

Supplementary Information

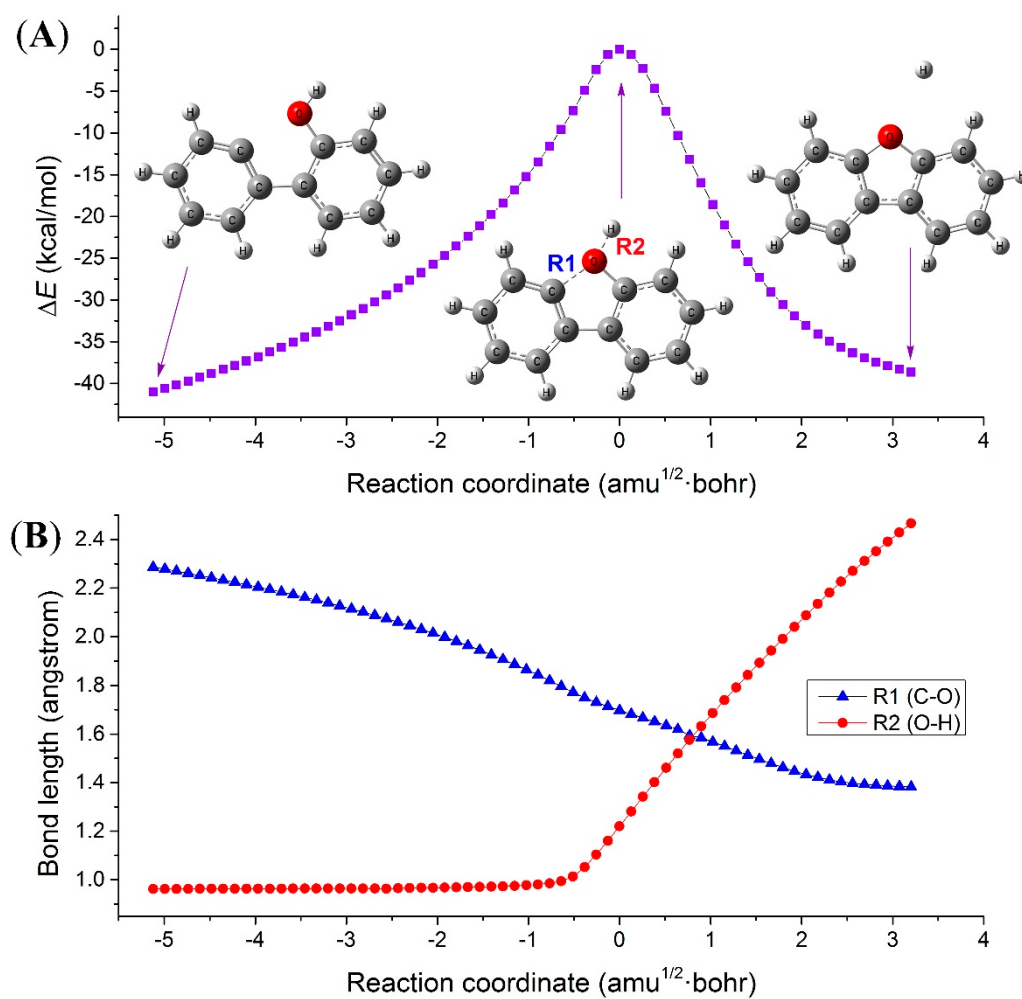


Figure S1. Intrinsic reaction coordinate (IRC) analysis of the reaction $\text{Phe-B5} \rightarrow \text{DF} + \cdot\text{H}$; (A) The energy changes along with the reaction coordinate; (B) The changes of bond lengths along with the reaction coordinate.

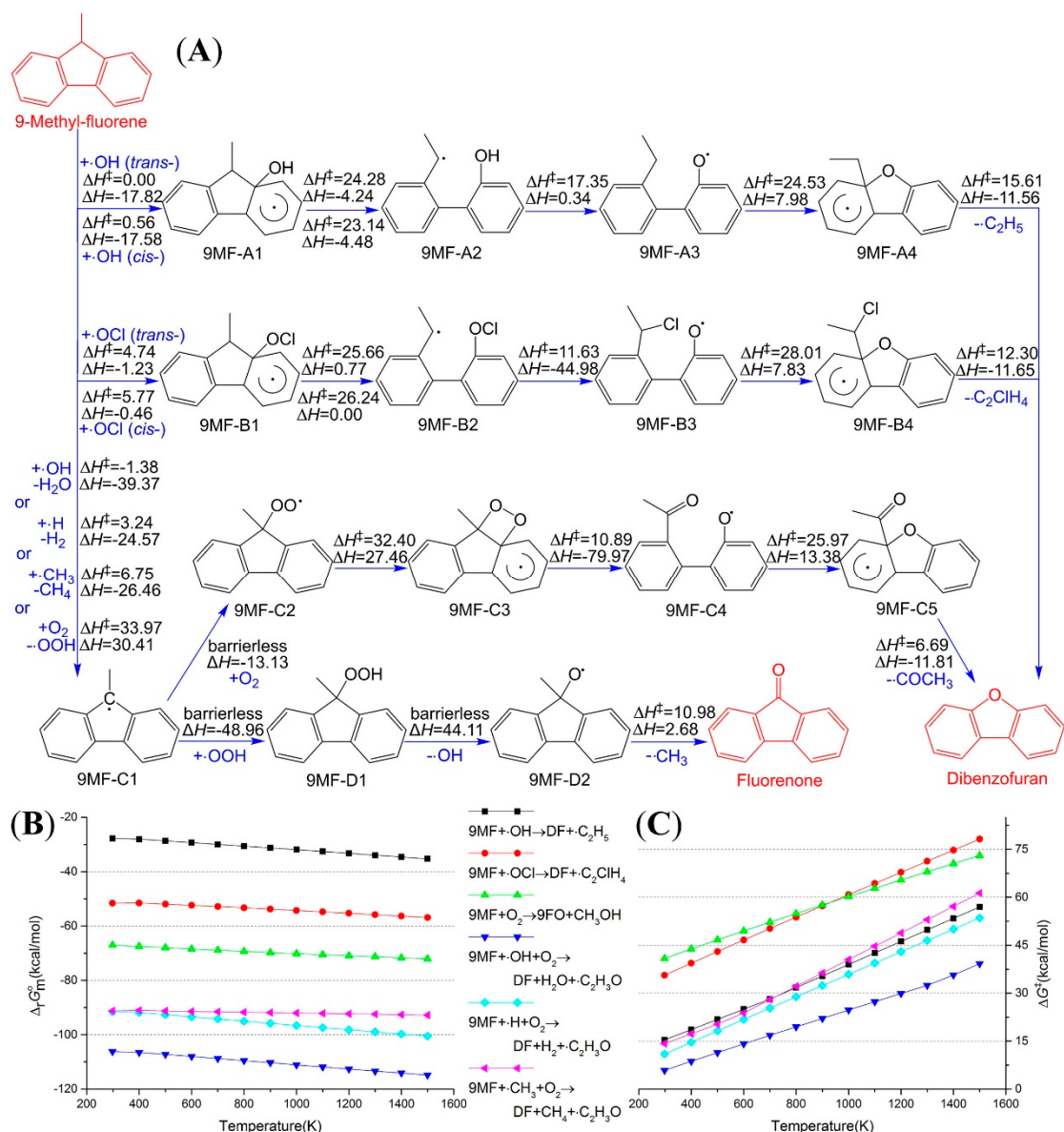


Figure S2. Dibenzofuran and 9-fluorenone formation paths from 9-methylfluorene (9MF); (A) Reaction scheme, enthalpies is were calculated at 1000 K, and energy unit is kcal/mol; (B) Standard Gibbs energy changes for the overall reactions; (C) Activation Gibbs energies for the overall reactions.

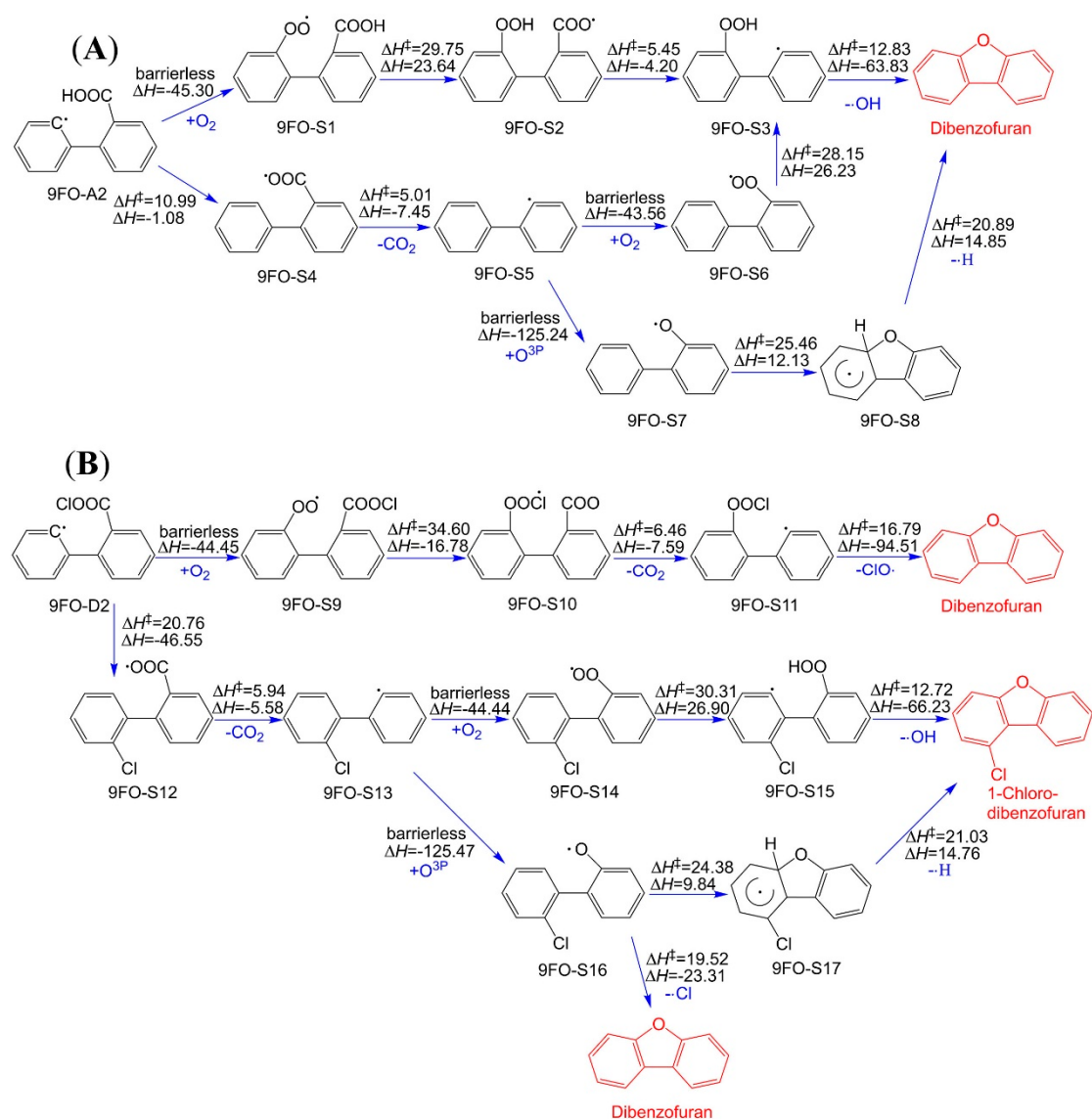


Figure S3. (A) Supplementary reaction channels for 9FO-A2 (9FO stands for 9-fluorenone); (B) Supplementary reaction channels for 9FO-D2.

Table S1. Calculated activation enthalpies and standard enthalpy changes (in kcal/mol) for the reactions from phenanthrene (Phe) to dibenzofuran (DF).

