

Supporting Information

for

Formation of 2- and 1-Methyl-1,4-Dihydronaphthalene Isomers via the Crossed Beam Reactions of Phenyl Radicals (C₆H₅) with Isoprene (CH₂C(CH₃)CHCH₂) and 1,3-Pentadiene (CH₂CHCHCHCH₃)

By

Tao Yang, Lloyd Muzangwa, Dorian S. N. Parker, Ralf I. Kaiser*

Department of Chemistry, University of Hawaii at Manoa, Honolulu, HI 96822

Alexander M. Mebel*

Department of Chemistry and Biochemistry, Florida International University, Miami, Florida

List of Contents:

Table S1. RRKM calculated energy-dependent rate constants (s^{-1}) for unimolecular reaction steps in the reaction systems of phenyl with isoprene and 1,3-pentadiene at different collision energies.....	3
--	---

(a) p-tolyl + isoprene

From	To	Collision Energy, kJ mol ⁻¹							
		0	10	20	30	40	50	55	60
i0	i1	1.21E+09	3.22E+09	4.16E+09	4.75E+09	5.18E+09	5.52E+09	5.66E+09	5.79E+09
i1	i0	4.00E-06	8.72E-04	1.81E-02	1.72E-01	1.06E+00	4.88E+00	9.68E+00	1.83E+01
i0	i2	1.94E+01	5.04E+05	6.58E+06	1.74E+07	3.09E+07	4.60E+07	5.38E+07	6.19E+07
i2	i0	4.47E-10	7.49E-04	1.25E-01	2.23E+00	1.82E+01	9.77E+01	2.02E+02	3.96E+02
i0	i4	1.05E+10	1.45E+10	1.60E+10	1.68E+10	1.74E+10	1.79E+10	1.81E+10	1.83E+10
i4	i0	1.92E-05	2.25E-03	4.13E-02	3.73E-01	2.24E+00	1.03E+01	2.03E+01	3.85E+01
i0	i3	1.56E-02	2.37E+02	1.34E+05	8.05E+05	2.08E+06	3.89E+06	4.98E+06	6.17E+06
i3	i0	8.84E-12	7.82E-06	5.38E-02	2.06E+00	2.34E+01	1.50E+02	3.33E+02	6.87E+02
i0	CH ₂ C(CH ₃)CCH ₂	1.20E+06	1.68E+06	2.74E+06	4.81E+06	8.61E+06	1.48E+07	1.90E+07	2.40E+07
i0	CH ₂ CHC(CH ₃)CH	8.04E+04	1.07E+05	1.69E+05	2.93E+05	5.57E+05	1.11E+06	1.57E+06	2.17E+06
i0	CH ₂ C(CH ₃)CHCH	3.40E+04	4.16E+04	6.24E+04	1.03E+05	1.89E+05	3.73E+05	5.25E+05	7.34E+05
i0	CH ₂ C(CH ₂)CHCH ₂	3.35E+07	5.45E+07	1.12E+08	2.11E+08	3.44E+08	5.05E+08	5.96E+08	6.92E+08
i1	i5	2.81E+10	3.50E+10	4.28E+10	5.17E+10	6.15E+10	7.24E+10	7.82E+10	8.43E+10
i5	i1	1.92E+10	2.39E+10	2.91E+10	3.52E+10	4.16E+10	4.89E+10	5.27E+10	5.68E+10
i1	i2	1.69E+02	3.81E+02	7.89E+02	1.52E+03	2.77E+03	4.77E+03	6.16E+03	7.88E+03
i2	i1	1.19E+06	2.09E+06	3.44E+06	4.92E+06	7.99E+06	1.14E+07	1.35E+07	1.59E+07
i1	i7	1.82E-04	1.40E-03	7.21E-03	2.87E-02	9.47E-02	2.71E-01	4.38E-01	6.91E-01
i7	i1	7.49E+03	4.09E+04	1.55E+05	4.63E+05	1.17E+06	2.62E+06	3.80E+06	5.32E+06
i1	p1	2.16E-02	1.90E-01	1.11E+00	4.91E+00	1.78E+01	5.53E+01	9.30E+01	1.52E+02
i5	i6	2.89E+04	4.77E+04	7.54E+04	1.14E+05	1.68E+05	2.39E+05	2.83E+05	3.32E+05
i6	i5	3.70E+07	6.16E+07	9.78E+07	1.49E+08	2.20E+08	3.16E+08	3.74E+08	4.41E+08
i5	p2	3.32E-04	6.65E-03	6.30E-02	3.90E-01	1.81E+00	6.85E+00	1.25E+01	2.21E+01
i6	p3	5.23E+05	1.12E+06	2.23E+06	4.15E+06	7.32E+06	1.23E+07	1.57E+07	1.99E+07
i2	p4	5.83E-04	2.83E-02	4.10E-01	3.12E+00	1.61E+01	6.41E+01	1.19E+02	2.10E+02
i2	p6	1.67E-04	1.35E-01	3.72E+00	3.75E+01	2.27E+02	9.96E+02	1.91E+03	3.50E+03
i7	p5	2.78E+03	1.45E+04	5.48E+04	1.66E+05	4.27E+05	9.75E+05	1.42E+06	2.02E+06
i4	i8	2.56E+09	3.33E+09	4.24E+09	5.32E+09	6.56E+09	7.98E+09	8.76E+09	9.59E+09
i8	i4	4.72E+09	6.15E+09	7.87E+09	9.88E+09	1.22E+10	1.49E+10	1.64E+10	1.79E+10
i4	i3	7.41E+02	1.60E+03	3.10E+03	6.01E+03	1.07E+04	1.81E+04	2.32E+04	2.94E+04
i3	i4	2.27E+08	3.45E+08	5.18E+08	6.93E+08	9.32E+08	1.22E+09	1.38E+09	1.55E+09
i4	i10	1.04E-06	1.79E-05	1.49E-04	8.31E-04	3.55E-03	1.25E-02	2.22E-02	3.82E-02
i10	i4	6.90E+01	8.16E+02	4.83E+03	1.96E+04	6.28E+04	1.69E+05	2.63E+05	3.99E+05
i4	p7	1.01E-04	1.16E-03	8.38E-03	4.36E-02	1.79E-01	6.16E-01	1.08E+00	1.84E+00
i8	i9	7.51E+04	1.26E+05	2.02E+05	3.11E+05	4.63E+05	6.70E+05	7.86E+05	9.21E+05
i9	i8	5.16E+07	8.37E+07	1.30E+08	1.95E+08	2.82E+08	3.98E+08	4.68E+08	5.48E+08
i8	p8	3.70E-05	1.30E-03	1.64E-02	1.22E-01	6.54E-01	2.76E+00	5.31E+00	9.80E+00
i9	p3	4.79E+05	1.03E+06	2.06E+06	3.85E+06	6.82E+06	1.15E+07	1.47E+07	1.87E+07

