.4869 1476.0666 1516.0989 1526.4433 1571.3198 1584.7161 1606.6407 1646.6292 1663.0110 1981.7767 3153.8752 3155.6459 3158.7915 3162.5063 3163.1448 3165.9155 3176.5819 3176.5819 3188.6395 3203.5871 3230.2490							
*Vibration frequency replaced by unsymmetrical 1-D hindered rotor (hrd 5 3 1)			(Vhrd2) 1 0 436.12 -241.25 -41.24 57.26 -53.47	(Ihrd1) 1 0 12.57 1.68 -0.74						
1,2-benzanthracene oxyradicals IV	ZPE: -767.730853 Energy: -767.717755	0	37.9850 69.8629 109.7454 158.0149 178.0719 197.0654 263.6689 295.5232 329.1907 344.4243 372.2221 410.2673 436.5827 444.7437 510.1346 523.4257 525.7892 539.8904	1.00402 0.25054 0.20051	0.7851 （0.75）	1	1	Doublet	7.9497	969.155

			544.2794 561.0327 629.3118 646.3049 649.1707 689.6563 704.8174 754.6397 765.4733 770.0105 770.0443 803.8218 807.4825 821.7017 853.4483 890.1074 892.2520 892.5689 913.3519 977.9579 985.2475 991.5002 1009.4789 1018.2748 1019.5064 1048.6309 1064.9816 1085.2555 1129.6937 1164.1386 1174.5537 1177.6568 1189.0727 1200.8644 1234.1287 1250.8555 1275.0669 1291.4777 1303.3491 1343.7633 1359.9574 1372.0710 1400.9536 1434.6520 1455.8881 1466.7989 1495.7061 1504.7933							

			1542.1772 1572.1718 1588.3586 1601.5563 1625.1264 1639.9456 1645.0167 3159.1507 3161.3893 3162.6629 3166.3525 3171.7311 3174.8675 3179.7201 3187.1658 3187.6915 3202.9054 3254.9989							
S4-CS2	ZPE: -654.361354 Energy: -654.349774	80.1	60.7233 78.9356 159.4200 167.3163 196.5225 291.8565 325.4556 328.4721 376.3893 414.6346 428.4930 481.4558 513.1660 533.2830 540.1974 546.6535 575.5469 610.8762 643.2757 671.9511 702.9668 723.3947 749.4446 752.3560 759.6821 777.4675 788.4815 826.1821 826.8200 862.3355	1.04505 0.35561 0.26533	0.7848 (0.75)	1	1	Doublet	7.9497	969.155

			875.7907 877.0499 942.1464 955.1815 960.5729 973.2745 982.7969 992.6123 1018.6856 1039.6072 1059.9748 1106.2193 1119.4492 1152.2063 1164.9885 1174.7055 1181.5641 1200.8515 1227.7814 1250.5908 1270.3270 1296.6571 1337.3495 1366.3472 1366.6634 1390.3577 1423.2927 1462.6186 1465.9930 1478.7726 1495.8769 1549.4447 1575.1591 1605.7053 1606.2169 1615.8723 1643.4077 3159.1621 3162.5060 3163.7082 3171.5480 3172.9910 3179.8983 3186.9393 3188.0529 3202.6109 3209.1401 3234.3875							

S4-TS12	ZPE: -767.603155 Energy: -767.589649	16.0	-774.4717 67.9189* 78.2769 109.2711 132.4844 144.9942 189.3090 196.8600 282.9603 299.4018 324.1872 363.6874 382.4865 425.5939 467.0905 485.7907 510.9732 514.5297 536.0708 538.3798 552.7686 576.5247 616.9771 649.4465 670.3260 691.5495 715.9977 753.1492 756.9064 767.2355 787.5739 801.2406 811.1646 838.6105 874.6671 881.0083 890.3363 924.6341 954.5458 964.8785 970.1237 977.1476 987.4116 993.9372 1010.9828 1059.8511 1068.6155 1115.7502	0.79076 0.31622 0.25762	0.7974 (0.75)	1	1	Doublet	-	-

			1154.7715 1159.9775 1169.4436 1184.8250 1192.1655 1209.7037 1229.3474 1281.8973 1295.2975 1331.3599 1352.5465 1358.3490 1374.9196 1397.9447 1433.7623 1453.7345 1465.9354 1522.5507 1536.9306 1558.4749 1571.6394 1600.4154 1641.2002 1650.6348 1829.8827 3161.2458 3163.8161 3165.2590 3170.0067 3174.0835 3181.9208 3186.6091 3189.3932 3198.2525 3201.1719 3208.0409							
*Vibration frequency replaced by unsymmetrical 1-D hindered rotor (hrd 5 6 1)			(Vhrd2) 1 0 267.12 108.47 -121.54 12.36 0.57	(Ihrd1) 1 0 14.07 0.81 0.26 -0.43 -0.47 1.15						
3H-cydopenta[a]a	ZPE:	0	56.9745 84.8957 117.1289	1.24504	0(0)	1	1	Singlet	7.7448	930.35

nthracene oxyradicals	-728.953007 Energy: -728.940203		154.3198 191.9106 199.8436 255.5566 281.8241 293.0181 341.5690 374.2613 428.2909 442.7960 467.3061 478.2781 523.3862 528.7596 540.4632 549.2447 607.9109 655.0592 659.7956 696.3295 704.8361 723.4388 750.1528 766.9099 794.1397 818.2747 832.5764 839.3761 848.2281 871.8479 890.1314 893.8449 918.4589 926.7534 966.9533 977.3175 978.8360 1001.4396 1045.1404 1094.5827 1111.9093 1167.4189 1182.3272 1188.6207 1190.9949 1217.0308 1229.8144 1246.4462	0.23465 0.19744						

			1275.2432 1284.0199 1302.7889 1329.8577 1357.3972 1390.3323 1414.0180 1450.5620 1468.4034 1505.7076 1548.5360 1578.4891 1591.1148 1624.6521 1647.1417 1661.4522 1681.6149 3164.0696 3165.9361 3169.9271 3174.9272 3182.1781 3189.3048 3195.6428 3201.9127 3205.0364 3212.0699							
S5-CS2	ZPE: -728.937324 Energy: -728.924639	9.1	49.5917 75.3519 95.9512 159.8684 186.5854 208.2658 272.6378 302.1452 325.0249 353.8483 393.5723 418.9643 434.7056 452.6956 490.2729 520.3767 538.1903 543.7432 563.1854 614.7141 665.2187	1.19412 0.23750 0.20337	0(0)	1	1	Singlet	7.7448	930.35

			676.2507 719.6189 731.6334 740.8586 757.3198 785.9926 788.5223 817.1779 823.7907 872.5229 874.5811 886.3264 896.2439 907.7739 912.3477 964.6735 970.8309 982.3054 996.3554 1032.3711 1052.3516 1057.7208 1089.3831 1128.8037 1169.3534 1173.5857 1183.0782 1186.7487 1206.5372 1229.9192 1240.3644 1251.7276 1275.2932 1316.1427 1369.8541 1393.1672 1415.4425 1461.2262 1470.7479 1477.9873 1533.1273 1560.4544 1628.2046 1648.5241 1662.7860 1674.6926 1859.6904 3157.8061							

			3161.0573 3170.8236 3171.8723 3173.0148 3175.8280 3177.4596 3185.8128 3194.7347 3209.9345							
S5-CS3	ZPE: -615.599316 Energy: -615.588345	6.1	78.5940 91.1839 174.9924 202.1655 223.0241 265.9280 339.2394 352.6993 389.3040 396.9042 436.7996 476.9395 513.4028 541.2813 545.5591 567.5710 628.2568 690.3964 711.9484 745.5350 752.1744 755.2674 758.8698 789.0286 823.1232 828.2752 846.3267 869.7329 879.7185 887.0440 894.8063 926.7505 946.4534 962.4397 976.2301 994.0524 1037.8388 1053.5073 1068.7620	1.40765 0.36491 0.28979	0(0)	1	1	Singlet	7.7448	930.35

			1080.0009 1113.0521 1174.0624 1180.3925 1205.1446 1227.8656 1238.1904 1262.3245 1273.1135 1312.4316 1374.9484 1384.9616 1400.4121 1431.0196 1458.6045 1483.8153 1540.6942 1543.0397 1567.9427 1629.5796 1650.6574 1682.1496 1709.8023 3155.9214 3158.8061 3168.7856 3170.2915 3175.7888 3184.2451 3193.0445 3207.0397 3210.4018 3235.3055							
S5-TS12	ZPE: -728.937436 Energy: -728.925271	9.8	-165.3243 62.5774 80.0962 139.0518 160.4040 203.7944 231.5019 278.0447 312.8730 347.4125 373.9412 396.2690 434.1041 447.1465 485.7296	1.21965 0.23532 0.20027	0(0)	1	1	Singlet	-	-