No.	Elementary Reactions		Temperature (K)												
			298.15	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500
1	Phe + ·H → Phe-A1	$\Delta_r H_m^0$	-28.99	-29.27	-29.50	-29.69	-29.84	-29.97	-30.07	-30.15	-30.21	-30.26	-30.28	-30.30	-30.30
2	Phe-A1 + O ₂ → Phe-A2	$\Delta_r H_m^0$	-22.79	-22.86	-22.85	-22.76	-22.63	-22.47	-22.27	-22.06	-21.84	-21.60	-21.36	-21.11	-20.85
3	Phe-A2 → Phe-A3	$\Delta H^\ddagger$	35.22	35.12	35.01	34.90	34.78	34.65	34.51	34.36	34.21	34.05	33.88	33.72	33.55
		$\Delta_r H_m^0$	28.38	28.39	28.43	28.50	28.56	28.62	28.68	28.73	28.78	28.82	28.86	28.90	28.93
4	Phe-A3 → Phe-A4	$\Delta H^\ddagger$	13.72	13.70	13.64	13.55	13.43	13.30	13.16	13.00	12.84	12.67	12.50	12.32	12.14
		$\Delta_r H_m^0$	-71.40	-71.17	-71.03	-70.95	-70.91	-70.89	-70.88	-70.88	-70.88	-70.89	-70.89	-70.90	-70.91
5	Phe-A4 → Phe-A5	$\Delta H^\ddagger$	27.16	26.98	26.82	26.65	26.49	26.32	26.15	25.97	25.79	25.61	25.42	25.24	25.05
		$\Delta_r H_m^0$	10.48	10.43	10.43	10.44	10.46	10.49	10.51	10.53	10.55	10.57	10.59	10.60	10.61
6	Phe-A5 → DF + ·C ₂ H ₃ O	$\Delta H^\ddagger$	9.59	9.51	9.40	9.27	9.12	8.96	8.79	8.62	8.43	8.25	8.06	7.87	7.67
		$\Delta_r H_m^0$	-2.43	-2.60	-2.85	-3.14	-3.46	-3.80	-4.16	-4.53	-4.90	-5.29	-5.67	-6.07	-6.46
7	Phe + ·OH → Phe-B1	$\Delta H^\ddagger$	5.77	5.77	5.81	5.87	5.94	6.02	6.11	6.20	6.30	6.39	6.49	6.58	6.68
		$\Delta_r H_m^0$	-5.57	-5.52	-5.38	-5.19	-4.96	-4.71	-4.44	-4.17	-3.89	-3.61	-3.32	-3.03	-2.74
8	Phe-B1 → Phe-B2	$\Delta H^\ddagger$	32.25	32.29	32.27	32.21	32.12	32.00	31.87	31.73	31.58	31.42	31.26	31.09	30.92
		$\Delta_r H_m^0$	22.43	22.62	22.75	22.85	22.91	22.96	23.00	23.02	23.04	23.06	23.08	23.09	23.10
9	Phe-B2 → Phe-B3	$\Delta H^\ddagger$	6.62	6.39	6.21	6.07	5.96	5.87	5.79	5.72	5.65	5.57	5.49	5.41	5.32
		$\Delta_r H_m^0$	-20.41	-20.55	-20.67	-20.77	-20.84	-20.90	-20.95	-20.98	-21.00	-21.01	-21.02	-21.02	-21.02
10	Phe-B3 → Phe-B4	$\Delta H^\ddagger$	27.05	26.87	26.70	26.54	26.37	26.20	26.03	25.85	25.67	25.49	25.31	25.12	24.93
		$\Delta_r H_m^0$	11.74	11.67	11.65	11.66	11.68	11.69	11.71	11.73	11.75	11.76	11.78	11.79	11.80
11	Phe-B4 → DF + ·C ₂ H ₃	$\Delta H^\ddagger$	21.58	21.60	21.56	21.47	21.36	21.23	21.09	20.93	20.77	20.60	20.43	20.25	20.07
		$\Delta_r H_m^0$	14.71	14.57	14.34	14.06	13.74	13.40	13.04	12.68	12.30	11.93	11.55	11.16	10.78
12	Phe-B2 → Phe-B5 + C ₂ H ₂	$\Delta H^\ddagger$	43.23	43.38	43.46	43.49	43.46	43.40	43.30	43.18	43.05	42.89	42.73	42.56	42.39
		$\Delta_r H_m^0$	40.13	40.18	40.15	40.07	39.93	39.75	39.54	39.31	39.06	38.79	38.52	38.23	37.95
13	Phe-B5 → DF + ·H	$\Delta H^\ddagger$	43.96	43.88	43.83	43.80	43.78	43.76	43.73	43.71	43.67	43.63	43.58	43.52	43.45
		$\Delta_r H_m^0$	2.51	2.59	2.66	2.73	2.81	2.88	2.95	3.01	3.07	3.12	3.16	3.19	3.21
14	Phe + ·OCl → Phe-C1	$\Delta H^\ddagger$	11.69	11.83	11.99	12.14	12.29	12.43	12.56	12.70	12.82	12.95	13.07	13.18	13.30
		$\Delta_r H_m^0$	8.89	9.16	9.47	9.80	10.14	10.48	10.82	11.15	11.48	11.81	12.13	12.46	12.77

Table S1. Cont.

No.	Elementary Reactions		Temperature (K)												
			298.15	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500
15	Phe-C1 $\rightarrow$ Phe-C2	$\Delta H^\ddagger$	35.94	35.95	35.91	35.84	35.73	35.61	35.48	35.33	35.18	35.02	34.85	34.68	34.51
		$\Delta_r H_m^\circ$	28.86	29.05	29.18	29.28	29.35	29.40	29.44	29.47	29.50	29.52	29.54	29.55	29.57
16	Phe-C2 $\rightarrow$ Phe-C3	$\Delta H^\ddagger$	11.25	11.09	10.93	10.76	10.59	10.42	10.24	10.06	9.87	9.69	9.50	9.31	9.12
		$\Delta_r H_m^\circ$	-65.91	-66.04	-66.15	-66.25	-66.32	-66.39	-66.44	-66.48	-66.52	-66.55	-66.58	-66.61	-66.63
17	Phe-C3 $\rightarrow$ Phe-C4	$\Delta H^\ddagger$	29.63	29.45	29.28	29.11	28.95	28.77	28.60	28.42	28.24	28.06	27.87	27.68	27.49
		$\Delta_r H_m^\circ$	15.19	15.14	15.13	15.14	15.15	15.17	15.19	15.21	15.23	15.25	15.26	15.27	15.29
18	Phe-C4 $\rightarrow$ DF + $\cdot\text{C}_2\text{ClH}_2$	$\Delta H^\ddagger$	20.63	20.62	20.56	20.46	20.34	20.20	20.04	19.88	19.71	19.53	19.36	19.17	18.99
		$\Delta_r H_m^\circ$	-8.42	-8.59	-8.79	-9.00	-9.21	-9.42	-9.64	-9.85	-10.07	-10.28	-10.49	-10.71	-10.92
19	Phe-C2 $\rightarrow$ Phe-C5 + C_2H_2	$\Delta H^\ddagger$	43.28	43.43	43.51	43.54	43.51	43.45	43.35	43.23	43.10	42.95	42.78	42.61	42.44
		$\Delta_r H_m^\circ$	40.27	40.32	40.29	40.21	40.07	39.89	39.68	39.45	39.20	38.93	38.66	38.38	38.09
20	Phe-C5 $\rightarrow$ DF + $\cdot\text{Cl}$	$\Delta H^\ddagger$	8.08	7.97	7.84	7.69	7.53	7.36	7.19	7.01	6.82	6.63	6.45	6.26	6.06
		$\Delta_r H_m^\circ$	-79.62	-79.83	-80.04	-80.24	-80.42	-80.60	-80.76	-80.91	-81.06	-81.20	-81.34	-81.47	-81.60
21	Phe + $\cdot\text{OH} \rightarrow$ Phe-D1	$\Delta_r H_m^\circ$	-23.45	-23.46	-23.40	-23.27	-23.10	-22.90	-22.68	-22.43	-22.18	-21.92	-21.65	-21.38	-21.10
22	Phe-D1 + $\text{O}_2 \rightarrow$ <i>trans</i> -Phe-D2	$\Delta_r H_m^\circ$	-23.85	-23.93	-23.92	-23.84	-23.71	-23.54	-23.35	-23.14	-22.91	-22.68	-22.43	-22.18	-21.92
23	<i>trans</i> -Phe-D2 $\rightarrow$ <i>trans</i> -Phe-D3	$\Delta H^\ddagger$	36.25	36.15	36.04	35.93	35.80	35.67	35.54	35.39	35.24	35.08	34.92	34.76	34.59
		$\Delta_r H_m^\circ$	29.72	29.73	29.78	29.84	29.91	29.98	30.04	30.09	30.14	30.19	30.23	30.27	30.30
24	<i>trans</i> -Phe-D3 $\rightarrow$ <i>trans</i> -Phe-D4	$\Delta H^\ddagger$	12.20	12.17	12.12	12.03	11.92	11.79	11.65	11.50	11.34	11.17	10.99	10.82	10.64
		$\Delta_r H_m^\circ$	-72.12	-71.87	-71.72	-71.63	-71.58	-71.55	-71.53	-71.52	-71.52	-71.52	-71.52	-71.52	-71.52
25	<i>trans</i> -Phe-D4 $\rightarrow$ <i>trans</i> -Phe-D5	$\Delta H^\ddagger$	26.51	26.34	26.18	26.01	25.85	25.68	25.51	25.33	25.16	24.97	24.79	24.60	24.42
		$\Delta_r H_m^\circ$	7.78	7.71	7.69	7.69	7.70	7.72	7.73	7.75	7.76	7.77	7.79	7.80	7.80
26	<i>trans</i> -Phe-D5 $\rightarrow$ DF + $\cdot\text{C}_2\text{H}_3\text{O}_2$	$\Delta H^\ddagger$	6.74	6.63	6.49	6.33	6.16	5.98	5.79	5.60	5.41	5.21	5.02	4.82	4.62
		$\Delta_r H_m^\circ$	-10.27	-10.57	-10.92	-11.31	-11.71	-12.11	-12.52	-12.94	-13.35	-13.76	-14.17	-14.59	-15.00
27	Phe-D1 + $\text{O}_2 \rightarrow$ <i>cis</i> -Phe-D2	$\Delta_r H_m^\circ$	-25.24	-25.34	-25.34	-25.27	-25.14	-24.98	-24.79	-24.58	-24.35	-24.11	-23.87	-23.61	-23.35
28	<i>cis</i> -Phe-D2 $\rightarrow$ <i>cis</i> -Phe-D3	$\Delta H^\ddagger$	37.63	37.55	37.46	37.36	37.25	37.12	36.99	36.85	36.70	36.54	36.38	36.22	36.05
		$\Delta_r H_m^\circ$	31.08	31.11	31.17	31.24	31.32	31.39	31.45	31.51	31.56	31.60	31.64	31.68	31.71
29	<i>cis</i> -Phe-D3 $\rightarrow$ <i>cis</i> -Phe-D4	$\Delta_r H_m^\circ$	13.97	13.95	13.89	13.80	13.69	13.56	13.41	13.26	13.10	12.93	12.75	12.57	12.39
		$\Delta_r H_m^\circ$	-76.63	-76.43	-76.32	-76.26	-76.24	-76.23	-76.23	-76.24	-76.25	-76.26	-76.27	-76.28	-76.29

Table S1. Cont.

No.	Elementary Reactions		Temperature (K)												
			298.15	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500
30	<i>cis</i> -Phe-D4 → <i>cis</i> -Phe-D5	$\Delta H^\ddagger$	26.90	26.73	26.58	26.43	26.27	26.10	25.93	25.76	25.58	25.40	25.22	25.04	24.85
		$\Delta_r H_m^\circ$	10.78	10.72	10.72	10.74	10.76	10.79	10.81	10.84	10.86	10.88	10.90	10.92	10.93
31	<i>cis</i> -Phe-D5 → DF + ·C ₂ H ₃ O ₂	$\Delta H^\ddagger$	10.74	10.66	10.54	10.39	10.23	10.05	9.87	9.68	9.49	9.30	9.11	8.91	8.71
		$\Delta_r H_m^\circ$	-14.99	-15.33	-15.73	-16.14	-16.57	-17.00	-17.42	-17.85	-18.28	-18.70	-19.13	-19.55	-19.96

Table S2. Calculated Gibbs energies of activation and standard Gibbs energy changes (in kcal/mol) for the reactions from phenanthrene (Phe) to dibenzofuran (DF).

No.	Elementary Reactions		Temperature (K)												
			298.15	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500
1	Phe + ·H → Phe-A1	$\Delta_r G_m^o$	-23.05	-20.97	-18.87	-16.72	-14.55	-12.35	-10.15	-7.93	-5.70	-3.47	-1.24	1.00	3.23
2	Phe-A1 + O ₂ → Phe-A2	$\Delta_r G_m^o$	-10.58	-6.39	-2.28	1.83	5.92	9.99	14.03	18.05	22.05	26.03	29.99	33.94	37.86
3	Phe-A2 → Phe-A3	$\Delta G^\ddagger$	36.14	36.47	36.82	37.20	37.59	38.00	38.43	38.87	39.33	39.80	40.29	40.79	41.30
		$\Delta_r G_m^o$	29.09	29.33	29.56	29.78	29.99	30.19	30.38	30.57	30.75	30.92	31.10	31.27	31.44
4	Phe-A3 → Phe-A4	$\Delta G^\ddagger$	13.75	13.76	13.78	13.81	13.87	13.94	14.02	14.13	14.25	14.39	14.53	14.70	14.87
		$\Delta_r G_m^o$	-73.90	-74.79	-75.71	-76.66	-77.62	-78.58	-79.54	-80.50	-81.46	-82.42	-83.38	-84.34	-85.30
5	Phe-A4 → Phe-A5	$\Delta G^\ddagger$	27.94	28.24	28.57	28.94	29.33	29.75	30.19	30.65	31.13	31.62	32.13	32.65	33.19
		$\Delta_r G_m^o$	11.46	11.81	12.15	12.50	12.84	13.17	13.51	13.84	14.17	14.50	14.82	15.15	15.47
6	Phe-A5 → DF + ·C ₂ H ₃ O	$\Delta G^\ddagger$	10.12	10.32	10.53	10.77	11.03	11.31	11.62	11.94	12.28	12.64	13.01	13.40	13.80
		$\Delta_r G_m^o$	-14.53	-18.07	-21.92	-25.71	-29.45	-33.14	-36.78	-40.39	-43.96	-47.49	-50.99	-54.46	-57.91
7	Phe + ·OH → Phe-B1	$\Delta G^\ddagger$	14.95	18.08	21.16	24.22	27.27	30.32	33.35	36.37	39.38	42.39	45.38	48.37	51.35
		$\Delta_r G_m^o$	4.00	7.27	10.46	13.61	16.72	19.80	22.84	25.86	28.85	31.82	34.76	37.67	40.57
8	Phe-B1 → Phe-B2	$\Delta G^\ddagger$	31.68	31.47	31.27	31.08	30.89	30.73	30.57	30.44	30.32	30.21	30.11	30.03	29.96
		$\Delta_r G_m^o$	20.28	19.52	18.72	17.91	17.08	16.24	15.40	14.55	13.70	12.85	12.00	11.15	10.30
9	Phe-B2 → Phe-B3	$\Delta G^\ddagger$	8.55	9.25	9.98	10.75	11.54	12.34	13.15	13.98	14.81	15.64	16.48	17.33	18.19
		$\Delta_r G_m^o$	-20.29	-20.23	-20.13	-20.01	-19.88	-19.74	-19.59	-19.44	-19.28	-19.13	-18.97	-18.81	-18.66
10	Phe-B3 → Phe-B4	$\Delta_r G_m^o$	28.93	29.60	30.30	31.04	31.80	32.59	33.40	34.23	35.08	35.94	36.82	37.71	38.62
		$\Delta_r G_m^o$	13.46	14.06	14.66	15.26	15.86	16.46	17.05	17.65	18.24	18.82	19.41	20.00	20.59

