Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

The mechanism and rate constants for oxidation of indenyl radical C_9H_7 with molecular oxygen O_2: A theoretical study

A. R. Ghildina,[1,2] D. P. Porfiriev,[1,2] V. N. Azyazov,[1,2,*] and A. M. Mebel[1,3,†]

[1] *Samara University, Samara, 443086, Russia*

[2] *Lebedev Physical Institute, Samara, 443011, Russia*

[3] *Department of Chemistry and Biochemistry, Florida International University, Miami, FL 33199, USA*

Supplementary Information

* E-mail: azyazov@ssau.ru

† E-mail: mebela@fiu.edu

Figure S1. Comparison of rate constants for the phenoxy (P14) + propynal and CO loss (P7/P8) channels calculated in the present work with those proposed by Lindstedt et al. in Ref. 15.

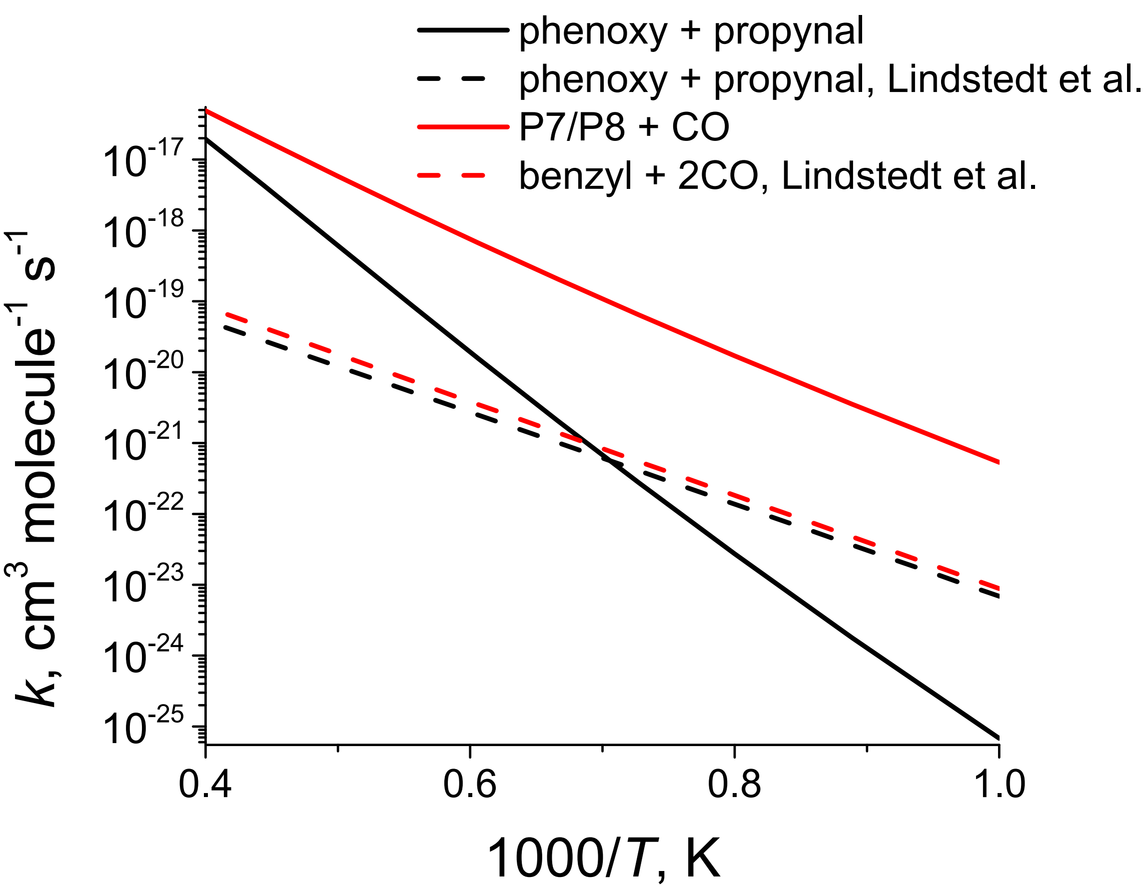

Figure S2. (a) The ratios of eigenvalue over the relaxation limit for six lowest eigenvalues from the master equation solution as functions of temperature at the lowest pressure of 0.01 atm; (b) The ratio of the lowest eigenvalue over the relaxation limit from the master equation solution as a function of temperature at various pressure in the 0.01 – 100 atm range.