			522.7200 537.2801 543.7390 562.1254 611.6285 669.7603 675.2863 712.7861 728.0224 737.0928 756.8617 781.6435 785.7624 787.9630 824.0340 861.6240 870.9277 874.4379 888.2785 901.3599 907.9196 965.6022 976.1975 981.7425 997.2076 1026.5374 1055.6046 1091.3850 1117.0386 1143.8342 1172.5600 1179.7905 1187.3239 1199.9919 1206.2833 1241.5213 1246.4173 1257.3996 1279.4787 1318.9717 1373.0936 1397.8013 1414.6877 1460.6523 1470.4225 1490.1071 1537.0338 1560.0945							

			1628.3629 1649.1613 1662.6500 1676.7756 1797.9289 3158.8380 3161.8272 3169.0156 3171.1524 3171.5758 3171.7858 3178.0864 3186.0845 3194.1097 3208.9058							
S5-TS23	ZPE: -728.893308 Energy: -728.880424	37.5	-208.9700 50.2378* 60.6054 100.9323 132.0154 190.1299 206.7317 239.4215 307.4118 322.7693 337.2085 389.1338 397.1662 430.8433 458.7089 480.1283 500.5234 521.8871 532.6914 566.8455 568.9902 633.7809 673.1984 718.4385 726.0723 752.2531 753.9058 780.8494 806.3080 812.8789 828.0757 841.0551 873.3830	1.13618 0.24327 0.21427	0(0)	1	1	Singlet	-	-

			883.9964 897.3452 903.8046 951.6699 961.2396 970.2951 988.9659 992.2013 1045.0470 1057.0622 1063.9014 1123.9988 1167.7204 1171.4901 1184.4778 1211.1723 1213.9994 1228.1712 1234.7449 1248.5195 1268.9745 1303.9568 1364.7038 1374.4609 1411.8799 1443.5071 1458.0281 1471.1870 1530.4613 1556.7125 1605.7171 1629.3918 1646.1219 1663.9013 2086.3750 3072.3152 3153.3282 3157.9691 3169.1024 3170.1845 3176.0323 3183.6319 3196.2214 3214.1739 3232.1448							
*Vibration frequency replaced by			(Vhrd2) 1 0 379.12 105.4	(Ihrd1) 1 0 12.67 4.85 -3.12 -0.48 2.15						

unsymmetrical 1-D hindered rotor (hrd 3 5 1)			-204.66	-0.47						
phenoxy(S6-CS1)	ZPE: -306.822305 Energy: -306.817001	0	185.4723 376.6101 446.3815 479.3320 531.1065 596.9364 647.7147 792.2480 800.7119 804.6808 923.3036 983.3764 987.3146 994.1137 1008.5550 1089.8171 1165.4728 1166.0753 1275.6166 1339.0056 1417.3826 1442.1676 1481.0426 1544.4213 1585.1980 3164.6787 3171.2326 3185.6821 3193.6738 3196.6225	5.51912 2.78930 1.85288	0.7862 (0.75)	2	1	Doublet	5.5077	514.96
S6-CS2	ZPE: -306.745762 Energy: -306.740068	48.0	139.5496 226.4459 457.6320 468.3256 557.2317 602.5758 668.5135 705.7514 726.9632 796.5307 876.6735 908.8947	5.81677 2.56197 2.18128	0.7717 (0.75)	1	1	Doublet	5.5077	514.96

			930.5168 951.5127 1004.1947 1006.2169 1053.1628 1072.7600 1107.5436 1220.8761 1249.1600 1308.7435 1396.3516 1455.6337 1909.0565 3124.5225 3130.3641 3197.2463 3219.9670 3229.0158							
S6-CS3	ZPE: -306.763964 Energy: -306.757807	33.6	44.1663 169.4183 242.4817 431.5085 535.6175 628.6869 689.4604 726.6809 801.3225 814.6417 861.4467 943.0207 956.4076 959.1415 1009.3684 1026.5344 1108.5186 1117.7137 1154.4442 1199.6633 1305.4293 1389.9475 1544.9394 1634.1949 1908.1253 2992.4163 3196.3453 3207.6658 3232.5290 3236.7144	6.47687 2.13970 1.76224	0.7532 (0.75)	1	2	Doublet	5.5077	514.96

S6-CS4	ZPE: -193.438137 Energy: -193.433334	25.2	47.9722 498.2325 513.7050 679.7107 720.5125 818.2636 846.0864 894.5680 900.6908 928.4062 944.0213 1058.4649 1070.9209 1141.7061 1216.6960 1294.5301 1384.7352 1484.6505 1528.1171 3201.1494 3205.5230 3216.9913 3232.9931 3240.7480	9.28591 8.50822 4.44004	0.7679 (0.75)	1	1	Doublet	5.5077	514.96
S6-CS5	ZPE: -306.721185 Energy: -306.713879	63.5	94.0218 112.2050 129.2707 220.6007 378.6915 398.8170 220.6007 378.6915 398.8170 525.6942 600.5714 620.1877 659.3533 688.5927 738.1885 849.9193 854.5885 970.1834 979.8970 1077.2047 1141.1616 1270.1165 1275.3473 1348.0393	7.80109 1.30742 1.11975	0.7659 (0.75)	1	1	Doublet	5.5077	514.96

			1467.9054 1598.3829 1657.4555 2199.0645 3009.4600 3116.7030 3157.8448 3180.2907 3244.6788							
S6-TS12	ZPE: -306.741819 Energy: -306.736506	50.5	-362.4507 208.2182 293.5510 434.9777 511.6426 590.0674 623.0039 702.6298 739.1792 773.4442 869.7245 892.3558 916.0544 963.3750 981.6524 1062.4929 1063.9284 1099.3118 1125.3698 1245.2150 1291.4637 1342.0945 1421.3118 1485.4481 1840.6859 3124.3008 3126.0816 3191.1762 3195.1383 3218.4295	6.16868 2.52249 1.99648	0.7681 (0.75)	1	1	Doublet	-	-
S6-TS15	ZPE: -306.709746 Energy:	70.6	-124.3717 96.7405* 134.8778 182.1664 320.1487 397.5096 482.4382 550.1472 601.1717	4.70939 1.87217 1.48548	0.7658 (0.75)	1	1	Doublet	-	-

	-306.702990		667.2634 718.8907 758.4955 868.8113 876.8343 947.8257 998.3014 1014.7846 1129.4355 1239.9869 1272.8447 1377.8089 1420.0251 1617.8055 1669.3585 2204.6732 3026.2244 3127.9221 3144.8876 3156.9463 3230.7606							
*Vibration frequency replaced by unsymmetrical 1-D hindered rotor (hrd 5 6 1)			(Vhrd2) 1 0 435.15 -214.21 -204.66 78.36 24.64	(Ihrd1) 1 0 11.67 3.48 -1.34 -0.46 0.44 -0.12						
S6-TS23	ZPE: -306.734121 Energy: -306.728674	55.3	-619.9380 152.5677 288.0065 409.8300 434.1091 550.8898 718.4539 753.9894 762.0013 781.9619 829.2843 890.1059 948.3019 974.1193 1001.3928 1067.9230 1072.9313 1084.9766	6.23764 2.41306 2.04830	0.7744 (0.75)	1	1	Doublet	-	-

			1127.2114 1233.8637 1285.4732 1364.6152 1416.8352 1516.4429 1880.5343 3009.7016 3199.5551 3208.3444 3224.2479 3231.9229							
S6-TS53	ZPE: -306.704260 Energy: -306.697816	74.1	-501.0767 91.5053 149.7424 268.2430 394.5511 435.7119 494.9933 581.3118 640.6451 668.7695 713.7815 778.6071 882.3467 907.8591 972.1445 982.6323 1011.3950 1098.7034 1178.4661 1238.8734 1304.3599 1389.7437 1565.6627 1650.3691 2143.7734 3081.2244 3094.4703 3173.9177 3195.7809 3203.5086	6.07642 1.79909 1.48976	0.7742 (0.75)	1	1	Doublet	-	-
S6-TS34	ZPE: -306.757801	40.5	-410.0415 81.9257* 121.0810 195.2638 362.0919 553.8380	4.84129 2.32290	0.7611 (0.75)	1	1	Doublet	-	-

	Energy: -306.751537		579.4640 721.5608 736.6618 789.1417 835.4788 917.1249 932.0065 948.1601 991.6300 993.5409 1039.4620 1100.6044 1134.7563 1271.4952 1299.6431 1389.9380 1495.7968 1575.9631 2011.0670 3187.6315 3201.5589 3212.5696 3230.6192 3236.3480	2.17582						
*Vibration frequency replaced by unsymmetrical 1-D hindered rotor (hrd 3 6 1)			(Vhrd2) 1 0 238.43 102.61 -78.14	(Ihrd1) 1 0 13.47 1.06 -3.12 -0.47 1.34 -0.77						

Note: The relaxed potential energy surface scans calculation were carried out to obtain 1-D hindered rotors based on DFT B3LYP with 6-31G basis set, and the step-sizes is 3 degrees.

Table S20. Cartesian coordinates for optimized structures at B3LYP/6-311+G(d,p) level of theory.

