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On the mechanism of soot nucleation. II. E-bridge formation at PAH bay

Alexander S. Semenikhin[a], Anna S. Savchenkova[a], Ivan V. Chechet[a], Sergey G. Matveev[a], Michael Frenklach[b], and Alexander M. Mebel[a,c]

[a.] *Samara National Research University, Samara 443086, Russia*
[b.] *Department of Mechanical Engineering, University of California, Berkeley, California 94720, USA.*
[c.] *Department of Chemistry and Biochemistry, Florida International University, Miami, Florida 33199, USA.*

Table S1 Parameters of fitted modified Arrhenius expressions $k = A\,T^{\alpha}\exp(-E_a/RT)$ or $k = A_1\,T^{\alpha_1}\exp(-E_a^1/RT) + A_2\,T^{\alpha_2}\exp(-E_a^2/RT)$ for the most relevant reactions considered. Pre-exponential factors A are in $cm^3\ mol^{-1}\ s^{-1}$ for bimolecular reactions and in s^{-1} for unimolecular reactions, E_a are in cal mol^{-1}

Reaction	p, atm	A_1	α_1	E_a^1	A_2	α_2	E_a^2	T-range, K
1-naphthyl + acenaphthylene								
R → P1 + H	1	5.69E+57	-12.754	42664				1000-2500
	3	1.15E+72	-16.567	58199				1000-2500
	10	5.66E+80	-18.797	70557				1000-2500
	100	2.60E+79	-18.077	81986				1000-2500
R → P2 + H	1	3.79E+46	-9.1442	42415				1000-2500
	3	3.09E+58	-12.323	55249				1000-2500
	10	4.57E+65	-14.172	65105				1000-2500
	100	2.05E+58	-11.924	67208				1000-2500
R → W1	1	3.42E+103	-26.619	56390	3.73E+32	-6.5426	8663.9	500-1375
	3	2.09E+68	-16.261	37365	1.32E+29	-5.4902	7257.6	500-1375
	10	3.96E+63	-14.742	36880	6.93E+23	-3.8095	5561.3	500-1500
	100	1.96E+60	-13.509	39927	1.50E+16	-1.372	3086.1	500-1800
P1 + H → R	1	3.77E+68	-14.728	66117				1000-2500
	3	6.82E+82	-18.529	81605				1000-2500
	10	3.00E+91	-20.746	93920				1000-2500
	100	1.22E+90	-20.011	1.05E+05				1000-2500
P1 + H → P2 + H	1	9.95E+65	-14.108	63412				1000-2500
	3	2.21E+80	-17.931	79035				1000-2500
	10	5.41E+88	-20.076	91201				1000-2500
	100	3.81E+86	-19.131	102030				1000-2500
P1 + H → W1	1	9.66E+118	-30.264	75212	1.30E+68	-16.191	40811	500-1375
	3	8.38E+99	-24.484	68275	1.84E+53	-11.667	35865	500-1375
	10	-1.53E+84	-20.441	53144	1.55E+59	-12.742	43027	500-1500
	100	2.79E+74	-16.534	66159	4.40E+27	-3.8174	29249	500-1800
P2 + H → R	1	1.72E+55	-11.065	52678				1000-2500
	3	1.73E+67	-14.268	65588				1000-2500
	10	2.81E+74	-16.128	75481				1000-2500
	100	1.32E+67	-13.886	77602				1000-2500
P2 + H → P1 + H	1	1.27E+64	-14.127	50454				1000-2500
	3	2.42E+78	-17.932	66020				1000-2500
	10	5.50E+86	-20.068	78161				1000-2500
	100	4.33E+84	-19.137	89025				1000-2500
P2 + H → W1	1	3.48E+99	-25.011	57453	1.72E+40	-8.3954	15991	500-1375
	3	3.99E+85	-20.808	51831	1.52E+28	-4.6094	11786	500-1375
	10	1.01E+68	-15.576	43011	4.70E+28	-4.7624	11967	500-1500
	100	5.50E+64	-14.367	45872	2.70E+21	-2.4587	9641.2	500-1800
W1 → R	1	1.39E+97	-24.006	94521	1.74E+42	-8.546	56898	500-1375
	3	6.26E+73	-17.09	82439	1.23E+41	-8.2041	56375	500-1375
	10	2.51E+78	-18.263	88047	6.06E+31	-5.2382	53402	500-1500
	100	9.42E+54	-11.34	76089	1.05E+30	-4.6829	52803	500-1800