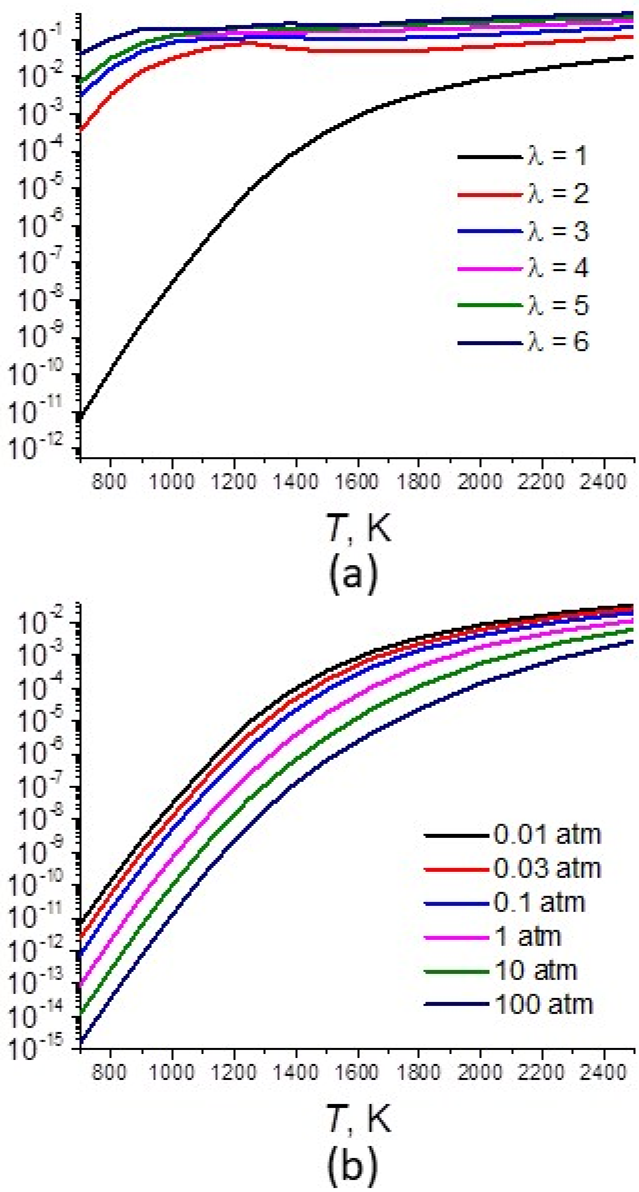

Table S1. Calculated rate constants (in cm^3 $molecule^{-1}$ s^{-1}) for individual bimolecular reaction channels. The values given are obtained at 0.03-1 atm (identical) but are also valid at higher pressures of 10 and 100 atm beginning from the temperatures of 1125 and 1500 K, respectively.