Species	Geometry (Å)

1,2-benzanthracene oxyradicals I	C	-2.83616100	-1.36284100	0.00003700
	C	-4.21722200	-0.93057600	-0.00001400
	C	-4.45357600	0.51845700	0.00003500
	C	-3.42715200	1.39812500	0.00003800
	H	-2.65597800	-2.43241000	0.00006300
	H	-5.48764900	0.84259700	0.00005200
	C	4.77269200	-1.17007400	-0.00000200
	C	4.42706100	0.16515200	-0.00001000
	C	3.07271800	0.56575000	-0.00001600
	C	2.04544900	-0.42059100	-0.00001200
	C	2.43116800	-1.77763000	0.00000800
	C	3.76328100	-2.14686100	0.00001200
	C	2.72291700	1.95646700	-0.00002700
	C	0.65005000	0.01051300	0.00000800
	C	0.35476900	1.41448700	-0.00000900
	C	1.42375800	2.36142600	-0.00003000

	C	-0.98863500	1.84825500	0.00000200
	H	-1.18687500	2.91577600	-0.00000500
	C	-2.04939800	0.96172800	0.00001900
S1-CS2	C	-3.05216000	-1.12477900	-0.58135900
	C	-4.06155600	-1.02514300	0.49893400
	C	-4.19032200	-0.00548100	-0.58089400
	C	-3.46065800	1.26448100	-0.36857500
	H	-3.09560100	-1.99202100	-1.23351800
	H	-5.06306000	-0.05523100	-1.22700000
	C	4.67828800	-1.20701600	0.07010100
	C	4.34983800	0.12457600	0.21504100
	C	3.00713900	0.55676700	0.15196700
	C	1.96716700	-0.39618400	-0.06519700
	C	2.33935200	-1.75451700	-0.21008000
	C	3.65955000	-2.15209100	-0.14457900
	C	2.67660000	1.94324300	0.30537300

	C	0.59086100	0.05723200	-0.12701900
	C	0.30668900	1.45170300	0.03022200
	C	1.38985900	2.36935400	0.24746100
	C	-1.01724400	1.92369600	-0.02849300
	H	-1.20690900	2.98490500	0.09234400
	C	-2.07628700	1.03614400	-0.25352700
	C	-1.78196100	-0.36492800	-0.39706600
	C	-0.49904300	-0.83588500	-0.33466400
	H	3.48284900	2.65020200	0.47055700
	H	5.71331500	-1.52494800	0.12132300
	H	5.12609100	0.86420500	0.38195600
	H	1.58150000	-2.50899300	-0.37578500
	H	3.91087200	-3.20052600	-0.25904400
	H	1.15373200	3.42165900	0.36540700
	H	-0.31844800	-1.89737900	-0.44262000
	H	-3.95734600	2.21864200	-0.26034400

	O	-4.53545900	-1.51594400	1.47510800
S1-CS3	C	-2.85360000	-1.37997400	-0.64494100
	C	-4.82424100	-0.82578300	0.66950100
	C	-4.03307800	-0.44526100	-0.67084200
	C	-3.45583400	0.91492000	-0.57317000
	H	-2.93123900	-2.45495000	-0.71608500
	H	-4.74344000	-0.61414900	-1.48128700
	C	4.80211100	-1.01104800	0.22432900
	C	4.37292700	0.30465400	0.26995200
	C	3.01024100	0.63005700	0.14668700
	C	2.05100200	-0.40193300	-0.02774800
	C	2.51466500	-1.72891600	-0.07076100
	C	3.86242800	-2.03276700	0.05230600
	C	2.58240600	2.01079000	0.19726600
	C	0.62455400	-0.05358900	-0.15659800
	C	0.24562100	1.36672800	-0.10001700

	C	1.28172400	2.35458200	0.08111600
	C	-1.07194100	1.76020600	-0.21201600
	H	-1.32058200	2.81521600	-0.16447700
	C	-2.09744400	0.79686900	-0.39729300
	C	-1.72522700	-0.62765600	-0.45090400
	C	-0.35621600	-1.00354500	-0.32238300
	H	3.34142100	2.77412300	0.33262200
	H	5.85563900	-1.24687200	0.32109800
	H	5.09058600	1.10756400	0.40306600
	H	1.81514700	-2.54412800	-0.20260100
	H	4.18455400	-3.06721600	0.01469600
	H	0.98347000	3.39685000	0.12228900
	H	-0.11136300	-2.05709900	-0.36285400
	H	-4.04171600	1.82240300	-0.55422800
	O	-4.71288300	-0.46271800	1.77510500
S1-CS4	C	3.44162600	-1.64840300	0.00024100

	C	4.56313800	-0.80575400	0.00009600
	C	4.14339700	0.53052900	-0.00015900
	H	3.45615400	-2.72990900	0.00081300
	H	5.59226700	-1.13712000	0.00030600
	C	-4.28536300	-0.82971600	0.00004100
	C	-3.80170700	0.45956200	0.00013500
	C	-2.41098700	0.71929600	0.00007000
	C	-1.48867700	-0.37099700	-0.00006600
	C	-2.02146600	-1.68295300	-0.00019900
	C	-3.38209200	-1.90930200	-0.00014900
	C	-1.91821400	2.06082100	0.00010400
	C	-0.06353000	-0.09557500	-0.00003000
	C	0.37981800	1.26083100	-0.00002500
	C	-0.58083800	2.31733900	0.00003100
	C	1.77119100	1.56344600	-0.00002600
	H	2.07823700	2.60490100	0.00018800

	C	2.69825100	0.54859600	-0.00029400
	C	2.25692700	-0.82349000	-0.00008600
	C	0.91359600	-1.12957700	0.00011900
	H	-2.63429900	2.87577900	0.00018300
	H	-5.35348500	-1.01458700	0.00009700
	H	-4.48640100	1.30142400	0.00025500
	H	-1.35615400	-2.53638700	-0.00042400
	H	-3.75724400	-2.92655100	-0.00026500
	H	-0.22055200	3.34091800	0.00004500
	H	0.60669000	-2.16796800	0.00044500
	H	4.78437800	1.40157100	-0.00046200
S1-CS5	C	-2.21041600	-2.21717900	-0.00047000
	C	-5.70961700	-0.02658200	0.00034400
	C	-4.42356600	-0.35128900	-0.00010100
	C	-3.34521500	0.58828700	-0.00014800
	H	-2.02743300	-3.28153000	-0.00053100

	H	-4.21557100	-1.42214100	-0.00030100
	C	5.14249500	-0.58763900	0.00033300
	C	4.54989400	0.66398300	0.00019300
	C	3.15061500	0.80765100	0.00003900
	C	2.32565700	-0.34883400	0.00000900
	C	2.95316300	-1.60708200	0.00016500
	C	4.33480800	-1.72991700	0.00032500
	C	2.55104200	2.12508700	-0.00005900
	C	0.86118200	-0.18614200	-0.00015100
	C	0.31057900	1.16585700	-0.00018200
	C	1.21006600	2.29174400	-0.00014700
	C	-1.05207600	1.34759000	-0.00023400
	H	-1.44031700	2.36169000	-0.00022400
	C	-1.99812600	0.27698700	-0.00026100
	C	-1.45379300	-1.09997100	-0.00034600
	C	-0.00918300	-1.24466500	-0.00026500

	H	3.21219400	2.98519000	-0.00003800
	H	6.22246300	-0.68133500	0.00045600
	H	5.16538200	1.55772100	0.00021000
	H	2.35638600	-2.51030300	0.00018200
	H	4.78630000	-2.71555700	0.00045200
	H	0.77943400	3.28774600	-0.00019100
	H	0.36431300	-2.26001300	-0.00029900
	H	-3.60783600	1.64098100	-0.00003200
	O	-6.84004700	0.22878100	0.00075600
S1-TS12	C	-2.98668800	-1.17029300	-0.44337000
	C	-4.12311500	-0.99120000	0.43495900
	C	-4.26182900	0.17914900	-0.44830900
	C	-3.41144400	1.33928900	-0.36117700
	H	-2.97422000	-2.06777000	-1.05839700
	H	-5.19011100	0.21452400	-1.01496700
	C	4.69214900	-1.24510300	0.04227300

	C	4.38059400	0.09163100	0.17454100
	C	3.04103200	0.53678400	0.13255600
	C	1.98848200	-0.40899100	-0.05018200
	C	2.34302500	-1.77277000	-0.18182100
	C	3.66021300	-2.18300600	-0.13731300
	C	2.72853000	1.92907400	0.27365800
	C	0.61480300	0.05927500	-0.09069100
	C	0.35069000	1.45781600	0.05522800
	C	1.44530800	2.36821800	0.23686800
	C	-0.97077900	1.93676600	0.00492100
	H	-1.15056400	3.00293800	0.09595300
	C	-2.03893800	1.05880000	-0.18551400
	C	-1.77468100	-0.34521400	-0.29985900
	C	-0.48572800	-0.82046500	-0.27140100
	H	3.54559300	2.62911200	0.41248300
	H	5.72475300	-1.57292400	0.07722700