Table S2. *Cont.*

No.	Elementary Reactions		Temperature (K)												
			298.15	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500
11	Phe-B4 $\rightarrow$ DF + $\cdot$ C ₂ H ₃	$\Delta G^\ddagger$	20.94	20.71	20.50	20.29	20.10	19.93	19.77	19.64	19.52	19.41	19.32	19.24	19.17
		$\Delta_r G_m^\circ$	2.44	-1.17	-5.10	-8.96	-12.77	-16.54	-20.26	-23.94	-27.58	-31.19	-34.77	-38.32	-41.84
12	Phe-B2 $\rightarrow$ Phe-B5 + C ₂ H ₂	$\Delta G^\ddagger$	41.77	41.24	40.69	40.14	39.58	39.03	38.49	37.96	37.44	36.94	36.45	35.97	35.51
		$\Delta_r G_m^\circ$	29.29	25.57	21.92	18.29	14.67	11.07	7.49	3.95	0.42	-3.08	-6.56	-10.01	-13.45
13	Phe-B5 $\rightarrow$ DF + $\cdot$ H	$\Delta G^\ddagger$	45.04	45.43	45.82	46.22	46.63	47.03	47.44	47.86	48.27	48.69	49.12	49.55	49.98
		$\Delta_r G_m^\circ$	-2.81	-4.07	-5.76	-7.45	-9.15	-10.86	-12.59	-14.31	-16.05	-17.79	-19.53	-21.28	-23.03
14	Phe + $\cdot$ Ocl $\rightarrow$ Phe-C1	$\Delta G^\ddagger$	22.30	25.90	29.40	32.87	36.32	39.74	43.14	46.54	49.91	53.28	56.64	59.98	63.32
		$\Delta_r G_m^\circ$	19.57	23.19	26.66	30.07	33.42	36.72	39.98	43.20	46.39	49.55	52.68	55.79	58.87
15	Phe-C1 $\rightarrow$ Phe-C2	$\Delta G^\ddagger$	35.60	35.48	35.37	35.26	35.18	35.10	35.05	35.01	34.98	34.97	34.98	34.99	35.02
		$\Delta_r G_m^\circ$	25.86	24.81	23.73	22.63	21.52	20.40	19.27	18.14	17.01	15.87	14.73	13.59	12.45
16	Phe-C2 $\rightarrow$ Phe-C3	$\Delta G^\ddagger$	13.42	14.18	14.98	15.80	16.66	17.53	18.43	19.36	20.29	21.25	22.22	23.21	24.21
		$\Delta_r G_m^\circ$	-65.29	-65.05	-64.79	-64.51	-64.22	-63.91	-63.60	-63.28	-62.96	-62.63	-62.31	-61.98	-61.65
17	Phe-C3 $\rightarrow$ Phe-C4	$\Delta G^\ddagger$	31.53	32.21	32.93	33.67	34.44	35.24	36.06	36.90	37.76	38.63	39.52	40.42	41.34
		$\Delta_r G_m^\circ$	16.87	17.45	18.03	18.61	19.19	19.76	20.33	20.90	21.47	22.03	22.60	23.16	23.73
18	Phe-C4 $\rightarrow$ DF + $\cdot$ C ₂ ClH ₂	$\Delta G^\ddagger$	19.78	19.49	19.21	18.95	18.70	18.48	18.27	18.08	17.91	17.76	17.62	17.49	17.38
		$\Delta_r G_m^\circ$	-20.03	-23.41	-27.10	-30.75	-34.36	-37.93	-41.48	-45.01	-48.52	-52.00	-55.47	-58.92	-62.36
19	Phe-C2 $\rightarrow$ Phe-C5 + C ₂ H ₂	$\Delta G^\ddagger$	42.01	41.55	41.07	40.58	40.09	39.61	39.13	38.67	38.22	37.78	37.36	36.95	36.55
		$\Delta_r G_m^\circ$	29.72	26.11	22.55	19.02	15.49	11.99	8.52	5.07	1.64	-1.76	-5.14	-8.50	-11.84
20	Phe-C5 $\rightarrow$ DF + $\cdot$ Cl	$\Delta G^\ddagger$	8.05	8.06	8.09	8.16	8.25	8.37	8.50	8.66	8.82	9.02	9.23	9.45	9.68
		$\Delta_r G_m^\circ$	-85.58	-87.02	-88.80	-90.54	-92.24	-93.91	-95.57	-97.21	-98.83	-100.44	-102.03	-103.62	-105.20
21	Phe + $\cdot$ OH $\rightarrow$ Phe-D1	$\Delta_r G_m^\circ$	-14.44	-11.36	-8.34	-5.34	-2.37	0.58	3.50	6.40	9.27	12.12	14.94	17.75	20.53
22	Phe-D1 + O ₂ $\rightarrow$ <i>trans</i> -Phe-D2	$\Delta_r G_m^\circ$	-11.86	-7.75	-3.71	0.33	4.34	8.34	12.32	16.27	20.20	24.11	28.00	31.86	35.72
23	<i>trans</i> -Phe-D2 $\rightarrow$ <i>trans</i> -Phe-D3	$\Delta G^\ddagger$	36.92	37.16	37.43	37.72	38.03	38.35	38.70	39.06	39.43	39.82	40.22	40.63	41.06
		$\Delta_r G_m^\circ$	30.44	30.69	30.92	31.14	31.35	31.56	31.75	31.94	32.12	32.30	32.47	32.64	32.81
24	<i>trans</i> -Phe-D3 $\rightarrow$ <i>trans</i> -Phe-D4	$\Delta G^\ddagger$	12.26	12.29	12.32	12.37	12.44	12.52	12.62	12.73	12.86	13.01	13.17	13.34	13.53
		$\Delta_r G_m^\circ$	-74.16	-74.90	-75.67	-76.47	-77.29	-78.10	-78.93	-79.75	-80.57	-81.39	-82.21	-83.04	-83.86

Table S2. *Cont.*

No.	Elementary Reactions		Temperature (K)												
			298.15	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500
25	<i>trans</i> -Phe-D4 → <i>trans</i> -Phe-D5	$\Delta G^\ddagger$	27.97	28.49	29.05	29.64	30.26	30.90	31.56	32.24	32.94	33.66	34.39	35.14	35.90
		$\Delta_r G_m^\circ$	9.00	9.43	9.87	10.30	10.74	11.17	11.60	12.03	12.46	12.88	13.31	13.73	14.16
26	<i>trans</i> -Phe-D5 → DF + ·C ₂ H ₃ O ₂	$\Delta G^\ddagger$	6.90	6.97	7.06	7.19	7.35	7.53	7.74	7.96	8.21	8.47	8.75	9.04	9.35
		$\Delta_r G_m^\circ$	-23.08	-26.84	-30.89	-34.84	-38.73	-42.57	-46.35	-50.08	-53.78	-57.44	-61.06	-64.65	-68.21
27	Phe-D1 + O ₂ → <i>cis</i> -Phe-D2	$\Delta_r G_m^\circ$	-12.78	-8.51	-4.30	-0.09	4.09	8.26	12.40	16.52	20.62	24.70	28.76	32.80	36.82
28	<i>cis</i> -Phe-D2 → <i>cis</i> -Phe-D3	$\Delta G^\ddagger$	38.14	38.33	38.54	38.76	39.01	39.27	39.54	39.83	40.14	40.46	40.79	41.14	41.50
		$\Delta_r G_m^\circ$	31.43	31.54	31.65	31.73	31.81	31.88	31.93	31.98	32.03	32.07	32.11	32.14	32.17
29	<i>cis</i> -Phe-D3 → <i>cis</i> -Phe-D4	$\Delta G^\ddagger$	13.91	13.89	13.88	13.88	13.90	13.94	14.00	14.07	14.16	14.27	14.39	14.52	14.66
		$\Delta_r G_m^\circ$	-78.84	-79.62	-80.44	-81.27	-82.10	-82.94	-83.78	-84.62	-85.46	-86.29	-87.13	-87.96	-88.80
30	<i>cis</i> -Phe-D 4→ <i>cis</i> -Phe-D5	$\Delta G^\ddagger$	28.30	28.80	29.34	29.91	30.50	31.11	31.75	32.41	33.08	33.77	34.48	35.19	35.93
		$\Delta_r G_m^\circ$	12.37	12.92	13.47	14.02	14.57	15.11	15.65	16.19	16.72	17.25	17.78	18.31	18.84
31	<i>cis</i> -Phe-D5 → DF + ·C ₂ H ₃ O ₂	$\Delta G^\ddagger$	10.57	10.52	10.50	10.51	10.54	10.60	10.68	10.78	10.90	11.03	11.19	11.35	11.53
		$\Delta_r G_m^\circ$	-27.80	-31.56	-35.58	-39.51	-43.37	-47.17	-50.92	-54.62	-58.28	-61.89	-65.47	-69.02	-72.54

Table S3. Calculated activation enthalpies and standard enthalpy changes (in kcal/mol) for the reactions from fluorene (Flu) to dibenzofuran (DF) and 9-fluorenone (9FO).

No.	Elementary Reactions		Temperature (K)												
			298.15	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500
32	Flu + ·OH → Flu-A1	$\Delta H^\ddagger$	−0.28	−0.30	−0.28	−0.23	−0.17	−0.09	−0.01	0.07	0.16	0.25	0.34	0.43	0.52
		$\Delta_r H_m^o$	−18.44	−18.43	−18.33	−18.16	−17.96	−17.74	−17.49	−17.24	−16.97	−16.70	−16.43	−16.15	−15.88
33	Flu-A1 → Flu-A2	$\Delta H^\ddagger$	27.35	27.38	27.36	27.30	27.21	27.10	26.96	26.82	26.66	26.50	26.33	26.16	25.98
		$\Delta_r H_m^o$	−4.13	−3.93	−3.78	−3.67	−3.59	−3.54	−3.50	−3.47	−3.45	−3.44	−3.43	−3.42	−3.42
34	Flu-A2 → Flu-A3	$\Delta H^\ddagger$	18.33	18.01	17.75	17.53	17.35	17.20	17.07	16.96	16.85	16.74	16.64	16.54	16.43
		$\Delta_r H_m^o$	−2.51	−2.66	−2.81	−2.95	−3.06	−3.15	−3.22	−3.27	−3.30	−3.32	−3.34	−3.34	−3.34
35	Flu-A3 → Flu-A4	$\Delta H^\ddagger$	26.62	26.44	26.27	26.10	25.93	25.76	25.59	25.41	25.23	25.05	24.87	24.68	24.49
		$\Delta_r H_m^o$	9.24	9.17	9.15	9.16	9.17	9.19	9.21	9.23	9.25	9.26	9.27	9.29	9.30

Table S3. *Cont.*

No.	Elementary Reactions		Temperature (K)												
			298.15	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500
36	Flu-A4 → DF + ·CH ₃	$\Delta H^\ddagger$	18.92	18.97	18.97	18.92	18.84	18.73	18.60	18.46	18.30	18.14	17.96	17.79	17.61
		$\Delta_r H_m^\circ$	-11.73	-11.69	-11.74	-11.83	-11.96	-12.11	-12.28	-12.45	-12.63	-12.82	-13.01	-13.20	-13.40
37	Flu + ·OC1 → Flu-B1	$\Delta H^\ddagger$	4.11	4.22	4.34	4.47	4.60	4.72	4.84	4.95	5.07	5.18	5.29	5.40	5.51
		$\Delta_r H_m^\circ$	-2.60	-2.38	-2.10	-1.80	-1.48	-1.17	-0.85	-0.53	-0.21	0.10	0.41	0.73	1.04
38	Flu-B1 → Flu-B2	$\Delta H^\ddagger$	28.72	28.72	28.67	28.60	28.49	28.37	28.23	28.08	27.91	27.74	27.57	27.39	27.21
		$\Delta_r H_m^\circ$	0.85	1.05	1.19	1.30	1.38	1.44	1.48	1.52	1.54	1.55	1.57	1.57	1.58
39	Flu-B2 → Flu-B3	$\Delta H^\ddagger$	18.24	18.07	17.88	17.67	17.45	17.24	17.03	16.81	16.60	16.39	16.18	15.97	15.77
		$\Delta_r H_m^\circ$	-46.41	-46.58	-46.74	-46.89	-47.01	-47.11	-47.20	-47.26	-47.32	-47.37	-47.41	-47.45	-47.48
40	Flu-B3 → Flu-B4	$\Delta H^\ddagger$	30.01	29.85	29.69	29.54	29.38	29.22	29.06	28.88	28.71	28.54	28.36	28.17	27.99
		$\Delta_r H_m^\circ$	9.86	9.80	9.78	9.79	9.81	9.83	9.85	9.87	9.89	9.91	9.93	9.94	9.95
41	Flu-B4 → DF + ·CClH ₂	$\Delta H^\ddagger$	15.35	15.32	15.25	15.15	15.02	14.88	14.72	14.55	14.38	14.20	14.02	13.83	13.64
		$\Delta_r H_m^\circ$	-10.71	-10.71	-10.79	-10.91	-11.06	-11.22	-11.40	-11.58	-11.77	-11.96	-12.15	-12.35	-12.55
42	Flu + ·OH → Flu-C1 + H ₂ O	$\Delta H^\ddagger$	-1.20	-1.16	-1.06	-0.93	-0.77	-0.60	-0.42	-0.24	-0.06	0.12	0.29	0.46	0.62
		$\Delta_r H_m^\circ$	-35.28	-35.21	-35.18	-35.17	-35.19	-35.23	-35.30	-35.38	-35.48	-35.58	-35.69	-35.81	-35.93
43	Flu + ·H → Flu-C1 + H ₂	$\Delta H^\ddagger$	5.18	5.05	4.98	4.94	4.93	4.93	4.93	4.93	4.93	4.92	4.91	4.89	4.87
		$\Delta_r H_m^\circ$	-20.66	-20.50	-20.40	-20.35	-20.35	-20.39	-20.47	-20.58	-20.72	-20.87	-21.05	-21.23	-21.42
44	Flu + ·CH ₃ → Flu-C1 + CH ₄	$\Delta H^\ddagger$	6.19	6.04	5.99	6.00	6.04	6.11	6.19	6.27	6.36	6.45	6.53	6.61	6.68
		$\Delta_r H_m^\circ$	-21.77	-21.92	-22.05	-22.17	-22.27	-22.35	-22.41	-22.47	-22.52	-22.56	-22.60	-22.63	-22.65
45	Flu + O ₂ → Flu-C1 + ·OOH	$\Delta H^\ddagger$	34.76	34.96	35.21	35.48	35.77	36.05	36.32	36.59	36.84	37.08	37.30	37.52	37.72
		$\Delta_r H_m^\circ$	34.14	34.23	34.31	34.38	34.42	34.43	34.42	34.40	34.35	34.29	34.23	34.15	34.07
46	Flu-C1 + O ₂ → Flu-C2	$\Delta_r H_m^\circ$	-14.53	-14.56	-14.51	-14.41	-14.26	-14.08	-13.87	-13.65	-13.41	-13.16	-12.90	-12.64	-12.37
47	Flu-C2 → Flu-C3	$\Delta_r H_m^\circ$	34.63	34.50	34.38	34.26	34.14	34.00	33.86	33.71	33.55	33.39	33.22	33.05	32.88
		$\Delta_r H_m^\circ$	28.97	28.97	29.00	29.06	29.12	29.18	29.23	29.28	29.33	29.37	29.40	29.43	29.46
48	Flu-C3 → Flu-C4	$\Delta H^\ddagger$	12.87	12.81	12.71	12.59	12.45	12.30	12.13	11.96	11.79	11.61	11.43	11.24	11.05
		$\Delta_r H_m^\circ$	-79.56	-79.36	-79.25	-79.21	-79.20	-79.20	-79.21	-79.23	-79.24	-79.25	-79.27	-79.28	-79.29
49	Flu-C4 → Flu-C5	$\Delta H^\ddagger$	27.01	26.83	26.67	26.51	26.35	26.18	26.01	25.84	25.66	25.48	25.30	25.11	24.93
		$\Delta_r H_m^\circ$	13.91	13.86	13.87	13.89	13.92	13.95	13.97	14.00	14.02	14.04	14.06	14.07	14.08