T, K	P1 + CO_2	P2 + CO_2	P3 + OH	P4 + H	P5 + CO	P6 + HCO	P7 + CO	P8 + CO	P10 + HCCO	P11 + H	P12 + CO	P13 + HCO	P14 + C_3H_2O
1000	6.45E-23	5.24E-25	4.26E-19	8.64E-23	1.73E-19	4.92E-23	3.83E-28	5.35E-22	6.65E-29	4.81E-20	2.55E-23	7.22E-25	6.78E-26
1125	3.45E-22	4.76E-24	2.16E-18	6.23E-22	7.69E-19	3.99E-22	6.87E-27	3.52E-21	1.16E-27	2.45E-19	2.82E-22	1.09E-23	1.78E-24
1250	1.38E-21	2.99E-23	8.22E-18	3.26E-21	2.60E-18	2.30E-21	6.52E-26	1.70E-20	1.31E-26	9.19E-19	2.11E-21	1.06E-22	2.73E-23
1375	4.44E-21	1.42E-22	2.51E-17	1.33E-20	7.19E-18	1.02E-20	3.95E-25	6.46E-20	1.06E-25	2.76E-18	1.17E-20	7.33E-22	2.77E-22
1500	1.20E-20	5.41E-22	6.51E-17	4.49E-20	1.70E-17	3.70E-20	1.75E-24	2.04E-19	6.55E-25	6.97E-18	5.09E-20	3.88E-21	2.03E-21
1650	3.35E-20	2.13E-21	1.72E-16	1.57E-19	4.06E-17	1.39E-19	7.81E-24	6.69E-19	4.35E-24	1.78E-17	2.31E-19	2.15E-20	1.56E-20
1800	8.01E-20	6.80E-21	3.92E-16	4.62E-19	8.44E-17	4.32E-19	2.77E-23	1.85E-18	2.24E-23	3.89E-17	8.39E-19	9.26E-20	8.87E-20
2000	2.13E-19	2.48E-20	9.85E-16	1.56E-18	1.90E-16	1.55E-18	1.14E-22	5.82E-18	1.45E-22	9.17E-17	3.54E-18	4.73E-19	6.13E-19
2250	5.74E-19	9.00E-20	2.51E-15	5.42E-18	4.24E-16	5.67E-18	4.87E-22	1.88E-17	1.00E-21	2.12E-16	1.50E-17	2.43E-18	4.24E-18
2500	1.28E-18	2.46E-19	5.32E-15	1.50E-17	8.00E-16	1.62E-17	1.57E-21	4.89E-17	4.97E-21	3.98E-16	4.64E-17	8.83E-18	1.94E-17

Table S2. Calculated branching ratios for individual bimolecular reaction channels. The values given are obtained at 0.03-1 atm (identical) but are also valid at higher pressures of 10 and 100 atm beginning from the temperatures of 1125 and 1500 K, respectively.

T, K	P1 + CO_2	P2 + CO_2	P3 + OH	P4 + H	P5 + CO	P6 + HCO	P7 + CO	P8 + CO	P10 + HCCO	P11 + H	P12 + CO	P13 + HCO	P14 + C_3H_2O
1000	0.000100	0.000001	0.657839	0.000133	0.266628	0.000076	0.000000	0.000827	0.000000	0.074356	0.000039	0.000001	0.000000
1125	0.000108	0.000001	0.679717	0.000196	0.241731	0.000125	0.000000	0.001107	0.000000	0.076922	0.000089	0.000003	0.000001
1250	0.000117	0.000003	0.698285	0.000277	0.221351	0.000196	0.000000	0.001443	0.000000	0.078138	0.000179	0.000009	0.000002
1375	0.000126	0.000004	0.714251	0.000379	0.204354	0.000291	0.000000	0.001836	0.000000	0.078399	0.000332	0.000021	0.000008
1500	0.000135	0.000006	0.728143	0.000502	0.189918	0.000414	0.000000	0.002283	0.000000	0.077964	0.000569	0.000043	0.000023
1650	0.000145	0.000009	0.742620	0.000680	0.175151	0.000601	0.000000	0.002888	0.000000	0.076747	0.000998	0.000093	0.000068
1800	0.000154	0.000013	0.755170	0.000890	0.162499	0.000832	0.000000	0.003560	0.000000	0.074916	0.001617	0.000178	0.000171
2000	0.000166	0.000019	0.769524	0.001217	0.148066	0.001208	0.000000	0.004546	0.000000	0.071639	0.002765	0.000369	0.000479
2250	0.000180	0.000028	0.784503	0.001697	0.132854	0.001776	0.000000	0.005895	0.000000	0.066293	0.004685	0.000760	0.001327
2500	0.000192	0.000037	0.796979	0.002245	0.119880	0.002431	0.000000	0.007335	0.000001	0.059714	0.006955	0.001323	0.002909