	H	5.16757500	0.82530800	0.31492000
	H	1.57422200	-2.52185600	-0.31911800
	H	3.89869700	-3.23552300	-0.24050600
	H	1.22214000	3.42438000	0.34490900
	H	-0.31629700	-1.88398500	-0.37788700
	H	-3.81580000	2.33501300	-0.49159400
	O	-4.85446600	-1.65847200	1.11809600
S1-TS15	C	-2.53109500	-1.76947300	-0.49087300
	C	-5.12797300	-0.39148100	0.42061500
	C	-4.51236300	0.15380500	-0.60335500
	C	-3.36084200	1.06354000	-0.41662300
	H	-2.41132000	-2.84249900	-0.56912000
	H	-4.93325300	-0.04577200	-1.58746100
	C	4.94528800	-0.92930700	0.18412300
	C	4.47679700	0.37321900	0.23664900
	C	3.10285800	0.65635300	0.14230700

	C	2.17362500	-0.40636600	-0.01047000
	C	2.67537800	-1.71847300	-0.06023100
	C	4.03460400	-1.98016200	0.03460100
	C	2.63253300	2.02461800	0.20190200
	C	0.73672000	-0.09609600	-0.11005300
	C	0.31556900	1.30455400	-0.04212300
	C	1.31976000	2.32931800	0.11626100
	C	-1.01433100	1.63159000	-0.12945400
	H	-1.30315000	2.67660000	-0.07665000
	C	-2.05777500	0.65856000	-0.29186000
	C	-1.64428100	-0.76422400	-0.34807800
	C	-0.22722200	-1.05754900	-0.26093700
	H	3.37119200	2.81054800	0.31975500
	H	6.00749200	-1.13197500	0.25856400
	H	5.17249800	1.19779900	0.35319200
	H	1.99719100	-2.55438500	-0.17455100

	H	4.38794900	-3.00419600	-0.00733600
	H	0.98934100	3.36155600	0.16469900
	H	0.04483600	-2.10366500	-0.31283200
	H	-3.56772100	2.13064300	-0.41102800
	O	-5.67232200	-0.87365200	1.32604600
S1-TS23	C	-2.87408600	-1.43432400	-0.65025900
	C	-4.46798000	-0.49770400	0.69006900
	C	-4.07139700	-0.53813400	-0.70565700
	C	-3.50989500	0.85572900	-0.55146100
	H	-2.94959000	-2.51131700	-0.63868900
	H	-4.87351600	-0.74714300	-1.42129200
	C	4.78546100	-0.97979600	0.22198500
	C	4.35287500	0.33135700	0.25791800
	C	2.98519200	0.65325800	0.13434200
	C	2.02710700	-0.38687000	-0.03126100
	C	2.50073900	-1.71580200	-0.06432300

	C	3.84690100	-2.01004900	0.05902800
	C	2.54924900	2.02217700	0.17402000
	C	0.61010800	-0.04756300	-0.16005400
	C	0.22323300	1.34606100	-0.11357200
	C	1.23722800	2.34685300	0.05686400
	C	-1.12309200	1.72112400	-0.22501100
	H	-1.38428600	2.77308200	-0.17913800
	C	-2.11373600	0.75516300	-0.40194100
	C	-1.73185300	-0.65139300	-0.45508900
	C	-0.38265900	-1.01732600	-0.31992700
	H	3.29790900	2.79712000	0.30107700
	H	5.83991600	-1.21202000	0.31870800
	H	5.06715500	1.13872400	0.38347200
	H	1.80456700	-2.53498300	-0.18906600
	H	4.17562300	-3.04287500	0.02919200
	H	0.92592700	3.38586700	0.09001200

	H	-0.12863300	-2.06873100	-0.35349400
	H	-4.12072100	1.74393300	-0.59396500
	O	-4.58934100	-0.52977900	1.84489500
S1-TS34	C	-2.90143800	-1.32883000	-0.74856100
	C	-4.77699700	-0.54892700	0.82439100
	C	-4.03689400	-0.42437900	-0.71188500
	C	-3.47053900	0.95869200	-0.57291800
	H	-2.97336800	-2.40167500	-0.85193800
	H	-4.87226200	-0.57442500	-1.38978700
	C	4.75879700	-1.03782300	0.19910100
	C	4.34411900	0.27974400	0.27975600
	C	2.98482900	0.62439500	0.15957400
	C	2.01485000	-0.39402800	-0.04904100
	C	2.46664700	-1.72613400	-0.12648600
	C	3.80909800	-2.04630000	-0.00578900
	C	2.57186800	2.00526700	0.24795300

	C	0.59795000	-0.02999900	-0.17550400
	C	0.23400600	1.38355500	-0.07766100
	C	1.27304600	2.36034700	0.13648900
	C	-1.08509600	1.78577300	-0.18527600
	H	-1.33132600	2.83956500	-0.10602000
	C	-2.10912600	0.83158400	-0.40462200
	C	-1.74984200	-0.58917100	-0.50242500
	C	-0.39776700	-0.97452200	-0.37800100
	H	3.33637600	2.75803600	0.40829100
	H	5.80935700	-1.28755900	0.29396800
	H	5.06974000	1.07067300	0.43881400
	H	1.75924800	-2.52978100	-0.28347800
	H	4.12192800	-3.08226500	-0.07023400
	H	0.98025000	3.40271200	0.20642300
	H	-0.15528100	-2.02670100	-0.45170600
	H	-4.06302000	1.86147200	-0.54722800

	O	-4.35583900	-0.85068900	1.86229100
S1-TS53	C	-2.60687700	-1.63978100	-0.33875300
	C	-5.34598700	-0.31550200	0.27212400
	C	-4.25004900	-0.18631500	-0.50033800
	C	-3.33382100	0.95803300	-0.30023400
	H	-2.58660300	-2.72209600	-0.39598000
	H	-4.36746800	-0.61981300	-1.49699500
	C	4.97785300	-0.95804300	0.17766900
	C	4.52243700	0.35022800	0.19338300
	C	3.15011000	0.64354200	0.11022900
	C	2.20790600	-0.41301700	0.00772300
	C	2.69653500	-1.73072700	-0.00600600
	C	4.05466900	-2.00332500	0.07699600
	C	2.69452900	2.01823400	0.12925400
	C	0.77006100	-0.09448400	-0.07785400
	C	0.36369100	1.31791900	-0.05568900

	C	1.38471500	2.33404700	0.05158700
	C	-0.96134200	1.66808900	-0.13777200
	H	-1.23562000	2.71826100	-0.12390700
	C	-1.99615900	0.68719200	-0.24345300
	C	-1.60441700	-0.73772200	-0.26812400
	C	-0.19944800	-1.05682400	-0.18023800
	H	3.44293700	2.79979500	0.20881800
	H	6.03907800	-1.16889900	0.24283000
	H	5.22758100	1.17137500	0.27107900
	H	2.00892800	-2.56317000	-0.08244500
	H	4.39688300	-3.03193000	0.06363100
	H	1.06689900	3.37127400	0.06762600
	H	0.06182500	-2.10691300	-0.20236400
	H	-3.72454400	1.96339000	-0.20495200
	O	-6.18454100	-0.60756600	1.02370400
1,2-benzanthracene oxyradicals II	C	2.83980500	-2.00498800	0.00011100

	C	4.19624100	-1.73949100	0.00045100
	C	4.65731700	-0.41245500	0.00049800
	C	3.75107100	0.63888400	0.00022900
	H	2.48294100	-3.02963500	-0.00003800
	H	5.72239800	-0.21113800	0.00067400
	C	-4.68941500	-0.89439300	0.00017100
	C	-4.20016400	0.39235600	0.00042300
	C	-2.80688800	0.64342500	0.00027200
	C	-1.89346000	-0.45340200	-0.00012000
	C	-2.42989000	-1.76081300	-0.00038700
	C	-3.79290700	-1.97912100	-0.00024700
	C	-2.30541000	1.97884400	0.00048100
	C	-0.46190600	-0.17854900	-0.00021800
	C	-0.02440300	1.17255200	-0.00011900
	C	-0.95882500	2.23027300	0.00024000
	C	1.41543500	1.51249900	-0.00052000

	H	4.90728300	-2.55788000	0.00032900
	C	2.37473800	0.38936200	-0.00008700
	C	1.89755400	-0.94795600	-0.00014200
	C	0.49976600	-1.20498200	-0.00032200
	H	-3.01556500	2.79898100	0.00080600
	H	-5.75837500	-1.07387300	0.00028400
	H	-4.87981700	1.23797000	0.00073100
	H	-1.77012900	-2.61860700	-0.00072900
	H	-4.17415200	-2.99393000	-0.00047100
	H	-0.57299600	3.24204000	0.00029300
	H	0.18848800	-2.24154200	-0.00037000
	H	4.08412500	1.66968700	0.00015900
	O	1.79673200	2.68570700	-0.00074300
S2-CS2	C	3.30251400	-1.54732600	-0.00014200
	C	4.44407000	-0.74048200	-0.00004000
	C	4.33350300	0.65186000	0.00012900