i3	p9	1.49E+00	3.51E+01	3.21E+02	1.80E+03	7.40E+03	2.45E+04	4.18E+04	6.90E+04
i3	p11	5.52E-13	3.81E-08	1.13E-03	1.50E-01	2.76E+00	2.36E+01	5.80E+01	1.31E+02
i10	p10	1.97E+03	1.08E+04	4.20E+04	1.30E+05	3.42E+05	7.92E+05	1.16E+06	1.67E+06

(b) p-tolyl + 1,3-pentadiene

		Collision Energy, kJ mol ⁻¹							
From	To	0	10	20	30	40	50	55	60
i0'	i1'	1.62E+09	5.89E+09	7.86E+09	9.07E+09	9.91E+09	1.06E+10	1.08E+10	1.11E+10
i1'	i0'	1.40E-06	8.17E-04	2.21E-02	2.40E-01	1.61E+00	7.96E+00	1.62E+01	3.16E+01
i0'	i2'	2.46E-01	1.36E+04	2.23E+06	9.66E+06	2.11E+07	3.54E+07	4.33E+07	5.17E+07
i2'	i0'	5.19E-13	4.06E-06	1.05E-02	3.38E-01	3.64E+00	2.30E+01	5.08E+01	1.05E+02
i0'	i4'	3.03E+07	3.70E+08	6.28E+08	8.08E+08	9.47E+08	1.06E+09	1.11E+09	1.16E+09
i4'	i0'	3.85E-07	7.24E-04	2.44E-02	2.90E-01	2.05E+00	1.04E+01	2.15E+01	4.22E+01
i0'	i3'	1.07E+01	3.19E+05	8.56E+06	2.65E+07	4.96E+07	7.56E+07	8.93E+07	1.03E+08
i3'	i0'	2.34E-11	1.02E-04	4.30E-02	9.90E-01	9.15E+00	5.27E+01	1.12E+02	2.25E+02
i0'	CH ₃ CHCHCCH ₂	1.37E+06	1.65E+06	2.60E+06	4.49E+06	7.99E+06	1.37E+07	1.75E+07	2.20E+07
i0'	CH ₃ CHCCHCH ₂	2.14E+06	2.60E+06	4.06E+06	6.91E+06	1.21E+07	2.04E+07	2.60E+07	3.26E+07
i0'	CH ₃ CCHCHCH ₂	2.49E+06	3.04E+06	4.80E+06	8.25E+06	1.46E+07	2.50E+07	3.20E+07	4.03E+07
i0'	CH ₃ CHCHCHCH	7.02E+04	7.78E+04	1.16E+05	1.95E+05	3.64E+05	7.11E+05	9.86E+05	1.35E+06
i0'	CH ₂ CHCHCHCHCH ₂	8.34E+06	2.29E+07	9.36E+07	2.37E+08	4.33E+08	6.67E+08	7.95E+08	9.29E+08
i1'	i5'	1.14E+10	1.47E+10	1.86E+10	2.31E+10	2.83E+10	3.42E+10	3.74E+10	4.08E+10
i5'	i1'	3.62E+09	4.67E+09	5.93E+09	7.37E+09	9.05E+09	1.11E+10	1.20E+10	1.31E+10
i1'	i2'	2.11E+02	5.02E+02	1.09E+03	2.19E+03	4.12E+03	7.34E+03	9.63E+03	1.24E+04
i2'	i1'	5.99E+05	1.08E+06	1.82E+06	2.89E+06	4.37E+06	6.35E+06	7.55E+06	8.92E+06
i1'	i7'	2.46E-07	7.67E-06	8.16E-05	5.25E-04	2.47E-03	9.37E-03	1.71E-02	3.01E-02
i7'	i1'	1.30E+01	2.77E+02	2.08E+03	9.70E+03	3.40E+04	9.77E+04	1.57E+05	2.43E+05