Table S3. *Cont.*

No.	Elementary Reactions		Temperature (K)												
			298.15	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500
50	Flu-C5 $\rightarrow$ DF + $\cdot$ CHO	$\Delta H^\ddagger$	8.12	8.05	7.95	7.81	7.66	7.49	7.32	7.14	6.96	6.77	6.59	6.40	6.21
		$\Delta_r H_m^\circ$	-10.60	-10.69	-10.85	-11.03	-11.22	-11.42	-11.62	-11.82	-12.02	-12.23	-12.43	-12.63	-12.83
51	Flu-C2 $\rightarrow$ 9FO + $\cdot$ OH	$\Delta H^\ddagger$	38.57	38.55	38.54	38.51	38.47	38.42	38.36	38.29	38.21	38.13	38.03	37.92	37.81
		$\Delta_r H_m^\circ$	-29.93	-29.74	-29.66	-29.67	-29.75	-29.89	-30.07	-30.28	-30.51	-30.76	-31.02	-31.29	-31.57
52	Flu-C1 + $\cdot$ OOH $\rightarrow$ Flu-D1	$\Delta_r H_m^\circ$	-51.19	-51.14	-51.03	-50.85	-50.64	-50.39	-50.11	-49.81	-49.50	-49.17	-48.84	-48.49	-48.14
53	Flu-D1 $\rightarrow$ 9FO + H ₂ O	$\Delta H^\ddagger$	54.20	54.29	54.37	54.43	54.46	54.47	54.47	54.45	54.42	54.37	54.30	54.23	54.15
		$\Delta_r H_m^\circ$	-62.69	-62.59	-62.63	-62.77	-62.98	-63.25	-63.56	-63.89	-64.25	-64.62	-65.01	-65.40	-65.80

Table S4. Calculated Gibbs energies of activation and standard Gibbs energy changes (in kcal/mol) for the reactions from fluorene (Flu) to dibenzofuran (DF) and 9-fluorenone (9FO).

No.	Elementary Reactions		Temperature (K)												
			298.15	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500
32	Flu + ·OH → Flu-A1	$\Delta G^\ddagger$	9.42	12.74	16.00	19.25	22.49	25.72	28.94	32.16	35.36	38.56	41.75	44.93	48.11
		$\Delta_r G_m^\circ$	−8.19	−4.68	−1.26	2.14	5.51	8.85	12.16	15.44	18.69	21.92	25.13	28.32	31.49
33	Flu-A1 → Flu-A2	$\Delta G^\ddagger$	26.97	26.84	26.71	26.58	26.47	26.37	26.28	26.22	26.16	26.13	26.10	26.09	26.09
		$\Delta_r G_m^\circ$	−5.61	−6.14	−6.72	−7.32	−7.93	−8.55	−9.18	−9.82	−10.45	−11.09	−11.73	−12.37	−13.00
34	Flu-A2 → Flu-A3	$\Delta G^\ddagger$	20.05	20.69	21.40	22.15	22.93	23.74	24.57	25.41	26.26	27.12	27.98	28.86	29.74
		$\Delta_r G_m^\circ$	−2.53	−2.51	−2.46	−2.38	−2.27	−2.15	−2.02	−1.89	−1.75	−1.61	−1.46	−1.32	−1.18
35	Flu-A3 → Flu-A4	$\Delta G^\ddagger$	28.35	28.97	29.62	30.31	31.02	31.76	32.52	33.30	34.09	34.91	35.74	36.58	37.44
		$\Delta_r G_m^\circ$	10.91	11.49	12.08	12.66	13.24	13.82	14.40	14.98	15.55	16.12	16.69	17.27	17.83
36	Flu-A4 → DF + ·CH ₃	$\Delta G^\ddagger$	18.49	18.33	18.17	18.02	17.88	17.75	17.63	17.53	17.45	17.37	17.32	17.28	17.25
		$\Delta_r G_m^\circ$	−23.47	−26.92	−30.74	−34.53	−38.30	−42.05	−45.78	−49.50	−53.19	−56.87	−60.54	−64.18	−67.82
37	Flu + ·OCl → Flu-B1	$\Delta G^\ddagger$	15.15	18.90	22.56	26.19	29.80	33.39	36.97	40.54	44.09	47.63	51.16	54.69	58.20
		$\Delta_r G_m^\circ$	8.70	12.52	16.22	19.85	23.43	26.97	30.47	33.93	37.36	40.77	44.14	47.49	50.82
38	Flu-B1 → Flu-B2	$\Delta G^\ddagger$	28.59	28.55	28.51	28.49	28.48	28.48	28.51	28.55	28.60	28.67	28.75	28.85	28.96
		$\Delta_r G_m^\circ$	−1.21	−1.95	−2.72	−3.51	−4.32	−5.14	−5.96	−6.79	−7.62	−8.46	−9.29	−10.13	−10.96
39	Flu-B2 → Flu-B3	$\Delta G^\ddagger$	19.09	19.40	19.76	20.15	20.58	21.04	21.53	22.04	22.58	23.13	23.70	24.28	24.88
		$\Delta_r G_m^\circ$	−45.99	−45.82	−45.61	−45.37	−45.11	−44.83	−44.54	−44.24	−43.94	−43.63	−43.32	−43.00	−42.68

Table S4. *Cont.*

No.	Elementary Reactions		Temperature (K)												
			298.15	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500
40	Flu-B3 $\rightarrow$ Flu-B4	$\Delta G^\ddagger$	31.93	32.62	33.33	34.07	34.84	35.63	36.44	37.27	38.11	38.98	39.85	40.74	41.65
		$\Delta_r G_m^\circ$	11.74	12.40	13.05	13.70	14.35	15.00	15.65	16.29	16.93	17.57	18.21	18.84	19.48
41	Flu-B4 $\rightarrow$ DF + $\cdot\text{CClH}_2$	$\Delta G^\ddagger$	14.79	14.60	14.43	14.27	14.14	14.02	13.92	13.84	13.78	13.73	13.70	13.68	13.68
		$\Delta_r G_m^\circ$	-23.74	-27.63	-31.87	-36.07	-40.25	-44.41	-48.55	-52.67	-56.77	-60.85	-64.92	-68.97	-73.01
42	Flu + $\cdot\text{OH} \rightarrow$ Flu-C1 + H_2O	$\Delta G^\ddagger$	6.46	9.07	11.62	14.14	16.64	19.12	21.57	24.01	26.42	28.82	31.21	33.58	35.94
		$\Delta_r G_m^\circ$	-36.19	-36.51	-36.84	-37.18	-37.51	-37.84	-38.16	-38.48	-38.78	-39.08	-39.37	-39.64	-39.92
43	Flu + $\cdot\text{H} \rightarrow$ Flu-C1 + H_2	$\Delta G^\ddagger$	11.95	14.28	16.60	18.93	21.26	23.60	25.93	28.27	30.60	32.93	35.27	37.60	39.94
		$\Delta_r G_m^\circ$	-21.53	-21.85	-22.20	-22.56	-22.93	-23.30	-23.66	-24.01	-24.34	-24.67	-24.98	-25.27	-25.55
44	Flu + $\cdot\text{CH}_3 \rightarrow$ Flu-C1 + CH_4	$\Delta G^\ddagger$	17.24	21.04	24.79	28.55	32.31	36.06	39.80	43.53	47.25	50.96	54.67	58.37	62.06
		$\Delta_r G_m^\circ$	-21.26	-21.06	-20.82	-20.57	-20.29	-20.01	-19.71	-19.40	-19.10	-18.78	-18.47	-18.15	-17.83
45	Flu + $\text{O}_2 \rightarrow$ Flu-C1 + $\cdot\text{OOH}$	$\Delta G^\ddagger$	43.51	46.47	49.32	52.12	54.87	57.58	60.25	62.90	65.52	68.11	70.69	73.25	75.80
		$\Delta_r G_m^\circ$	32.69	32.18	31.66	31.12	30.58	30.03	29.47	28.93	28.38	27.84	27.31	26.78	26.25
46	Flu-C1 + $\text{O}_2 \rightarrow$ Flu-C2	$\Delta_r G_m^\circ$	-3.88	-0.23	3.34	6.90	10.44	13.96	17.45	20.92	24.37	27.79	31.19	34.58	37.94
47	Flu-C2 $\rightarrow$ Flu-C3	$\Delta G^\ddagger$	35.82	36.24	36.69	37.16	37.66	38.17	38.70	39.24	39.81	40.38	40.97	41.57	42.19
		$\Delta_r G_m^\circ$	30.04	30.41	30.76	31.11	31.45	31.78	32.10	32.41	32.72	33.03	33.34	33.64	33.94
48	Flu-C3 $\rightarrow$ Flu-C4	$\Delta G^\ddagger$	13.21	13.34	13.48	13.64	13.83	14.04	14.27	14.51	14.78	15.06	15.35	15.66	15.98
		$\Delta_r G_m^\circ$	-81.82	-82.63	-83.47	-84.31	-85.17	-86.02	-86.87	-87.72	-88.57	-89.42	-90.26	-91.11	-91.95
49	Flu-C4 $\rightarrow$ Flu-C5	$\Delta G^\ddagger$	28.62	29.20	29.81	30.45	31.13	31.82	32.53	33.27	34.02	34.79	35.57	36.37	37.18
		$\Delta_r G_m^\circ$	14.99	15.37	15.75	16.13	16.50	16.87	17.23	17.59	17.95	18.31	18.66	19.01	19.37
50	Flu-C5 $\rightarrow$ DF + $\cdot\text{CHO}$	$\Delta G^\ddagger$	8.26	8.32	8.40	8.50	8.63	8.78	8.95	9.14	9.35	9.58	9.82	10.07	10.34
		$\Delta_r G_m^\circ$	-22.34	-25.78	-29.55	-33.28	-36.97	-40.63	-44.28	-47.89	-51.49	-55.07	-58.63	-62.18	-65.71
51	Flu-C2 $\rightarrow$ 9FO + $\cdot\text{OH}$	$\Delta G^\ddagger$	38.93	39.05	39.18	39.31	39.44	39.59	39.74	39.89	40.06	40.23	40.40	40.59	40.79
		$\Delta_r G_m^\circ$	-40.00	-43.48	-46.93	-50.38	-53.82	-57.25	-60.66	-64.05	-67.42	-70.76	-74.08	-77.39	-80.67
52	Flu-C1 + $\cdot\text{OOH} \rightarrow$ Flu-D1	$\Delta_r G_m^\circ$	-38.77	-34.53	-30.39	-26.28	-22.20	-18.15	-14.14	-10.16	-6.21	-2.29	1.61	5.48	9.32
53	Flu-D1 $\rightarrow$ 9FO + H_2O	$\Delta G^\ddagger$	53.85	53.71	53.56	53.39	53.22	53.04	52.86	52.68	52.51	52.34	52.17	52.01	51.85
		$\Delta_r G_m^\circ$	-74.00	-77.88	-81.70	-85.50	-89.27	-93.01	-96.71	-100.38	-104.01	-107.60	-111.17	-114.71	-118.22

Table S5. Calculated activation enthalpies and standard enthalpy changes (in kcal/mol) for the reactions from 9-methylfluorene (9MF) to dibenzofuran (DF) and 9-fluorenone (9FO).