	C	3.07541400	1.27460300	0.00021200
	H	3.39510200	-2.62822400	-0.00021100
	H	5.23071000	1.26038300	0.00020500
	C	-4.46576400	-0.28781100	0.00004400
	C	-3.73012800	0.87623800	-0.00011500
	C	-2.31303200	0.84579700	-0.00012300
	C	-1.64763700	-0.42316700	0.00001400
	C	-2.43012500	-1.59937700	0.00015900
	C	-3.80816400	-1.53557300	0.00018600
	C	-1.54717600	2.04830500	-0.00016200
	C	-0.21384700	-0.42279500	0.00000800
	C	0.50746400	0.80622100	0.00010100
	C	-0.16366900	2.03304200	-0.00002000
	H	5.42620700	-1.19936700	-0.00011200
	C	1.93690900	0.48504600	0.00006800
	C	2.04582100	-0.93868500	-0.00010300

	C	0.71610200	-1.48942700	-0.00024200
	H	-2.07705000	2.99500500	-0.00031700
	H	-5.54904700	-0.24871000	0.00000800
	H	-4.23083400	1.83902100	-0.00020200
	H	-1.93760900	-2.56505300	0.00034300
	H	-4.39099200	-2.44991000	0.00036200
	H	0.38913900	2.96625500	0.00005900
	H	0.48317900	-2.54555500	-0.00034500
	H	3.00767200	2.35734400	0.00036700
S2-TS12	C	3.01537400	1.86252700	0.09177500
	C	4.11789300	1.26704300	-0.44191200
	C	4.06153600	-0.07641100	-0.99414000
	C	2.96448000	-0.85311700	-0.87797900
	H	3.03836500	2.90458800	0.39256900
	H	4.92943400	-0.44788000	-1.52830900
	C	-4.66708300	0.35010600	-0.16167800

	C	-3.90646900	-0.78009100	-0.39422100
	C	-2.50025100	-0.74440600	-0.30198900
	C	-1.85707800	0.49036700	0.03443200
	C	-2.66037600	1.63298600	0.26267300
	C	-4.03549200	1.56384100	0.16906500
	C	-1.70908500	-1.91862700	-0.56066900
	C	-0.43126100	0.50903600	0.09883400
	C	0.30766900	-0.72566000	-0.00360100
	C	-0.35477800	-1.92785000	-0.43331200
	C	1.49301600	-1.03002200	1.21748700
	H	5.04576100	1.82058200	-0.52565500
	C	1.83925800	-0.35364600	-0.05210600
	C	1.78216700	1.13954400	0.15673200
	C	0.47990000	1.58369700	0.24763000
	H	-2.22504600	-2.82034700	-0.87371200
	H	-5.74757700	0.30394000	-0.23281100

	H	-4.38932300	-1.71749000	-0.65050400
	H	-2.18689300	2.57300600	0.52141100
	H	-4.63358800	2.44937400	0.35257100
	H	0.21640100	-2.83140700	-0.61248900
	H	0.20518200	2.61829800	0.40577600
	H	2.92802600	-1.85668900	-1.28462400
	O	1.89784300	-1.86648600	1.96170500
1,2-benzanthracene oxyradicals III	C	-3.07139500	-1.68182200	0.00003000
	C	-4.40918300	-1.38962400	0.00002800
	C	-4.84994600	-0.03699800	0.00003300
	C	-3.94373700	0.99065900	0.00001900
	H	-2.72975900	-2.71125700	0.00003800
	H	-5.91305800	0.17618000	0.00004300
	C	4.53744800	-0.54966800	-0.00000800
	C	3.97320500	0.73136800	-0.00001500
	C	2.57160900	0.93259500	-0.00001500

	C	1.67600200	-0.16451200	-0.00000800
	C	2.26289700	-1.52773900	-0.00000700
	C	3.71358800	-1.64670300	-0.00000500
	C	2.07012600	2.28043800	-0.00002100
	C	0.24934500	0.08859000	-0.00000400
	C	-0.21442600	1.46237900	-0.00001000
	C	0.73968700	2.53178300	-0.00001900
	C	-1.57830300	1.74107000	-0.00000300
	H	-1.90149400	2.77761600	-0.00000600
	C	-2.54378200	0.72483600	0.00000800
	C	-2.09508300	-0.63990400	0.00001600
	C	-0.72168200	-0.92363700	0.00001000
	H	2.78652300	3.09471200	-0.00002800
	H	5.61543200	-0.66623700	-0.00000600
	H	4.61724000	1.60415300	-0.00002100
	H	-5.14185500	-2.18863400	0.00004700

	H	4.09860500	-2.65938600	-0.00000400
	H	0.37037700	3.55189000	-0.00002500
	H	-0.39940700	-1.95331400	0.00001500
	H	-4.28064800	2.02204200	0.00001800
	O	1.58497900	-2.57330400	-0.00002900
S3-CS2	C	3.03015100	-1.62852200	-0.36910000
	C	4.36668900	-1.30598500	-0.31321100
	C	4.76937200	0.02927000	-0.07351300
	C	3.82948200	1.01579000	0.10566200
	H	2.72137500	-2.65282600	-0.55053800
	H	5.82545800	0.27072800	-0.03153800
	C	-3.89555300	-0.92382100	-0.94602100
	C	-3.94593100	0.41402300	-0.68472700
	C	-2.70156000	0.89496000	-0.18742300
	C	-1.76396000	-0.24619100	-0.02110000
	C	-2.23961900	-1.40473200	0.83085800

	C	-2.57036100	-1.51507500	-0.59538200
	C	-2.25229000	2.19269900	0.06628300
	C	-0.30669300	0.03779600	-0.05581800
	C	0.09013700	1.40592600	0.17341100
	C	-0.90941700	2.43837100	0.28906700
	C	1.44729900	1.70382000	0.22729800
	H	1.75506400	2.73120600	0.39659500
	C	2.44087700	0.71647600	0.05461100
	C	2.03542900	-0.63532200	-0.18854400
	C	0.64880200	-0.93390200	-0.23317000
	H	-2.95746600	3.01707400	0.04523600
	H	-4.70987400	-1.53318300	-1.31377900
	H	-4.81641300	1.03863900	-0.83952800
	H	5.11748400	-2.07561700	-0.45177600
	H	-2.12515700	-2.30881600	-1.19232100
	H	-0.57118500	3.45081800	0.47834400

	H	0.35406900	-1.96420400	-0.40781500
	H	4.13689800	2.04001500	0.28945200
	O	-2.14592400	-1.94341300	1.88782200
S3-CS3	C	-2.90016900	1.68920700	-0.27349700
	C	-4.24656700	1.46680200	-0.18562600
	C	-4.75014500	0.15160700	0.03022200
	C	-3.89244100	-0.90652400	0.15274900
	H	-2.51691100	2.69118100	-0.43529800
	H	-5.82089100	-0.00421400	0.09734000
	C	3.97819200	0.59991600	-0.42214500
	C	3.96351100	-0.72912900	-0.21527300
	C	2.58234400	-1.19277100	-0.07136400
	C	1.73158900	-0.10790100	-0.19292500
	C	2.42224200	2.14465100	0.75307000
	C	2.56037200	1.13656500	-0.40956600
	C	2.07507200	-2.50348100	0.14220300

	C	0.31828900	-0.25096400	-0.11274600
	C	-0.19316700	-1.58850400	0.10476800
	C	0.72202300	-2.68304800	0.22819900
	C	-1.57535500	-1.78004300	0.18840800
	H	-1.95884300	-2.78272200	0.35165000
	C	-2.47887300	-0.71894800	0.06736600
	C	-1.96870200	0.61222500	-0.15141400
	C	-0.58635400	0.81011600	-0.23667200
	H	2.75286400	-3.34459900	0.23540400
	H	4.84415100	1.23118000	-0.56154000
	H	4.83327500	-1.37259800	-0.17452100
	H	-4.94145000	2.29374500	-0.27889400
	H	2.30984400	1.67072600	-1.33487100
	H	0.31281800	-3.67441100	0.39182200
	H	-0.21729300	1.81679100	-0.40144800
	H	-4.27422000	-1.90868000	0.31787600

	O	2.26318500	3.31061900	0.67724200
S3-CS4	C	-2.87711900	-1.65593000	-0.00024200
	C	-4.18090400	-1.23615400	-0.00008500
	C	-4.49468800	0.15201000	0.00021600
	C	-3.49324300	1.08484900	0.00036600
	H	-2.64177900	-2.71513800	-0.00051300
	H	-5.53259700	0.46487000	0.00031600
	C	4.06192400	-1.57826500	0.00046500
	C	4.28875300	-0.22637800	0.00002200
	C	2.98437600	0.44750400	-0.00032100
	C	1.97819700	-0.55250300	-0.00018000
	C	2.64126500	-1.80459700	0.00038700
	C	2.65576300	1.80703400	-0.00028000
	C	0.58796100	-0.19770900	-0.00021200
	C	0.26828700	1.21740100	0.00000300
	C	1.32145000	2.17967100	-0.00003500