W1 → P1 + H	1	3.87E+108	-27.622	94392	4.46E+65	-15.876	64666	500-1375
	3	6.34E+92	-22.818	89041	1.85E+55	-12.752	61289	500-1375
	10	-7.80E+45	-9.5454	57959	2.21E+34	-5.8948	54028	500-1500
	100	4.95E+65	-14.466	84895	2.54E+27	-4.1728	54027	500-1800
W1 → P2 + H	1	1.50E+91	-22.417	89411	3.76E+36	-7.0449	51920	500-1375
	3	2.16E+80	-19.124	85237	3.93E+29	-4.844	49540	500-1375
	10	4.46E+72	-16.753	82818	5.17E+26	-3.9258	48621	500-1500
	100	3.33E+50	-10.212	71537	2.35E+25	-3.5014	48176	500-1800
4-phenanthrenyl + acenaphthylene								
R → P1 + H	1	8.19E+40	-8.1214	29446				1000-2500
	3	1.79E+50	-10.633	38874				1000-2500
	10	8.11E+61	-13.744	51413				1000-2500
	100	1.45E+68	-15.222	64594				1000-2500
R → P2 + H	1	1.50E+30	-4.695	38030				1000-2500
	3	5.13E+37	-6.7252	45512				1000-2500
	10	3.40E+48	-9.6252	56766				1000-2500
	100	9.33E+57	-12.024	70971				1000-2500
R → W2	1	2.39E+111	-29.741	55806	1.65E+47	-11.442	16229	500-1125
	3	6.08E+98	-25.705	52901	1.56E+38	-8.531	13588	500-1250
	10	3.23E+81	-20.368	46898	2.08E+30	-5.9795	11502	500-1375
	100	1.05E+51	-11.192	32526	9.66E+52	-13.027	21191	500-1650
P1 + H → R	1	4.22E+51	-10.029	56228				1000-2500
	3	1.26E+61	-12.578	65781				1000-2500
	10	3.63E+72	-15.635	78143				1000-2500
	100	7.57E+78	-17.132	91383				1000-2500
P1 + H → P2 + H	1	4.25E+48	-9.3806	54612				1000-2500
	3	1.23E+58	-11.926	64160				1000-2500
	10	3.79E+69	-14.99	76542				1000-2500
	100	1.76E+76	-16.582	90081				1000-2500
P1 + H → W2	1	1.43E+89	-22.437	47763	3.90E+36	-7.4807	14099	500-1125
	3	4.95E+81	-20.04	46340	5.45E+31	-5.9178	12647	500-1250
	10	1.09E+58	-12.992	34477	2.80E+30	-5.541	12024	500-1375
	100	2.00E+50	-10.48	34416	6.07E+20	-2.4587	8944.1	500-1650
P2 + H → R	1	3.18E+38	-6.6689	42575				1000-2500
	3	8.23E+45	-8.666	49950				1000-2500
	10	6.63E+56	-11.59	61270				1000-2500
	100	2.04E+66	-14.002	7.55E+04				1000-2500
P2 + H → P1 + H	1	1.51E+46	-9.4287	32314				1000-2500
	3	4.31E+55	-11.972	41850				1000-2500
	10	1.47E+67	-15.049	54285				1000-2500
	100	5.26E+73	-16.61	67719				1000-2500
P2 + H → W2	1	1.13E+120	-32.038	60666	5.34E+53	-13.097	19915	500-1125
	3	1.81E+107	-27.938	57729	6.99E+44	-10.231	17318	500-1250
	10	3.75E+89	-22.48	51581	8.77E+36	-7.6654	15272	500-1375
	100	3.23E+56	-12.569	35416	6.36E+63	-16.048	26339	500-1650
W2 → R	1	2.34E+112	-28.667	1.01E+05	1.95E+64	-15.22	69619	500-1125
	3	9.65E+104	-26.2	1.01E+05	4.26E+51	-11.131	65926	500-1250
	10	4.04E+85	-20.314	92636	2.33E+45	-9.1133	64231	500-1375
	100	-1.18E+42	-7.9318	62575	1.05E+32	-4.7317	59274	500-1650
W2 → P1 + H	1	6.04E+73	-17.816	63021	5.48E+40	-8.6748	39767	500-1125
	3	7.83E+71	-17.098	64202	8.83E+34	-6.7785	38221	500-1250
	10	4.15E+59	-13.407	58586	3.99E+30	-5.4226	36654	500-1375
	100	2.76E+51	-10.849	56588	1.19E+27	-4.2721	35689	500-1650
W2 → P2 + H	1	2.27E+109	-28.014	99647	2.01E+61	-14.575	67933	500-1125
	3	6.07E+102	-25.784	99663	5.33E+48	-10.51	64296	500-1250
	10	2.09E+78	-18.425	88254	9.82E+45	-9.6271	63673	500-1375
	100	-6.64E+39	-7.5208	61177	1.77E+29	-4.1566	57696	500-1650