No.	Elementary Reactions		Temperature (K)												
			298.15	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500
54	9MF + $\cdot\text{OH}$ $\rightarrow$ <i>trans</i> -9MF-A1	$\Delta H^\ddagger$	-0.42	-0.43	-0.39	-0.33	-0.26	-0.17	-0.09	0.00	0.09	0.19	0.28	0.37	0.47
		$\Delta_r H_m^\circ$	-19.10	-19.08	-18.96	-18.78	-18.57	-18.33	-18.08	-17.82	-17.55	-17.27	-17.00	-16.72	-16.43
55	<i>trans</i> -9MF-A1 $\rightarrow$ 9MF-A2	$\Delta H^\ddagger$	24.94	24.95	24.91	24.82	24.71	24.58	24.44	24.28	24.12	23.95	23.78	23.60	23.42
		$\Delta_r H_m^\circ$	-4.66	-4.50	-4.40	-4.34	-4.29	-4.27	-4.25	-4.24	-4.23	-4.23	-4.23	-4.23	-4.23
56	9MF-A2 $\rightarrow$ 9MF-A3	$\Delta H^\ddagger$	18.65	18.35	18.10	17.89	17.72	17.58	17.46	17.35	17.24	17.14	17.04	16.93	16.82
		$\Delta_r H_m^\circ$	1.09	0.92	0.76	0.63	0.52	0.44	0.38	0.34	0.31	0.29	0.28	0.28	0.28
57	9MF-A3 $\rightarrow$ 9MF-A4	$\Delta H^\ddagger$	25.74	25.55	25.39	25.22	25.06	24.89	24.71	24.53	24.35	24.17	23.99	23.80	23.61
		$\Delta_r H_m^\circ$	7.96	7.9	7.88	7.89	7.91	7.93	7.96	7.98	7.99	8.01	8.02	8.03	8.04
58	9MF-A4 $\rightarrow$ DF + $\cdot\text{C}_2\text{H}_5$	$\Delta H^\ddagger$	16.32	16.31	16.25	16.17	16.05	15.91	15.77	15.61	15.44	15.27	15.09	14.91	14.73
		$\Delta_r H_m^\circ$	-10.63	-10.66	-10.75	-10.88	-11.03	-11.2	-11.38	-11.56	-11.75	-11.95	-12.14	-12.34	-12.53
59	9MF + $\cdot\text{OH}$ $\rightarrow$ <i>cis</i> -9MF-A1	$\Delta H^\ddagger$	0.13	0.13	0.17	0.23	0.30	0.38	0.47	0.56	0.65	0.74	0.83	0.93	1.02
		$\Delta_r H_m^\circ$	-18.86	-18.84	-18.72	-18.54	-18.33	-18.09	-17.84	-17.58	-17.31	-17.04	-16.76	-16.48	-16.20
60	<i>cis</i> -9MF-A1 $\rightarrow$ 9MF-A2	$\Delta H^\ddagger$	23.87	23.85	23.79	23.70	23.58	23.45	23.30	23.14	22.98	22.81	22.63	22.46	22.28
		$\Delta_r H_m^\circ$	-4.90	-4.74	-4.64	-4.58	-4.53	-4.51	-4.49	-4.48	-4.47	-4.46	-4.46	-4.46	-4.46
61	9MF + $\cdot\text{OCl}$ $\rightarrow$ <i>trans</i> -9MF-B1	$\Delta H^\ddagger$	3.82	3.95	4.09	4.22	4.36	4.49	4.62	4.74	4.86	4.97	5.08	5.19	5.30
		$\Delta_r H_m^\circ$	-3.37	-3.14	-2.85	-2.53	-2.21	-1.88	-1.56	-1.23	-0.91	-0.59	-0.28	0.04	0.35
62	<i>trans</i> -9MF-B1 $\rightarrow$ 9MF-B2	$\Delta H^\ddagger$	26.43	26.41	26.34	26.24	26.11	25.97	25.82	25.66	25.49	25.32	25.14	24.96	24.78
		$\Delta_r H_m^\circ$	0.33	0.49	0.59	0.66	0.70	0.74	0.76	0.77	0.78	0.79	0.79	0.80	0.80
63	9MF-B2 $\rightarrow$ 9MF-B3	$\Delta H^\ddagger$	12.81	12.68	12.53	12.36	12.19	12.00	11.82	11.63	11.44	11.25	11.05	10.86	10.66
		$\Delta_r H_m^\circ$	-44.44	-44.56	-44.66	-44.75	-44.82	-44.89	-44.94	-44.98	-45.02	-45.05	-45.08	-45.11	-45.13
64	9MF-B3 $\rightarrow$ 9MF-B4	$\Delta H^\ddagger$	29.15	28.99	28.83	28.68	28.52	28.35	28.18	28.01	27.83	27.65	27.47	27.28	27.10
		$\Delta_r H_m^\circ$	7.83	7.76	7.75	7.75	7.77	7.79	7.81	7.83	7.85	7.87	7.88	7.89	7.90
65	9MF-B4 $\rightarrow$ DF + $\cdot\text{C}_2\text{ClH}_4$	$\Delta H^\ddagger$	13.29	13.23	13.12	12.98	12.83	12.66	12.48	12.30	12.12	11.93	11.75	11.56	11.37
		$\Delta_r H_m^\circ$	-10.45	-10.55	-10.70	-10.87	-11.05	-11.25	-11.45	-11.65	-11.85	-12.05	-12.25	-12.46	-12.66

Table S5. *Cont.*

No.	Elementary Reactions		Temperature (K)												
			298.15	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500
66	9MF + ·OCl → <i>cis</i> -9MF-B1	$\Delta H^\ddagger$	4.86	4.99	5.13	5.26	5.40	5.53	5.65	5.77	5.89	6.01	6.12	6.23	6.34
		$\Delta_r H_m^0$	-2.60	-2.36	-2.08	-1.76	-1.44	-1.11	-0.79	-0.46	-0.14	0.17	0.49	0.80	1.12
67	<i>cis</i> -9MF-B1 → 9MF-B2	$\Delta H^\ddagger$	27.09	27.04	26.95	26.84	26.71	26.56	26.41	26.24	26.07	25.90	25.72	25.54	25.35
		$\Delta_r H_m^0$	-0.44	-0.28	-0.18	-0.11	-0.07	-0.03	-0.01	0.00	0.01	0.02	0.03	0.03	0.03
68	9MF + ·OH → 9MF-C1 + H ₂ O	$\Delta H^\ddagger$	-2.33	-2.28	-2.18	-2.05	-1.9	-1.73	-1.56	-1.38	-1.21	-1.04	-0.87	-0.71	-0.55
		$\Delta_r H_m^0$	-39.31	-39.21	-39.16	-39.15	-39.17	-39.22	-39.29	-39.37	-39.46	-39.57	-39.68	-39.79	-39.91
69	9MF + ·H → 9MF-C1 + H ₂	$\Delta H^\ddagger$	3.44	3.34	3.28	3.25	3.24	3.24	3.24	3.24	3.24	3.23	3.22	3.20	3.18
		$\Delta_r H_m^0$	-24.69	-24.50	-24.38	-24.33	-24.33	-24.37	-24.46	-24.57	-24.71	-24.86	-25.03	-25.21	-25.41
70	9MF + ·CH ₃ → 9MF-C1 + CH ₄	$\Delta H^\ddagger$	5.14	5.25	5.42	5.64	5.90	6.17	6.46	6.75	7.04	7.33	7.61	7.89	8.17
		$\Delta_r H_m^0$	-25.80	-25.91	-26.03	-26.15	-26.25	-26.33	-26.40	-26.46	-26.51	-26.55	-26.58	-26.61	-26.63
71	9MF + O ₂ → 9MF-C1 + ·OOH	$\Delta H^\ddagger$	32.09	32.33	32.60	32.88	33.16	33.44	33.71	33.97	34.22	34.46	34.69	34.90	35.11
		$\Delta_r H_m^0$	30.11	30.24	30.33	30.40	30.44	30.45	30.44	30.41	30.36	30.31	30.24	30.17	30.09
72	9MF-C1 + O ₂ → 9MF-C2	$\Delta_r H_m^0$	-14.29	-14.29	-14.19	-14.03	-13.84	-13.62	-13.38	-13.13	-12.87	-12.61	-12.34	-12.07	-11.80
73	9MF-C2 → 9MF-C3	$\Delta_r H_m^0$	33.30	33.19	33.07	32.96	32.83	32.69	32.55	32.40	32.24	32.08	31.91	31.74	31.57
		$\Delta_r H_m^0$	27.15	27.16	27.20	27.25	27.31	27.36	27.41	27.46	27.50	27.53	27.57	27.60	27.62
74	9MF-C3 → 9MF-C4	$\Delta H^\ddagger$	11.94	11.85	11.72	11.58	11.42	11.25	11.07	10.89	10.71	10.53	10.34	10.15	9.96
		$\Delta_r H_m^0$	-80.21	-80.04	-79.96	-79.93	-79.92	-79.93	-79.95	-79.97	-79.99	-80.01	-80.03	-80.05	-80.07
75	9MF-C4 → 9MF-C5	$\Delta H^\ddagger$	27.15	26.97	26.81	26.64	26.48	26.31	26.14	25.97	25.79	25.60	25.42	25.23	25.05
		$\Delta_r H_m^0$	13.30	13.25	13.25	13.27	13.30	13.33	13.35	13.38	13.40	13.42	13.43	13.45	13.46
76	9MF-C5 → DF + ·COCH ₃	$\Delta H^\ddagger$	7.81	7.73	7.60	7.44	7.27	7.08	6.89	6.69	6.49	6.29	6.09	5.89	5.69
		$\Delta_r H_m^0$	-10.27	-10.45	-10.67	-10.90	-11.13	-11.36	-11.59	-11.81	-12.03	-12.25	-12.47	-12.69	-12.90
77	9MF-C1 + ·OOH → 9MF-D1	$\Delta_r H_m^0$	-50.60	-50.53	-50.37	-50.14	-49.88	-49.59	-49.28	-48.96	-48.63	-48.29	-47.94	-47.59	-47.23
78	9MF-D1 → 9MF-D2 + ·OH	$\Delta_r H_m^0$	44.34	44.50	44.57	44.57	44.52	44.41	44.28	44.11	43.93	43.73	43.52	43.30	43.06
79	9MF-D2 → 9FO + ·CH ₃	$\Delta H^\ddagger$	11.34	11.40	11.41	11.38	11.32	11.23	11.11	10.98	10.84	10.68	10.51	10.34	10.17
		$\Delta_r H_m^0$	3.60	3.74	3.75	3.65	3.48	3.25	2.98	2.68	2.36	2.03	1.68	1.32	0.95

Table S6. Calculated Gibbs energies of activation and standard Gibbs energy changes (in kcal/mol) for the reactions from 9-methylfluorene (9MF) to dibenzofuran (DF) and 9-fluorenone (9FO).

No.	Elementary Reactions		Temperature (K)												
			298.15	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500
54	9MF + ·OH → <i>trans</i> -9MF-A1	$\Delta G^\ddagger$	9.28	12.60	15.85	19.09	22.32	25.54	28.75	31.95	35.14	38.33	41.50	44.67	47.83
		$\Delta_r G_m^\circ$	-8.72	-5.17	-1.71	1.73	5.13	8.50	11.84	15.14	18.43	21.69	24.92	28.14	31.33
55	<i>trans</i> -9MF-A1 → 9MF-A2	$\Delta G^\ddagger$	24.08	23.78	23.49	23.21	22.95	22.71	22.48	22.27	22.08	21.90	21.74	21.59	21.45
		$\Delta_r G_m^\circ$	-6.85	-7.63	-8.42	-9.23	-10.05	-10.88	-11.71	-12.54	-13.36	-14.20	-15.03	-15.86	-16.69
56	9MF-A2 → 9MF-A3	$\Delta G^\ddagger$	20.96	21.80	22.69	23.63	24.60	25.60	26.61	27.63	28.66	29.70	30.76	31.81	32.88
		$\Delta_r G_m^\circ$	1.46	1.61	1.80	2.02	2.26	2.52	2.78	3.05	3.32	3.60	3.87	4.15	4.43
57	9MF-A3 → 9MF-A4	$\Delta G^\ddagger$	27.74	28.45	29.19	29.97	30.78	31.60	32.45	33.32	34.21	35.12	36.04	36.97	37.92
		$\Delta_r G_m^\circ$	9.78	10.41	11.04	11.67	12.30	12.92	13.55	14.17	14.79	15.40	16.02	16.63	17.25
58	9MF-A4 → DF + ·C ₂ H ₅	$\Delta G^\ddagger$	15.80	15.63	15.46	15.31	15.18	15.07	14.97	14.89	14.83	14.78	14.74	14.72	14.72
		$\Delta_r G_m^\circ$	-23.43	-27.23	-31.38	-35.50	-39.59	-43.66	-47.70	-51.73	-55.74	-59.73	-63.70	-67.66	-71.61
59	9MF + ·OH → <i>cis</i> -9MF-A1	$\Delta G^\ddagger$	9.77	13.06	16.29	19.51	22.72	25.91	29.10	32.28	35.44	38.60	41.75	44.90	48.04
		$\Delta_r G_m^\circ$	-8.51	-4.97	-1.51	1.91	5.30	8.66	11.99	15.29	18.57	21.82	25.04	28.25	31.43
60	<i>cis</i> -9MF-A1 → 9MF-A2	$\Delta G^\ddagger$	23.13	22.87	22.64	22.41	22.21	22.02	21.85	21.70	21.56	21.44	21.33	21.24	21.16
		$\Delta_r G_m^\circ$	-7.07	-7.83	-8.62	-9.42	-10.23	-11.04	-11.86	-12.68	-13.50	-14.33	-15.15	-15.97	-16.79
61	9MF + ·OCl → <i>trans</i> -9MF-B1	$\Delta G^\ddagger$	14.91	18.68	22.34	25.98	29.59	33.19	36.77	40.34	43.89	47.43	50.97	54.49	58.01
		$\Delta_r G_m^\circ$	8.06	11.93	15.66	19.34	22.96	26.53	30.06	33.56	37.02	40.45	43.86	47.25	50.61
62	<i>trans</i> -9MF-B1 → 9MF-B2	$\Delta G^\ddagger$	26.15	26.06	25.98	25.92	25.87	25.85	25.84	25.85	25.88	25.92	25.98	26.05	26.14
		$\Delta_r G_m^\circ$	-2.45	-3.42	-4.41	-5.42	-6.44	-7.46	-8.49	-9.51	-10.54	-11.57	-12.60	-13.63	-14.66
63	9MF-B2 → 9MF-B3	$\Delta G^\ddagger$	13.19	13.34	13.52	13.73	13.97	14.24	14.53	14.84	15.17	15.52	15.89	16.26	16.66
		$\Delta_r G_m^\circ$	-43.72	-43.46	-43.17	-42.86	-42.54	-42.21	-41.87	-41.53	-41.18	-40.83	-40.48	-40.12	-39.76
64	9MF-B3 → 9MF-B4	$\Delta G^\ddagger$	31.57	32.42	33.29	34.20	35.13	36.09	37.07	38.06	39.08	40.11	41.15	42.21	43.29
		$\Delta_r G_m^\circ$	10.25	11.09	11.93	12.76	13.60	14.43	15.26	16.08	16.91	17.73	18.55	19.37	20.19
65	9MF-B4 → DF + ·C ₂ ClH ₄	$\Delta G^\ddagger$	12.72	12.54	12.38	12.24	12.13	12.05	11.98	11.93	11.91	11.89	11.90	11.92	11.95
		$\Delta_r G_m^\circ$	-23.72	-27.68	-31.95	-36.19	-40.40	-44.57	-48.73	-52.86	-56.97	-61.07	-65.14	-69.20	-73.25
66	9MF + ·OCl → <i>cis</i> -9MF-B1	$\Delta G^\ddagger$	15.95	19.73	23.39	27.03	30.65	34.25	37.83	41.4	44.96	48.51	52.04	55.57	59.09
		$\Delta_r G_m^\circ$	8.82	12.69	16.42	20.09	23.70	27.27	30.80	34.29	37.75	41.18	44.59	47.97	51.33