	C	-1.07389700	1.61594400	0.00013400
	H	-1.30748400	2.67649600	0.00037300
	C	-2.12152600	0.68876900	0.00014000
	C	-1.80314500	-0.71704700	-0.00016500
	C	-0.45811200	-1.11820300	-0.00040100
	H	3.43253600	2.56432500	-0.00036700
	H	4.81298900	-2.35507300	0.00081700
	H	5.24770400	0.27304900	-0.00008900
	H	-4.98513500	-1.96341800	-0.00025400
	H	2.17097000	-2.77893000	0.00072900
	H	1.05450400	3.23122600	0.00015100
	H	-0.23616400	-2.18020200	-0.00062100
	H	-3.72760100	2.14442200	0.00058600
S3-TS12	C	3.01771500	-1.62951000	-0.28146200
	C	4.35447400	-1.30738700	-0.28959100
	C	4.76674700	0.04022900	-0.14993100

	C	3.83511600	1.03893200	-0.00349200
	H	2.70179900	-2.66222900	-0.38530400
	H	5.82401300	0.27987500	-0.15773400
	C	-4.00830400	-0.79203300	-0.91447800
	C	-3.98756000	0.50853800	-0.51480800
	C	-2.70385000	0.90026100	-0.04035300
	C	-1.76268600	-0.22739900	0.07409700
	C	-2.20838100	-1.50766200	0.68079300
	C	-2.76705000	-1.53916000	-0.65779900
	C	-2.23755000	2.20454700	0.17986200
	C	-0.31109900	0.06032500	0.01834900
	C	0.10043100	1.43469300	0.16670400
	C	-0.89052600	2.46828200	0.30480500
	C	1.45826000	1.73546900	0.16059000
	H	1.76885600	2.76968200	0.27408200
	C	2.44504400	0.74047000	0.00968700

	C	2.02900000	-0.62282000	-0.13381100
	C	0.64483300	-0.92203500	-0.11744700
	H	-2.95286500	3.02031800	0.19157700
	H	-4.85473400	-1.28903700	-1.37188900
	H	-4.82755100	1.18697000	-0.58552200
	H	5.10002300	-2.08637600	-0.40158400
	H	-2.42792400	-2.32821700	-1.32720500
	H	-0.54912400	3.48741000	0.44714000
	H	0.34667400	-1.96064200	-0.21402500
	H	4.14948000	2.07170600	0.10540100
	O	-1.86579000	-2.24898800	1.55934700
S3-TS23	C	2.99303100	-1.61078600	-0.40306600
	C	4.32801200	-1.30635600	-0.31272000
	C	4.74386400	0.02067000	-0.02848500
	C	3.81596800	1.01273700	0.15892800
	H	2.67503000	-2.62583000	-0.61725100

	H	5.80221000	0.24562100	0.04013900
	C	-3.93880500	-0.89441700	-0.74910200
	C	-3.98857800	0.44283700	-0.51087000
	C	-2.69032400	0.94703800	-0.17804300
	C	-1.76881500	-0.15199500	-0.14002300
	C	-2.24362000	-1.59310700	0.78439300
	C	-2.53385300	-1.42623700	-0.61726200
	C	-2.24624400	2.25352300	0.09928500
	C	-0.33555000	0.09235000	-0.10727000
	C	0.07989100	1.45090700	0.16326700
	C	-0.90480600	2.49020700	0.29113800
	C	1.44330400	1.72815800	0.25172000
	H	1.76075500	2.74612000	0.45631000
	C	2.42120900	0.73477300	0.07291500
	C	2.00143700	-0.60859200	-0.21456700
	C	0.62240400	-0.89074800	-0.29481400

	H	-2.95898400	3.06987500	0.14265900
	H	-4.77474000	-1.54849800	-0.95347000
	H	-4.89107500	1.04058300	-0.52929000
	H	5.07312900	-2.08053100	-0.45679300
	H	-2.14114000	-2.11694400	-1.37270700
	H	-0.55642300	3.49575200	0.49933900
	H	0.31999200	-1.91290700	-0.49846000
	H	4.13239400	2.02765000	0.37611400
	O	-1.90403700	-2.31083100	1.66510900
S3-TS34	C	-2.90860100	1.75482400	-0.35497000
	C	-4.25830100	1.57596400	-0.22361900
	C	-4.79197100	0.28927400	0.07520000
	C	-3.95962400	-0.78418300	0.23455800
	H	-2.50354200	2.73564000	-0.58140800
	H	-5.86449400	0.16751200	0.17585400
	C	3.91195100	0.47866300	-0.61151800

	C	3.89040500	-0.84556700	-0.31392600
	C	2.50274000	-1.26914300	-0.11215800
	C	1.67498700	-0.16430700	-0.29279700
	C	2.55326700	2.15263900	0.96386500
	C	2.53368100	0.99845400	-0.56585500
	C	1.96546400	-2.54352500	0.19330700
	C	0.26039200	-0.26431400	-0.17086300
	C	-0.28157300	-1.57227900	0.13810600
	C	0.60603200	-2.68090500	0.31236000
	C	-1.66668200	-1.71947000	0.26473100
	H	-2.07282600	-2.69974200	0.49563600
	C	-2.54399000	-0.64181100	0.10538500
	C	-2.00319100	0.66084800	-0.19712800
	C	-0.61784400	0.81305900	-0.32652800
	H	2.61980900	-3.39809400	0.32614600
	H	4.78220100	1.08415700	-0.81959400

	H	4.75060800	-1.49904800	-0.25009600
	H	-4.93250000	2.41619300	-0.34609400
	H	2.21884600	1.77938400	-1.25194500
	H	0.17485300	-3.64907100	0.54421000
	H	-0.22387900	1.79791400	-0.55482500
	H	-4.36380000	-1.76499100	0.46283700
	O	3.02648600	3.20010200	0.88629800
1,2-benzanthracene oxyradicals IV	C	3.08649800	-1.53912100	0.00013600
	C	4.42128500	-1.15640400	0.00030300
	C	4.76744500	0.20547700	0.00007400
	C	3.77951400	1.17089000	-0.00007100
	H	2.80186100	-2.58388100	0.00016200
	H	5.81144900	0.49770100	0.00005400
	C	-4.61569600	-0.75963900	0.00010800
	C	-4.14522600	0.53425200	0.00012900
	C	-2.75860100	0.80477900	0.00006800

	C	-1.81259600	-0.27641600	-0.00002800
	C	-2.33924600	-1.59896900	-0.00006500
	C	-3.69883200	-1.82734300	0.00000000
	C	-2.29773600	2.15491500	0.00008000
	C	-0.40146400	0.03067500	-0.00007100
	C	0.00878800	1.39321300	-0.00007400
	C	-0.96994900	2.43923200	-0.00001500
	C	1.37235100	1.75496300	-0.00012800
	H	1.62703700	2.80983100	-0.00018700
	C	2.41277400	0.79889600	-0.00006200
	C	2.07055700	-0.57749300	-0.00000400
	C	0.65041300	-1.01608500	-0.00012900
	H	-3.03233700	2.95334800	0.00016000
	H	-5.68202800	-0.95538200	0.00016600
	H	-4.83615000	1.37083600	0.00023500
	H	5.19998000	-1.91052500	0.00034200

	H	-4.06406600	-2.84834600	-0.00001300
	H	-0.62486000	3.46743300	-0.00002400
	H	-1.65061500	-2.42755400	-0.00016200
	H	4.03966400	2.22412600	-0.00019700
	O	0.40354800	-2.22656400	-0.00025400
S4-CS2	C	-1.89514300	-1.62878800	-0.00000500
	C	-3.28220400	-1.84853500	-0.00007300
	C	-4.18360100	-0.78384100	0.00001100
	C	-3.71526700	0.53090000	0.00010100
	H	-1.23838700	-2.48780300	0.00002800
	H	-5.24973400	-0.97928800	0.00008200
	C	3.90822300	-1.28975800	0.00014700
	C	3.68605000	0.06917300	0.00007800
	C	2.37494100	0.60079400	-0.00002900
	C	1.25149100	-0.30322400	-0.00007600
	C	1.52360800	-1.69930900	-0.00009700

	C	2.81288700	-2.17943300	0.00003200
	C	2.16476100	2.01305000	-0.00006900
	C	-0.05182100	0.26057900	-0.00005100
	C	-0.21464700	1.67365100	-0.00008200
	C	0.90451900	2.54464200	-0.00009800
	C	-1.59898200	1.98681300	0.00012400
	H	-2.02282800	2.98241800	0.00020200
	C	-2.33774100	0.76157800	0.00004000
	C	-1.40538200	-0.32861500	-0.00004200
	H	3.03446700	2.66135800	-0.00009500
	H	4.92043600	-1.67777000	0.00030100
	H	4.52406300	0.75856500	0.00012100
	H	-3.65499200	-2.86657300	-0.00011200
	H	2.98898800	-3.24927000	0.00001800
	H	0.75494400	3.61890900	-0.00004400
	H	0.70377900	-2.40199400	-0.00024300