i1'	p1'	3.30E-02	3.17E-01	1.97E+00	9.15E+00	3.45E+01	1.11E+02	1.89E+02	3.14E+02
i5'	i6'	3.30E+04	5.36E+04	8.35E+04	1.25E+05	1.82E+05	2.58E+05	3.04E+05	3.57E+05
i6'	i5'	3.19E+08	4.96E+08	7.39E+08	1.07E+09	1.49E+09	2.04E+09	2.36E+09	2.72E+09
i5'	p2'	1.98E-04	4.37E-03	4.38E-02	2.81E-01	1.35E+00	5.25E+00	9.72E+00	1.74E+01
i6'	p3'	1.89E+05	4.36E+05	9.19E+05	1.80E+06	3.31E+06	5.79E+06	7.52E+06	9.67E+06
i2'	p4'	1.17E-04	6.11E-03	1.14E-01	1.04E+00	6.03E+00	2.61E+01	5.01E+01	9.17E+01
i2'	p6'	2.15E-14	2.20E-08	8.42E-04	6.01E-02	8.99E-01	6.91E+00	1.64E+01	3.61E+01
i7'	p5'	1.25E+03	7.68E+03	3.21E+04	1.04E+05	2.83E+05	6.74E+05	9.98E+05	1.45E+06
i4'	i8'	3.82E+10	4.97E+10	6.34E+10	7.95E+10	9.80E+10	1.19E+11	1.31E+11	1.43E+11
i8'	i4'	7.02E+09	9.06E+09	1.15E+10	1.42E+10	1.74E+10	2.10E+10	2.30E+10	2.50E+10
i4'	i3'	1.81E+03	4.30E+03	9.32E+03	1.86E+04	3.50E+04	6.21E+04	8.12E+04	1.05E+05
i3'	i4'	3.81E+05	7.04E+05	1.24E+06	1.95E+06	2.99E+06	4.41E+06	5.28E+06	6.27E+06
i4'	i10'	7.24E-07	3.14E-05	3.71E-04	2.53E-03	1.23E-02	4.78E-02	8.80E-02	1.56E-01
i10'	i4'	5.54E+00	1.66E+02	1.40E+03	6.99E+03	2.56E+04	7.58E+04	1.23E+05	1.93E+05
i4'	p7'	9.35E-04	1.65E-02	1.48E-01	8.80E-01	3.99E+00	1.48E+01	2.62E+01	4.72E+01
i4'	p12'	2.13E+02	9.54E+02	3.45E+03	1.07E+04	2.87E+04	7.00E+04	1.06E+05	1.57E+05

i8'	i9'	4.59E+04	7.76E+04	1.25E+05	1.93E+05	2.88E+05	4.16E+05	4.96E+05	5.86E+05
i9'	i8'	8.52E+07	1.41E+08	2.21E+08	3.35E+08	4.90E+08	6.96E+08	8.22E+08	9.64E+08
i8'	p8'	1.37E-08	2.11E-07	3.18E-06	3.71E-05	2.96E-04	1.71E-03	3.74E-03	7.73E-03
i8'	p13'	4.47E+00	2.60E+01	1.14E+02	4.07E+02	1.24E+03	3.36E+03	5.32E+03	8.23E+03
i9'	p3'	1.91E+05	4.43E+05	9.38E+05	1.84E+06	3.40E+06	5.95E+06	7.74E+06	9.95E+06
i3'	p9'	1.27E-03	5.95E-02	8.39E-01	6.26E+00	3.18E+01	1.24E+02	2.28E+02	4.02E+02
i3'	p11'	1.14E-09	2.04E-04	5.95E-02	1.39E+00	1.33E+01	7.87E+01	1.70E+02	3.45E+02
i10'	p10'	1.26E+03	8.18E+03	3.54E+04	1.18E+05	3.25E+05	7.83E+05	1.17E+06	1.70E+06