Table S6. *Cont.*

No.	Elementary Reactions		Temperature (K)												
			298.15	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500
67	<i>cis</i> -9MF-B1 → 9MF-B2	$\Delta G^\ddagger$	26.79	26.69	26.61	26.55	26.52	26.50	26.50	26.52	26.56	26.61	26.67	26.75	26.85
		$\Delta_r G_m^\circ$	-3.21	-4.18	-5.17	-6.17	-7.18	-8.20	-9.22	-10.25	-11.27	-12.30	-13.33	-14.36	-15.38
68	9MF + ·OH → 9MF-C1 + H ₂ O	$\Delta G^\ddagger$	5.88	8.67	11.40	14.11	16.78	19.44	22.08	24.69	27.29	29.88	32.45	35.01	37.55
		$\Delta_r G_m^\circ$	-41.84	-42.73	-43.61	-44.51	-45.40	-46.29	-47.17	-48.04	-48.90	-49.75	-50.60	-51.43	-52.26
69	9MF + ·H → 9MF-C1 + H ₂	$\Delta G^\ddagger$	9.99	12.25	14.48	16.72	18.97	21.22	23.46	25.71	27.96	30.20	32.45	34.70	36.95
		$\Delta_r G_m^\circ$	-27.18	-28.06	-28.97	-29.89	-30.82	-31.74	-32.66	-33.57	-34.46	-35.34	-36.20	-37.06	-37.90
70	9MF + ·CH ₃ → 9MF-C1 + CH ₄	$\Delta G^\ddagger$	14.20	17.27	20.26	23.21	26.12	28.99	31.82	34.63	37.40	40.15	42.87	45.57	48.25
		$\Delta_r G_m^\circ$	-26.91	-27.27	-27.60	-27.90	-28.18	-28.45	-28.71	-28.96	-29.21	-29.46	-29.70	-29.94	-30.17
71	9MF + O ₂ → 9MF-C1 + ·OOH	$\Delta G^\ddagger$	40.87	43.83	46.67	49.46	52.20	54.90	57.57	60.21	62.82	65.41	67.98	70.53	73.07
		$\Delta_r G_m^\circ$	27.04	25.97	24.89	23.79	22.69	21.58	20.47	19.37	18.27	17.17	16.08	14.99	13.91
72	9MF-C1 + O ₂ → 9MF-C2	$\Delta_r G_m^\circ$	-1.52	2.85	7.12	11.37	15.59	19.78	23.94	28.07	32.18	36.26	40.32	44.37	48.39
73	9MF-C2 → 9MF-C3	$\Delta G^\ddagger$	34.09	34.38	34.69	35.03	35.38	35.75	36.15	36.55	36.98	37.41	37.87	38.33	38.81
		$\Delta_r G_m^\circ$	27.78	27.99	28.19	28.39	28.57	28.75	28.92	29.09	29.25	29.41	29.56	29.71	29.86
74	9MF-C3 → 9MF-C4	$\Delta G^\ddagger$	11.86	11.85	11.86	11.91	11.97	12.06	12.18	12.31	12.46	12.63	12.81	13.01	13.22
		$\Delta_r G_m^\circ$	-82.69	-83.57	-84.46	-85.36	-86.27	-87.17	-88.08	-88.98	-89.88	-90.77	-91.67	-92.57	-93.46
75	9MF-C4 → 9MF-C5	$\Delta G^\ddagger$	28.93	29.56	30.23	30.93	31.66	32.41	33.18	33.97	34.78	35.61	36.45	37.30	38.17
		$\Delta_r G_m^\circ$	14.38	14.75	15.13	15.50	15.87	16.24	16.60	16.96	17.32	17.67	18.02	18.38	18.73
76	9MF-C5 → DF + ·COCH ₃	$\Delta G^\ddagger$	7.21	7.01	6.84	6.71	6.60	6.51	6.46	6.42	6.40	6.40	6.42	6.45	6.50
		$\Delta_r G_m^\circ$	-22.30	-25.82	-29.65	-33.43	-37.16	-40.87	-44.54	-48.19	-51.82	-55.42	-59.01	-62.58	-66.14
77	9MF-C1 + ·OOH → 9MF-D1	$\Delta_r G_m^\circ$	-36.01	-31.03	-26.17	-21.36	-16.58	-11.84	-7.14	-2.48	2.16	6.76	11.33	15.88	20.40
78	9MF-D1 → 9MF-D2 + ·OH	$\Delta_r G_m^\circ$	32.72	28.73	24.78	20.82	16.86	12.92	8.99	5.08	1.18	-2.70	-6.56	-10.40	-14.23
79	9MF-D2 → 9FO + ·CH ₃	$\Delta G^\ddagger$	11.21	11.16	11.10	11.04	10.99	10.94	10.91	10.90	10.90	10.91	10.94	10.98	11.03
		$\Delta_r G_m^\circ$	-8.46	-12.61	-16.70	-20.78	-24.84	-28.87	-32.87	-36.84	-40.78	-44.68	-48.56	-52.41	-56.24

Table S7. Calculated activation enthalpies and standard enthalpy changes (in kcal/mol) for the reactions from 9-fluorenone (9FO) to dibenzofuran (DF).

No.	Elementary Reactions		Temperature (K)												
			298.15	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500
80	9FO + ·OH → 9FO-A1	$\Delta H^\ddagger$	7.86	7.80	7.81	7.85	7.91	7.98	8.07	8.16	8.25	8.35	8.44	8.54	8.64
		$\Delta_r H_m^\circ$	-14.52	-14.54	-14.45	-14.30	-14.11	-13.88	-13.64	-13.38	-13.12	-12.84	-12.57	-12.29	-12.01
81	9FO-A1 → 9FO-A2	$\Delta H^\ddagger$	10.31	10.22	10.09	9.94	9.77	9.59	9.41	9.23	9.04	8.85	8.66	8.47	8.27
		$\Delta_r H_m^\circ$	-1.07	-1.06	-1.08	-1.12	-1.15	-1.19	-1.22	-1.25	-1.28	-1.31	-1.33	-1.35	-1.36
82	9FO-A2 + O ^{3P} → 9FO-A3	$\Delta_r H_m^\circ$	-127.05	-127.16	-127.22	-127.24	-127.24	-127.22	-127.18	-127.14	-127.08	-127.02	-126.96	-126.89	-126.81
83	9FO-A3 → 9FO-A4	$\Delta H^\ddagger$	28.46	28.29	28.13	27.97	27.80	27.64	27.47	27.29	27.11	26.93	26.75	26.56	26.38
		$\Delta_r H_m^\circ$	15.45	15.40	15.39	15.40	15.42	15.44	15.47	15.49	15.51	15.52	15.54	15.55	15.56
84	9FO-A4 → DF + ·COOH	$\Delta H^\ddagger$	12.95	12.89	12.78	12.63	12.47	12.29	12.10	11.91	11.72	11.53	11.33	11.14	10.95
		$\Delta_r H_m^\circ$	4.55	4.29	3.94	3.55	3.15	2.74	2.32	1.91	1.49	1.07	0.66	0.25	-0.16
85	9FO + ·OH → 9FO-B1	$\Delta H^\ddagger$	0.97	0.97	1.00	1.06	1.13	1.21	1.30	1.39	1.48	1.57	1.66	1.76	1.85
		$\Delta_r H_m^\circ$	-16.74	-16.71	-16.59	-16.41	-16.20	-15.96	-15.71	-15.44	-15.17	-14.89	-14.61	-14.33	-14.05
86	9FO-B1 → 9FO-B2	$\Delta H^\ddagger$	16.84	16.77	16.67	16.53	16.38	16.21	16.03	15.85	15.66	15.47	15.28	15.09	14.90
		$\Delta_r H_m^\circ$	-2.70	-2.61	-2.58	-2.58	-2.60	-2.62	-2.64	-2.67	-2.69	-2.71	-2.73	-2.75	-2.77
87	9FO-B2 → Flu-C4	$\Delta H^\ddagger$	14.79	14.54	14.34	14.18	14.05	13.94	13.84	13.76	13.67	13.58	13.50	13.40	13.31
		$\Delta_r H_m^\circ$	-1.22	-1.33	-1.42	-1.48	-1.53	-1.55	-1.56	-1.56	-1.54	-1.53	-1.50	-1.48	-1.45
88	9FO-B2 → Phe-B5	$\Delta H^\ddagger$	24.24	24.27	24.25	24.19	24.09	23.97	23.84	23.69	23.53	23.37	23.20	23.02	22.85
		$\Delta_r H_m^\circ$	23.24	23.20	23.10	22.94	22.74	22.52	22.29	22.03	21.77	21.50	21.23	20.95	20.67
89	9FO + ·OCl → 9FO-C1	$\Delta H^\ddagger$	6.62	6.74	6.87	7.01	7.14	7.27	7.39	7.51	7.63	7.75	7.86	7.97	8.08
		$\Delta_r H_m^\circ$	-0.29	-0.05	0.24	0.55	0.88	1.21	1.53	1.86	2.18	2.51	2.82	3.14	3.46
90	9FO-C1 → 9FO-C2	$\Delta H^\ddagger$	19.13	19.07	18.96	18.83	18.67	18.50	18.32	18.14	17.95	17.76	17.57	17.38	17.18
		$\Delta_r H_m^\circ$	1.53	1.61	1.65	1.65	1.64	1.62	1.60	1.58	1.55	1.54	1.52	1.50	1.49
91	9FO-C2 → 9FO-C3	$\Delta H^\ddagger$	10.46	10.37	10.25	10.11	9.97	9.81	9.65	9.48	9.30	9.13	8.95	8.76	8.58
		$\Delta_r H_m^\circ$	-53.76	-53.80	-53.83	-53.84	-53.85	-53.86	-53.86	-53.86	-53.86	-53.86	-53.86	-53.86	-53.86
92	9FO-C3 → 9FO-C4	$\Delta H^\ddagger$	27.01	26.83	26.66	26.50	26.33	26.16	25.99	25.81	25.63	25.45	25.26	25.08	24.89
		$\Delta_r H_m^\circ$	12.27	12.21	12.19	12.20	12.21	12.23	12.25	12.27	12.28	12.30	12.31	12.32	12.33
93	9FO-C4 → DF + ·CClO	$\Delta H^\ddagger$	6.99	6.92	6.80	6.65	6.48	6.29	6.10	5.90	5.71	5.51	5.31	5.10	4.90
		$\Delta_r H_m^\circ$	-1.48	-1.73	-2.06	-2.44	-2.85	-3.26	-3.68	-4.10	-4.52	-4.94	-5.36	-5.77	-6.19