	H	-4.41089100	1.36338400	0.00027700
S4-TS12	C	1.86171400	-1.52903500	-0.67653700
	C	3.18947900	-1.62692500	-0.89481400
	C	4.10660900	-0.54366300	-0.58288100
	C	3.65248300	0.67695800	-0.19098900
	H	1.19029000	-2.34226900	-0.91838100
	H	5.16751300	-0.70548300	-0.73384400
	C	-4.02171500	-1.19883500	-0.37451900
	C	-3.79490300	0.16145800	-0.32356000
	C	-2.49040300	0.68244200	-0.16430300
	C	-1.39618200	-0.23250500	-0.06157900
	C	-1.65623700	-1.61566500	-0.10387100
	C	-2.94438700	-2.09385700	-0.26223900
	C	-2.26175500	2.09712600	-0.12720200
	C	-0.07505800	0.33993600	0.12506800
	C	0.11879800	1.76490300	-0.00081800

	C	-0.99496300	2.62497900	-0.05757000
	C	1.50778000	2.05364100	-0.03606800
	H	1.92866000	3.05103300	-0.05395300
	C	2.24445500	0.89299400	-0.03594900
	C	1.35008600	-0.32497000	0.02419600
	C	0.83292400	-0.42089400	1.41093100
	H	-3.12173600	2.75457700	-0.19070100
	H	-5.02997800	-1.57797900	-0.49598300
	H	-4.62484500	0.85570500	-0.40410800
	H	3.59526000	-2.53196400	-1.33384900
	H	-3.12213900	-3.16259800	-0.29249800
	H	-0.84480600	3.69908300	-0.07008300
	H	-0.84315000	-2.32152900	0.00916400
	H	4.33417400	1.51231400	-0.07176300
	O	0.74980200	-1.18492500	2.31902800
3H-cydopenta[a]anthracene oxyradicals	C	3.16596400	-1.40147300	0.00000200

	C	4.33496400	-0.52595100	0.00002500
	C	3.75297800	0.80956200	0.00000100
	H	3.23562800	-2.48292100	0.00001300
	C	-4.57806100	-1.00725600	0.00000300
	C	-4.18059000	0.30422900	-0.00000400
	C	-2.80221300	0.65194100	-0.00000600
	C	-1.80695400	-0.38992400	-0.00000300
	C	-2.26573500	-1.73888200	0.00000600
	C	-3.60522800	-2.03719200	0.00000800
	C	-2.39075100	2.00095600	-0.00001300
	C	-0.42436900	-0.03080600	-0.00000300
	C	-0.05797900	1.33180900	-0.00000900
	C	-1.05134400	2.32969500	-0.00001300
	C	1.35274600	1.70845500	-0.00000400
	H	1.60185200	2.76463300	0.00000100
	C	2.32033200	0.75310500	-0.00000600

	C	1.94983700	-0.64932200	0.00000000
	C	0.63930100	-1.02748300	0.00001200
	H	-3.14419800	2.78095400	-0.00001600
	H	-5.63155000	-1.26158500	0.00000600
	H	-4.91484800	1.10271700	-0.00000700
	H	-1.55322900	-2.55267200	0.00001000
	H	-3.92439500	-3.07320300	0.00001400
	H	-0.74905100	3.37144900	-0.00001600
	H	0.38914200	-2.08034100	0.00002900
	H	4.34526600	1.71658400	0.00001300
	O	5.52849900	-0.84679900	-0.00000400
S5-CS2	C	-3.30784500	-1.15530100	-0.50342200
	C	-4.26493700	-0.54579900	0.42700600
	C	-3.75950700	0.53762000	-0.42403200
	H	-3.62958000	-1.92530600	-1.19656800
	C	4.55620000	-1.00640800	0.15362900

	C	4.13967700	0.30518200	0.19773200
	C	2.76776200	0.64026400	0.11156900
	C	1.79517000	-0.39407800	-0.02443800
	C	2.25878300	-1.73137800	-0.06328700
	C	3.60217900	-2.03250800	0.02208500
	C	2.34501300	2.00460300	0.16058700
	C	0.38763300	-0.04408600	-0.11216100
	C	0.01377600	1.33338900	-0.05376700
	C	1.02810400	2.33311400	0.08106300
	C	-1.35707600	1.73257800	-0.14289400
	H	-1.61002300	2.78700600	-0.12457800
	C	-2.28328600	0.74480200	-0.28594200
	C	-1.92060700	-0.61287300	-0.34880800
	C	-0.62818400	-1.03914300	-0.26896700
	H	3.09899000	2.77766800	0.26420000
	H	5.61036600	-1.24966600	0.22130000

	H	4.86361300	1.10685500	0.30078300
	H	1.55408500	-2.54687000	-0.15847000
	H	3.92355700	-3.06745200	-0.01034600
	H	0.72080000	3.37291400	0.12002100
	H	-0.37499500	-2.08742100	-0.35231000
	H	-4.43766100	1.10307800	-1.05417900
	O	-5.24453300	-0.83633300	1.05430400
S5-CS3	C	3.90552500	-1.44220800	0.00091200
	C	4.37329300	-0.16912100	0.00084500
	H	4.37949500	-2.41413900	0.00201400
	C	-4.01978000	-0.72018500	0.00037700
	C	-3.48991100	0.54798500	0.00060600
	C	-2.08785800	0.75789700	0.00029600
	C	-1.20331300	-0.36744300	-0.00016500
	C	-1.78968000	-1.66150500	-0.00060200
	C	-3.15531100	-1.83498800	-0.00029200

	C	-1.54562900	2.07203300	0.00039700
	C	0.22327900	-0.15121300	-0.00032900
	C	0.71895300	1.17871800	-0.00050700
	C	-0.19388900	2.26901600	-0.00010500
	C	2.14679600	1.45338600	-0.00044000
	H	2.48604400	2.48360200	0.00024400
	C	2.97132600	0.38877100	-0.00128400
	C	2.47543500	-0.96083600	-0.00083100
	C	1.16158100	-1.26304700	0.00016100
	H	-2.22482900	2.91796500	0.00075200
	H	-5.09395200	-0.86633200	0.00062600
	H	-4.14229400	1.41523100	0.00099900
	H	-1.15891000	-2.54043200	-0.00128500
	H	-3.56928300	-2.83716400	-0.00065300
	H	0.20829400	3.27697100	-0.00015300
	H	0.80722000	-2.28469900	0.00148400

	H	5.36331600	0.26543600	0.00173600
S5-TS12	C	-3.26372800	-1.23239800	-0.38869900
	C	-4.31336300	-0.53830000	0.34500800
	C	-3.75553900	0.63407700	-0.31499000
	H	-3.52041500	-2.05327300	-1.05178200
	C	4.56776600	-1.01422000	0.11945100
	C	4.15818600	0.29911800	0.14984900
	C	2.78540100	0.63889100	0.08508300
	C	1.80576300	-0.39514500	-0.01512000
	C	2.26392100	-1.73596100	-0.03922100
	C	3.60694000	-2.03965100	0.02468600
	C	2.36805300	2.00289600	0.12069900
	C	0.40248100	-0.04040100	-0.08085800
	C	0.03390600	1.33412600	-0.03487700
	C	1.04819600	2.33365300	0.06279500
	C	-1.34398900	1.72894300	-0.11205500

	H	-1.59487100	2.78408400	-0.12845300
	C	-2.28060000	0.74795100	-0.19743600
	C	-1.92081600	-0.61555300	-0.25060000
	C	-0.62611100	-1.03281800	-0.21581400
	H	3.12519600	2.77598100	0.19685000
	H	5.62198000	-1.26116100	0.17054400
	H	4.88717200	1.09921600	0.22537400
	H	1.55421100	-2.55010700	-0.10379600
	H	3.92473200	-3.07599400	0.00485500
	H	0.74401500	3.37466400	0.09147800
	H	-0.37588800	-2.08030100	-0.31860600
	H	-4.39540700	1.26988500	-0.91957300
	O	-5.39868900	-0.84178000	0.78571200
S5-TS23	C	-2.82813278	-0.82248902	-0.46039229
	C	-4.21487373	0.36896814	0.85016513
	C	-3.27953853	0.59428655	-0.36510425

	H	-2.61992203	-1.95081644	-0.38276793
	C	4.42534470	-0.81225423	2.73181310
	C	3.95634881	0.48133167	2.78063102
	C	2.67191629	0.81278037	2.28846272
	C	1.84477087	-0.20624436	1.73014783
	C	2.35777304	-1.52558710	1.69882588
	C	3.61392557	-1.82346909	2.18465259
	C	2.19299147	2.15810686	2.34562964
	C	0.52647986	0.13989573	1.22651504
	C	0.09012372	1.49756260	1.30988336
	C	0.95870851	2.48270414	1.87693459
	C	-1.19533021	1.89302431	0.82228833
	H	-1.48941267	2.93569489	0.87218472
	C	-1.97852861	0.92145811	0.27759714
	C	-1.55221364	-0.41611243	0.18854559
	C	-0.33662569	-0.83801839	0.63885569