Table S7. *Cont.*

No.	Elementary Reactions		Temperature (K)												
			298.15	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500
94	9FO-C2 $\rightarrow$ Phe-C5	$\Delta H^\ddagger$	24.11	24.15	24.12	24.06	23.97	23.85	23.71	23.57	23.41	23.25	23.08	22.91	22.73
		$\Delta_r H_m^\circ$	23.60	23.56	23.45	23.30	23.10	22.89	22.65	22.40	22.14	21.87	21.60	21.32	21.04
95	9FO + $\cdot\text{OH}$ $\rightarrow$ 9FO-D1	$\Delta H^\ddagger$	18.09	18.19	18.31	18.44	18.57	18.71	18.84	18.97	19.10	19.22	19.35	19.47	19.58
		$\Delta_r H_m^\circ$	3.15	3.32	3.56	3.84	4.14	4.45	4.77	5.08	5.40	5.71	6.03	6.34	6.65
96	9FO-D1 $\rightarrow$ 9FO-D2	$\Delta H^\ddagger$	11.77	11.72	11.62	11.49	11.34	11.18	11.00	10.83	10.64	10.46	10.27	10.08	9.89
		$\Delta_r H_m^\circ$	2.54	2.60	2.62	2.61	2.60	2.58	2.56	2.54	2.52	2.50	2.49	2.47	2.46
97	9FO-D2 + O^3P $\rightarrow$ 9FO-D3	$\Delta_r H_m^\circ$	-126.66	-126.77	-126.83	-126.85	-126.85	-126.83	-126.79	-126.75	-126.70	-126.63	-126.57	-126.50	-126.42
98	9FO-D3 $\rightarrow$ DF + $\cdot\text{Cl}$ + CO_2	$\Delta H^\ddagger$	29.64	29.46	29.30	29.14	28.98	28.81	28.63	28.46	28.28	28.10	27.91	27.73	27.54
		$\Delta_r H_m^\circ$	-61.43	-61.75	-62.13	-62.54	-62.98	-63.42	-63.87	-64.32	-64.76	-65.21	-65.65	-66.09	-66.53
99	9FO-A2 + O_2 $\rightarrow$ 9FO-S1	$\Delta_r H_m^\circ$	-46.54	-46.50	-46.39	-46.22	-46.02	-45.80	-45.56	-45.30	-45.04	-44.78	-44.51	-44.23	-43.95
100	9FO-S1 $\rightarrow$ 9FO-S2	$\Delta H^\ddagger$	30.49	30.34	30.21	30.10	30.00	29.91	29.83	29.75	29.66	29.58	29.49	29.40	29.30
		$\Delta_r H_m^\circ$	23.18	23.28	23.37	23.44	23.50	23.55	23.60	23.64	23.67	23.70	23.73	23.75	23.78
101	9FO-S2 $\rightarrow$ 9FO-S3	$\Delta H^\ddagger$	6.32	6.28	6.20	6.08	5.95	5.79	5.63	5.45	5.27	5.09	4.90	4.71	4.52
		$\Delta_r H_m^\circ$	-2.54	-2.67	-2.85	-3.08	-3.33	-3.61	-3.90	-4.20	-4.50	-4.81	-5.12	-5.43	-5.74
102	9FO-S3 $\rightarrow$ DF + $\cdot\text{OH}$	$\Delta H^\ddagger$	13.48	13.47	13.42	13.34	13.24	13.12	12.98	12.83	12.67	12.51	12.34	12.17	11.99
		$\Delta_r H_m^\circ$	-62.34	-62.46	-62.64	-62.84	-63.06	-63.31	-63.56	-63.83	-64.10	-64.38	-64.66	-64.94	-65.23
103	9FO-A2 $\rightarrow$ 9FO-S4	$\Delta H^\ddagger$	11.63	11.49	11.38	11.28	11.20	11.12	11.06	10.99	10.92	10.85	10.77	10.69	10.60
		$\Delta_r H_m^\circ$	-0.95	-0.99	-1.03	-1.06	-1.07	-1.08	-1.08	-1.08	-1.07	-1.06	-1.04	-1.02	-1.01
104	9FO-S4 $\rightarrow$ 9FO-S5 + CO_2	$\Delta H^\ddagger$	5.84	5.80	5.73	5.62	5.49	5.34	5.18	5.01	4.83	4.65	4.46	4.28	4.09
		$\Delta_r H_m^\circ$	-5.77	-5.91	-6.09	-6.32	-6.58	-6.86	-7.15	-7.45	-7.76	-8.06	-8.37	-8.68	-8.99
105	9FO-S5 + O_2 $\rightarrow$ Phe-S6	$\Delta_r H_m^\circ$	-44.81	-44.77	-44.66	-44.49	-44.29	-44.06	-43.82	-43.56	-43.30	-43.04	-42.76	-42.49	-42.21
106	9FO-S6 $\rightarrow$ 9FO-S3	$\Delta H^\ddagger$	28.32	28.28	28.26	28.25	28.23	28.22	28.19	28.15	28.10	28.04	27.97	27.89	27.80
		$\Delta_r H_m^\circ$	-2.68	-2.50	-2.36	-2.24	-2.15	-2.07	-1.99	-1.92	-1.85	-1.77	-1.69	-1.60	-1.51
107	9FO-S5 + O^3P $\rightarrow$ 9FO-S7	$\Delta_r H_m^\circ$	-125.14	-125.26	-125.32	-125.34	-125.34	-125.32	-125.29	-125.24	-125.19	-125.13	-125.06	-125.00	-124.92
108	9FO-S7 $\rightarrow$ 9FO-S8	$\Delta H^\ddagger$	26.77	26.56	26.38	26.19	26.01	25.83	25.64	25.46	25.27	25.09	24.90	24.72	24.53

Table S7. *Cont.*

No.	Elementary Reactions		Temperature (K)												
			298.15	298.15	298.15	298.15	298.15	298.15	298.15	298.15	298.15	298.15	298.15	298.15	298.15
109	9FO-S8 $\rightarrow$ DF + $\cdot$ H	$\Delta_r H_m^\circ$	12.37	12.26	12.19	12.16	12.13	12.12	12.12	12.13	12.13	12.14	12.15	12.16	12.17
		$\Delta H^\ddagger$	20.91	20.95	20.98	20.99	20.99	20.98	20.94	20.89	20.83	20.75	20.67	20.57	20.46
		$\Delta_r H_m^\circ$	13.78	14.07	14.28	14.45	14.59	14.70	14.79	14.85	14.90	14.94	14.96	14.96	14.96
110	9FO-D2 + O ₂ $\rightarrow$ 9FO-S9	$\Delta_r H_m^\circ$	-45.68	-45.65	-45.54	-45.37	-45.17	-44.94	-44.70	-44.45	-44.19	-43.92	-43.65	-43.38	-43.10
111	9FO-S9 $\rightarrow$ 9FO-S10 + CO ₂	$\Delta H^\ddagger$	35.50	35.40	35.29	35.17	35.04	34.90	34.75	34.60	34.44	34.27	34.10	33.93	33.75
112	9FO-S10 $\rightarrow$ 9FO-S11	$\Delta_r H_m^\circ$	17.39	-17.93	-17.75	-17.56	-17.37	-17.18	-16.98	-16.78	-16.59	-16.39	-16.19	-15.99	-15.80
		$\Delta H^\ddagger$	7.26	7.22	7.15	7.05	6.92	6.78	6.63	6.46	6.30	6.12	5.94	5.76	5.58
		$\Delta_r H_m^\circ$	-4.51	-4.85	-5.24	-5.67	-6.13	-6.60	-7.09	-7.59	-8.09	-8.60	-9.11	-9.61	-10.12
113	9FO-S11 $\rightarrow$ DF + ClO $\cdot$	$\Delta H^\ddagger$	16.26	16.43	16.54	16.62	16.68	16.73	16.76	16.79	16.81	16.83	16.85	16.86	16.87
114	9FO-D2 $\rightarrow$ 9FO-S12	$\Delta_r H_m^\circ$	-92.97	-93.26	-93.53	-93.77	-93.98	-94.17	-94.35	-94.51	-94.67	-94.82	-94.96	-95.10	-95.23
		$\Delta H^\ddagger$	21.83	21.71	21.57	21.42	21.26	21.10	20.93	20.76	20.58	20.40	20.22	20.03	19.85
		$\Delta_r H_m^\circ$	-46.63	-46.61	-46.59	-46.58	-46.57	-46.56	-46.56	-46.55	-46.55	-46.55	-46.54	-46.54	-46.54
115	9FO-S12 $\rightarrow$ 9FO-S13 + CO ₂	$\Delta H^\ddagger$	6.78	6.74	6.65	6.54	6.41	6.27	6.11	5.94	5.77	5.59	5.41	5.23	5.04
116	9FO-S13 + O ₂ $\rightarrow$ Phe-S14	$\Delta_r H_m^\circ$	-3.83	-3.98	-4.18	-4.42	-4.69	-4.98	-5.27	-5.58	-5.89	-6.20	-6.51	-6.82	-7.13
		$\Delta_r H_m^\circ$	-45.71	-45.66	-45.54	-45.37	-45.17	-44.94	-44.69	-44.44	-44.17	-43.91	-43.63	-43.36	-43.08
		$\Delta H^\ddagger$	30.51	30.46	30.43	30.42	30.40	30.38	30.35	30.31	30.26	30.20	30.13	30.05	29.96
117	9FO-S14 $\rightarrow$ 9FO-S15	$\Delta_r H_m^\circ$	26.31	26.45	26.58	26.68	26.76	26.82	26.86	26.90	26.92	26.94	26.95	26.96	26.96
118	9FO-S15 $\rightarrow$ 1CDF + $\cdot$ OH	$\Delta H^\ddagger$	13.43	13.40	13.34	13.25	13.14	13.02	12.87	12.72	12.56	12.39	12.22	12.04	11.86
119	9FO-S13 + O ^{3P} $\rightarrow$ 9FO-S16	$\Delta_r H_m^\circ$	-64.71	-64.84	-65.01	-65.22	-65.45	-65.70	-65.96	-66.23	-66.51	-66.79	-67.07	-67.35	-67.64
		$\Delta_r H_m^\circ$	-125.40	-125.50	-125.56	-125.58	-125.57	-125.55	-125.51	-125.47	-125.41	-125.35	-125.29	-125.22	-125.14
		$\Delta H^\ddagger$	25.75	25.53	25.33	25.14	24.95	24.76	24.57	24.38	24.19	24.00	23.81	23.62	23.43
120	9FO-S16 $\rightarrow$ 9FO-S17	$\Delta_r H_m^\circ$	10.14	10.02	9.95	9.90	9.87	9.85	9.84	9.84	9.84	9.85	9.85	9.86	9.87
		$\Delta H^\ddagger$	21.03	21.07	21.11	21.12	21.12	21.11	21.07	21.03	20.96	20.89	20.80	20.71	20.60
		$\Delta_r H_m^\circ$	13.67	13.96	14.18	14.35	14.49	14.60	14.69	14.76	14.81	14.84	14.86	14.87	14.87
121	9FO-S17 $\rightarrow$ 1CDF + $\cdot$ H	$\Delta H^\ddagger$	20.40	20.35	20.26	20.15	20.01	19.86	19.69	19.52	19.34	19.15	18.96	18.77	18.57
122	9FO-S16 $\rightarrow$ DF + $\cdot$ Cl	$\Delta_r H_m^\circ$	-22.37	-22.45	-22.58	-22.72	-22.86	-23.01	-23.16	-23.31	-23.45	-23.59	-23.73	-23.87	-24.00

Table S8. Calculated Gibbs energies of activation and standard Gibbs energy changes (in kcal/mol) for the reactions from 9-fluorenone (9FO) to dibenzofuran (DF).

No.	Elementary Reactions		Temperature (K)												
			298.15	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500
80	9FO + ·OH → 9FO-A1	$\Delta G^\ddagger$	17.96	21.42	24.82	28.22	31.61	35.00	38.37	41.73	45.08	48.43	51.76	55.09	58.41
		$\Delta_r G_m^0$	-4.37	-0.89	2.51	5.89	9.24	12.56	15.85	19.11	22.35	25.56	28.75	31.91	35.06
81	9FO-A1 → 9FO-A2	$\Delta G^\ddagger$	10.27	10.27	10.30	10.36	10.44	10.55	10.68	10.84	11.00	11.19	11.39	11.61	11.84
		$\Delta_r G_m^0$	-2.75	-3.33	-3.89	-4.45	-5.00	-5.55	-6.09	-6.63	-7.17	-7.71	-8.24	-8.77	-9.30
82	9FO-A2 + O ^{3P} → 9FO-A3	$\Delta_r G_m^0$	-116.86	-113.37	-109.91	-106.45	-102.98	-99.52	-96.06	-92.60	-89.15	-85.70	-82.26	-78.83	-75.40
83	9FO-A3 → 9FO-A4	$\Delta G^\ddagger$	29.91	30.44	30.99	31.58	32.20	32.83	33.50	34.17	34.87	35.58	36.31	37.06	37.81
		$\Delta_r G_m^0$	16.02	16.23	16.44	16.64	16.85	17.05	17.25	17.45	17.64	17.84	18.03	18.22	18.41
84	9FO-A4 → DF + ·COOH	$\Delta G^\ddagger$	12.67	12.58	12.52	12.48	12.47	12.48	12.51	12.57	12.64	12.74	12.84	12.97	13.11
		$\Delta_r G_m^0$	-7.39	-10.87	-14.63	-18.31	-21.93	-25.48	-28.98	-32.44	-35.85	-39.23	-42.57	-45.88	-49.16
85	9FO + ·OH → 9FO-B1	$\Delta G^\ddagger$	10.36	13.56	16.71	19.84	22.97	26.08	29.19	32.28	35.36	38.44	41.51	44.57	47.63
		$\Delta_r G_m^0$	-6.69	-3.25	0.10	3.42	6.71	9.97	13.19	16.39	19.56	22.70	25.82	28.92	32.00
86	9FO-B1 → 9FO-B2	$\Delta G^\ddagger$	16.86	16.87	16.91	16.97	17.05	17.16	17.29	17.44	17.61	17.79	17.99	18.21	18.44
		$\Delta_r G_m^0$	-4.43	-5.04	-5.65	-6.26	-6.87	-7.48	-8.09	-8.70	-9.30	-9.90	-10.49	-11.09	-11.69
87	9FO-B2 → Flu-C4	$\Delta G^\ddagger$	16.72	17.42	18.16	18.94	19.75	20.57	21.40	22.25	23.10	23.96	24.83	25.70	26.59
		$\Delta_r G_m^0$	-0.66	-0.46	-0.23	0.02	0.27	0.53	0.79	1.05	1.31	1.57	1.83	2.08	2.34
88	9FO-B2 → Phe-B5	$\Delta G^\ddagger$	22.53	21.94	21.36	20.79	20.23	19.69	19.16	18.65	18.15	17.67	17.20	16.74	16.30
		$\Delta_r G_m^0$	12.33	8.60	4.97	1.36	-2.23	-5.78	-9.30	-12.80	-16.27	-19.72	-23.14	-26.54	-29.93
89	9FO + ·OCl → 9FO-C1	$\Delta G^\ddagger$	17.28	20.91	24.44	27.94	31.41	34.87	38.32	41.75	45.16	48.57	51.97	55.36	58.74
		$\Delta_r G_m^0$	10.87	14.65	18.29	21.88	25.40	28.89	32.33	35.73	39.10	42.44	45.76	49.05	52.32
90	9FO-C1 → 9FO-C2	$\Delta G^\ddagger$	18.79	18.68	18.60	18.54	18.50	18.49	18.50	18.52	18.57	18.64	18.72	18.81	18.92
		$\Delta_r G_m^0$	-0.64	-1.40	-2.16	-2.92	-3.68	-4.44	-5.19	-5.95	-6.70	-7.45	-8.19	-8.94	-9.69
91	9FO-C2 → 9FO-C3	$\Delta G^\ddagger$	11.33	11.63	11.96	12.32	12.70	13.10	13.52	13.96	14.42	14.89	15.38	15.88	16.39
		$\Delta_r G_m^0$	-53.11	-52.88	-52.65	-52.41	-52.17	-51.93	-51.69	-51.45	-51.21	-50.97	-50.73	-50.48	-50.24
92	9FO-C3 → 9FO-C4	$\Delta G^\ddagger$	28.96	29.66	30.38	31.14	31.93	32.74	33.58	34.43	35.30	36.19	37.09	38.01	38.94
		$\Delta_r G_m^0$	13.63	14.10	14.58	15.05	15.53	16.00	16.47	16.94	17.40	17.87	18.33	18.79	19.26
93	9FO-C4 → DF + ·CClO	$\Delta G^\ddagger$	6.63	6.52	6.43	6.37	6.34	6.33	6.35	6.38	6.44	6.52	6.61	6.72	6.84
		$\Delta_r G_m^0$	-13.91	-17.55	-21.49	-25.33	-29.12	-32.84	-36.52	-40.14	-43.72	-47.27	-50.78	-54.26	-57.71