	H	2.83614386	2.91971756	2.77359063
	H	5.41115495	-1.05299473	3.11291930
	H	4.56995742	1.27116307	3.20138424
	H	1.76044744	-2.32991135	1.29022963
	H	3.97634242	-2.84454834	2.14597613
	H	0.60725797	3.50794899	1.92686485
	H	-0.02158036	-1.86687249	0.52865960
	H	-3.60638034	1.61311984	-0.37239508
	O	-4.93838066	0.19467829	1.79020868
Phenoxy (S6-CS1)	C	1.78232500	0.00000000	-0.00000100
	C	1.08550100	1.22385600	0.00000000
	C	-0.28956100	1.23882600	0.00000100
	C	-1.04743500	0.00000000	0.00000000
	C	-0.28956100	-1.23882600	0.00000100
	C	1.08550100	-1.22385600	0.00000000
	H	2.86661200	0.00000000	-0.00000100

	H	1.64243200	2.15450000	0.00000000
	H	-0.85567800	2.16318300	0.00000100
	H	-0.85567800	-2.16318300	0.00000100
	H	1.64243200	-2.15450000	-0.00000100
	O	-2.30009300	0.00000000	-0.00000100
S6-CS2	C	1.19876400	0.00000000	-0.06946800
	C	0.18437300	0.80117300	0.66587800
	C	-1.05523100	1.15148300	-0.06776600
	C	-1.72002700	-0.00001500	-0.47434600
	C	-1.05520200	-1.15149100	-0.06776200
	C	0.18438900	-0.80115500	0.66590200
	H	0.53643500	1.39690500	1.50445000
	H	-1.35076100	2.17042100	-0.27296800
	H	-2.63202200	-0.00002900	-1.05765700
	H	-1.35069500	-2.17043700	-0.27297900
	H	0.53642700	-1.39686900	1.50449700

	O	2.22977800	0.00000400	-0.66499700
S6-CS3	C	-1.67085900	-0.51669600	-0.07122700
	C	0.78061200	-1.20231500	0.08075200
	C	1.83207500	-0.47452800	-0.33528400
	C	1.53186600	0.95656100	-0.18187800
	C	0.29730800	1.10729900	0.33256100
	C	-0.29568200	-0.25957100	0.56713100
	H	0.68026500	-2.27788600	0.08951100
	H	2.76156000	-0.86696300	-0.72640100
	H	2.20989400	1.75617500	-0.45107900
	H	-0.22322700	2.02942200	0.54544200
	H	-0.48428600	-0.42742300	1.63962900
	O	-2.47451500	0.26527200	-0.43117900
S6-CS4	C	0.00000000	1.18728800	0.00000000
	C	-1.16935900	0.35336200	0.00000000
	C	-0.74113100	-0.94730200	0.00000000

	C	0.74112200	-0.94732300	0.00000000
	C	1.16936800	0.35331600	0.00000000
	H	0.00001800	2.27001700	0.00000000
	H	-2.19120100	0.70207100	0.00000000
	H	-1.35864700	-1.83505600	0.00000000
	H	1.35861300	-1.83509300	0.00000000
	H	2.19121400	0.70201600	0.00000000
S6-CS5	C	-0.33019100	2.04289600	0.00000000
	C	1.86431700	-1.65306900	0.00000000
	C	0.68097100	-2.23656900	0.00000000
	C	-0.64996800	-1.63567300	0.00000000
	C	-0.95735200	-0.32043100	0.00000000
	C	0.00000000	0.76385500	0.00000000
	H	2.89815300	-1.96305900	0.00000000
	H	0.68278700	-3.33380900	0.00000000
	H	-1.47676300	-2.33677300	0.00000000

	H	-2.00684300	-0.04456100	0.00000000
	H	1.06617900	0.54977600	0.00000000
	O	-0.60127200	3.17029600	0.00000000
S6-TS12	C	-1.17190000	0.00000000	-0.14218900
	C	-0.23745700	-0.93423800	0.48333600
	C	1.10263800	-1.15058600	-0.02826600
	C	1.80591400	0.00000000	-0.35793700
	C	1.10263800	1.15058600	-0.02826600
	C	-0.23745700	0.93423800	0.48333500
	O	-2.32518000	0.00000000	-0.47795900
	H	-0.67938200	-1.61592300	1.20781300
	H	1.49272600	-2.15648700	-0.12111600
	H	2.78849900	0.00000000	-0.80979400
	H	1.49272700	2.15648700	-0.12111600
	H	-0.67938200	1.61592300	1.20781300
S6-TS15	C	-1.71611800	0.05777600	0.05065100

	C	1.23664900	1.54295600	0.32160700
	C	1.91674200	0.54171100	-0.20251900
	C	1.47031900	-0.84851600	-0.34592900
	C	0.29223800	-1.35780200	0.04502000
	C	-0.77655700	-0.57395900	0.71842400
	H	1.42138800	2.59343700	0.49523600
	H	2.92893100	0.74412100	-0.57014700
	H	2.18321200	-1.52672400	-0.80680800
	H	0.10767200	-2.41794600	-0.10995400
	H	-0.83230800	-0.51734400	1.80209400
	O	-2.54356500	0.61893200	-0.54174300
S6-TS23	C	1.23003800	-0.02287600	-0.21592600
	C	-0.06304800	0.98707500	0.46004600
	C	-1.32597800	1.02381300	-0.15066700
	C	-1.74832500	-0.30321500	-0.42104100
	C	-0.83181000	-1.20591100	0.05021300

	C	0.27917300	-0.50029800	0.76651800
	H	0.43491400	1.81394100	0.94761100
	H	-1.84386400	1.92500900	-0.44706200
	H	-2.63866800	-0.56327400	-0.97883200
	H	-0.84792600	-2.27846500	-0.07977600
	H	0.60782800	-0.84537800	1.75345400
	O	2.38092700	0.00957900	-0.51628100
S6-TS35	C	1.76313700	-0.04667000	0.08130600
	C	-0.98018300	1.40996300	0.11848700
	C	-1.95080300	0.57441300	-0.22859600
	C	-1.63942700	-0.85685400	-0.23643500
	C	-0.40184700	-1.22619700	0.12862400
	C	0.52000300	-0.14777200	0.58873600
	H	-0.94254000	2.48647000	0.22814600
	H	-2.94963000	0.90461800	-0.51800000
	H	-2.38511600	-1.58640300	-0.53255600

	H	-0.06809300	-2.25616100	0.11688400
	H	0.45272700	0.18503400	1.62553600
	O	2.75342200	0.25314300	-0.45409300
S6-TS34	C	-1.83652800	0.00000000	0.23643800
	C	0.55215000	-1.17664200	0.41085300
	C	1.41882700	-0.73265800	-0.53651600
	C	1.41882600	0.73265800	-0.53651600
	C	0.55215000	1.17664200	0.41085400
	C	-0.07755600	0.00000000	1.03000500
	H	0.32386800	-2.20152900	0.66372300
	H	2.02522200	-1.34897600	-1.18650000
	H	2.02522200	1.34897700	-1.18650000
	H	0.32386700	2.20152900	0.66372400
	H	-0.38050900	-0.00000100	2.06946900
	O	-2.06061100	0.00000000	-0.88932800

Table S21. The derived steady state approximation formula for the high-p limit rates.

Reaction	high-p limit rates formula
Phenoxy→C_5H_5 (cyclopentadienyl radical) +CO	$k=\frac{k_{1\to2}k_{2\to3}k_{3\to4}(k_{5\to1}+k_{5\to3})+k_{1\to5}k_{5\to3}k_{3\to4}(k_{2\to1}+k_{2\to3})}{k_{2\to1}k_{3\to2}(k_{5\to1}+k_{5\to3})+k_{5\to1}k_{3\to5}(k_{2\to1}+k_{2\to3})+k_{3\to4}(k_{2\to1}+k_{2\to3})(k_{5\to1}+k_{5\to3})}$
1,2-benzanthracene oxyradical I→S1-CS4+CO	$k=\frac{k_{1\to2}k_{2\to3}k_{3\to4}(k_{5\to1}+k_{5\to3})+k_{1\to5}k_{5\to3}k_{3\to4}(k_{2\to1}+k_{2\to3})}{k_{2\to1}k_{3\to2}(k_{5\to1}+k_{5\to3})+k_{5\to1}k_{3\to5}(k_{2\to1}+k_{2\to3})+k_{3\to4}(k_{2\to1}+k_{2\to3})(k_{5\to1}+k_{5\to3})}$
1,2-benzanthracene oxyradical III→S3-CS4+CO	$k=\frac{k_{1\to2}k_{2\to3}k_{3\to4}}{(k_{2\to1}+k_{2\to3})(k_{3\to2}+k_{3\to4})-k_{2\to3}k_{3\to2}}$
3H-cydopenta[a]anthracene oxyradical→S5-CS3+CO	$k=\frac{k_{1\to2}k_{2\to3}}{k_{2\to1}+k_{2\to3}}$

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