Table S8. *Cont.*

No.	Elementary Reactions		Temperature (K)												
			298.15	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500
94	9FO-C2 $\rightarrow$ Phe-C5	$\Delta G^\ddagger$	22.28	21.64	21.02	20.40	19.80	19.21	18.64	18.08	17.54	17.02	16.50	16.00	15.52
		$\Delta_r G_m^\circ$	12.57	8.80	5.13	1.47	-2.15	-5.74	-9.31	-12.84	-16.35	-19.84	-23.31	-26.75	-30.17
95	9FO + $\cdot$ OH $\rightarrow$ 9FO-D1	$\Delta G^\ddagger$	29.26	33.07	36.77	40.46	44.11	47.76	51.38	54.98	58.58	62.16	65.74	69.30	72.86
		$\Delta_r G_m^\circ$	14.40	18.21	21.91	25.55	29.15	32.70	36.21	39.69	43.13	46.55	49.94	53.31	56.65
96	9FO-D1 $\rightarrow$ 9FO-D2	$\Delta G^\ddagger$	11.44	11.33	11.24	11.18	11.14	11.12	11.12	11.15	11.19	11.25	11.32	11.41	11.51
		$\Delta_r G_m^\circ$	0.47	-0.25	-0.96	-1.68	-2.39	-3.10	-3.81	-4.52	-5.23	-5.93	-6.63	-7.33	-8.03
97	9FO-D2 + O ^{3P} $\rightarrow$ 9FO-D3	$\Delta_r G_m^\circ$	-116.45	-112.94	-109.48	-106.00	-102.53	-99.06	-95.59	-92.12	-88.66	-85.21	-81.76	-78.31	-74.87
98	9FO-D 3 $\rightarrow$ DF + $\cdot$ Cl + CO ₂	$\Delta G^\ddagger$	30.97	31.46	31.97	32.52	33.10	33.70	34.32	34.96	35.62	36.30	36.99	37.69	38.41
		$\Delta_r G_m^\circ$	-79.49	-85.05	-90.85	-96.56	-102.19	-107.76	-113.28	-118.74	-124.16	-129.55	-134.89	-140.20	-145.48
99	9FO-A2 + O ₂ $\rightarrow$ 9FO-S1	$\Delta_r G_m^\circ$	-34.96	-31.01	-27.15	-23.31	-19.51	-15.74	-11.99	-8.28	-4.59	-0.92	2.72	6.35	9.95
		$\Delta_r G_m^\circ$	-0.66	-0.46	-0.23	0.02	0.27	0.53	0.79	1.05	1.31	1.57	1.83	2.08	2.34
100	9FO-S1 $\rightarrow$ 9FO-S2	$\Delta G^\ddagger$	31.98	32.52	33.07	33.66	34.26	34.88	35.50	36.14	36.78	37.43	38.09	38.75	39.42
		$\Delta_r G_m^\circ$	23.56	23.68	23.76	23.83	23.90	23.95	24.00	24.04	24.07	24.11	24.14	24.17	24.20
101	9FO-S2 $\rightarrow$ 9FO-S3	$\Delta G^\ddagger$	5.47	5.18	4.92	4.67	4.45	4.24	4.06	3.90	3.75	3.62	3.50	3.40	3.32
		$\Delta_r G_m^\circ$	-14.26	-18.24	-22.11	-25.94	-29.73	-33.49	-37.20	-40.89	-44.54	-48.17	-51.77	-55.34	-58.90
102	9FO-S3 $\rightarrow$ DF + $\cdot$ OH	$\Delta G^\ddagger$	13.65	13.70	13.77	13.84	13.93	14.04	14.17	14.31	14.46	14.63	14.81	15.01	15.22
		$\Delta_r G_m^\circ$	-70.44	-72.63	-75.16	-77.65	-80.10	-82.52	-84.90	-87.26	-89.59	-91.89	-94.18	-96.44	-98.67
103	9FO-A2 $\rightarrow$ 9FO-S4	$\Delta G^\ddagger$	13.16	13.70	14.26	14.85	15.45	16.07	16.69	17.32	17.95	18.59	19.24	19.90	20.56
		$\Delta_r G_m^\circ$	-0.87	-0.83	-0.79	-0.74	-0.68	-0.62	-0.57	-0.51	-0.45	-0.40	-0.34	-0.29	-0.24
104	9FO-S4 $\rightarrow$ 9FO-S5 + CO ₂	$\Delta G^\ddagger$	5.46	5.33	5.22	5.13	5.05	5.00	4.97	4.95	4.95	4.97	5.01	5.06	5.12
		$\Delta_r G_m^\circ$	-16.89	-20.67	-24.34	-27.97	-31.55	-35.10	-38.61	-42.09	-45.54	-48.97	-52.36	-55.73	-59.08
105	9FO-S5 + O ₂ $\rightarrow$ Phe-S6	$\Delta_r G_m^\circ$	-33.37	-29.46	-25.64	-21.85	-18.10	-14.37	-10.68	-7.01	-3.36	0.26	3.85	7.43	10.98
106	9FO-S6 $\rightarrow$ 9FO-S3	$\Delta G^\ddagger$	29.78	30.29	30.79	31.30	31.81	32.32	32.83	33.35	33.87	34.40	34.93	35.47	36.02
		$\Delta_r G_m^\circ$	-4.31	-4.90	-5.52	-6.16	-6.82	-7.49	-8.18	-8.87	-9.57	-10.27	-10.98	-11.70	-12.42
107	9FO-S5 + O ^{3P} $\rightarrow$ 9FO-S7	$\Delta_r G_m^\circ$	-115.49	-112.18	-108.90	-105.61	-102.33	-99.04	-95.76	-92.48	-89.20	-85.93	-82.67	-79.41	-76.16
108	9FO-S7 $\rightarrow$ 9FO-S8	$\Delta G^\ddagger$	28.23	28.76	29.33	29.94	30.58	31.24	31.93	32.64	33.37	34.11	34.87	35.64	36.43
		$\Delta_r G_m^\circ$	13.71	14.19	14.68	15.18	15.68	16.19	16.70	17.21	17.72	18.22	18.73	19.24	19.74

Table S8. *Cont.*

No.	Elementary Reactions		Temperature (K)												
			298.15	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500
109	9FO-S8 $\rightarrow$ DF + $\cdot$ H	$\Delta G^\ddagger$	21.24	21.34	21.44	21.53	21.62	21.71	21.80	21.90	22.00	22.11	22.23	22.35	22.48
		$\Delta_r G_m^\circ$	6.76	4.89	2.55	0.19	-2.20	-4.61	-7.03	-9.45	-11.89	-14.33	-16.76	-19.20	-21.65
110	9FO-D2 + O ₂ $\rightarrow$ 9FO-S9	$\Delta_r G_m^\circ$	-33.72	-29.64	-25.65	-21.69	-17.76	-13.86	-9.99	-6.14	-2.32	1.47	5.24	8.99	12.73
111	9FO-S9 $\rightarrow$ 9FO-S10 + CO ₂	$\Delta G^\ddagger$	37.16	37.74	38.33	38.95	39.60	40.25	40.93	41.63	42.34	43.06	43.80	44.56	45.32
		$\Delta_r G_m^\circ$	16.86	-21.07	-21.87	-22.72	-23.59	-24.49	-25.42	-26.37	-27.33	-28.32	-29.32	-30.34	-31.37
112	9FO-S10 $\rightarrow$ 9FO-S11	$\Delta G^\ddagger$	6.69	6.50	6.33	6.18	6.04	5.93	5.83	5.75	5.69	5.64	5.60	5.59	5.58
		$\Delta_r G_m^\circ$	-14.30	-17.59	-20.73	-23.79	-26.77	-29.69	-32.55	-35.35	-38.10	-40.81	-43.47	-46.09	-48.68
113	9FO-S11 $\rightarrow$ DF + ClO $\cdot$	$\Delta G^\ddagger$	14.63	14.04	13.43	12.80	12.15	11.50	10.85	10.19	9.53	8.87	8.20	7.54	6.87
		$\Delta_r G_m^\circ$	-101.54	-103.86	-106.49	-109.06	-111.59	-114.10	-116.58	-119.04	-121.48	-123.92	-126.33	-128.74	-131.14
114	9FO-D2 $\rightarrow$ 9FO-S12	$\Delta G^\ddagger$	23.50	24.09	24.70	25.34	26.00	26.69	27.40	28.12	28.87	29.63	30.41	31.20	32.00
		$\Delta_r G_m^\circ$	-46.39	-46.31	-46.24	-46.17	-46.11	-46.04	-45.98	-45.91	-45.85	-45.79	-45.72	-45.66	-45.60
115	9FO-S12 $\rightarrow$ 9FO-S13 + CO ₂	$\Delta G^\ddagger$	7.13	7.25	7.39	7.55	7.72	7.92	8.14	8.37	8.62	8.89	9.17	9.47	9.78
		$\Delta_r G_m^\circ$	-14.74	-18.44	-22.04	-25.58	-29.09	-32.56	-35.99	-39.38	-42.75	-46.09	-49.40	-52.68	-55.95
116	9FO-S13 + O ₂ $\rightarrow$ Phe-S14	$\Delta_r G_m^\circ$	-34.43	-30.59	-26.83	-23.10	-19.40	-15.74	-12.10	-8.50	-4.91	-1.36	2.18	5.69	9.18
117	9FO-S14 $\rightarrow$ 9FO-S15	$\Delta G^\ddagger$	32.22	32.81	33.40	34.00	34.60	35.20	35.81	36.41	37.03	37.64	38.27	38.90	39.53
		$\Delta_r G_m^\circ$	26.06	25.95	25.80	25.64	25.46	25.27	25.08	24.87	24.67	24.47	24.26	24.05	23.84
118	9FO-S15 $\rightarrow$ 1CDF + $\cdot$ OH	$\Delta G^\ddagger$	13.38	13.36	13.36	13.37	13.40	13.45	13.51	13.59	13.68	13.79	13.91	14.05	14.20
		$\Delta_r G_m^\circ$	-72.65	-75.34	-77.95	-80.51	-83.04	-85.54	-88.00	-90.44	-92.84	-95.23	-97.59	-99.92	-102.24
119	9FO-S13 + O ^{3P} $\rightarrow$ 9FO-S16	$\Delta_r G_m^\circ$	-115.77	-112.46	-109.20	-105.92	-102.65	-99.38	-96.11	-92.84	-89.58	-86.33	-83.08	-79.83	-76.59
120	9FO-S16 $\rightarrow$ 9FO-S17	$\Delta G^\ddagger$	27.25	27.80	28.39	29.01	29.67	30.36	31.08	31.81	32.56	33.33	34.11	34.91	35.73
		$\Delta_r G_m^\circ$	11.44	11.90	12.38	12.88	13.37	13.88	14.38	14.88	15.39	15.89	16.40	16.90	17.40
121	9FO-S17 $\rightarrow$ 1CDF + $\cdot$ H	$\Delta G^\ddagger$	21.36	21.47	21.56	21.65	21.74	21.83	21.92	22.01	22.12	22.22	22.34	22.46	22.59
		$\Delta_r G_m^\circ$	6.63	4.18	1.70	-0.81	-3.34	-5.90	-8.47	-11.05	-13.63	-16.22	-18.81	-21.40	-23.99
122	9FO-S16 $\rightarrow$ DF + $\cdot$ Cl	$\Delta G^\ddagger$	20.59	20.66	20.74	20.85	20.98	21.13	21.29	21.48	21.69	21.91	22.14	22.40	22.66
		$\Delta_r G_m^\circ$	-30.48	-32.68	-35.23	-37.75	-40.25	-42.72	-45.18	-47.61	-50.04	-52.45	-54.85	-57.24	-59.61