Electronic Supplementary Information (ESI)

for

Understanding the Chemical Dynamics of the Reactions of Dicarbon with 1-Butyne, 2-Butyne, and 1,2-Butadiene – Toward the Formation of Resonantly Stabilized Free Radicals

by

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Table S1. Rate constants for various individual unimolecular reaction steps calculated using RRKM theory under single-collision conditions at different collision energies.

(a) $C_2(X^1\Sigma_g^+)$ + 2-butyne, Figure 4(a). RRKM calculations were not performed since product **p1$_{2b}$** is the only C_6H_5 isomer able to be formed on the singlet surface.

(b) $C_2(a^3\Pi_u)$ + 2-butyne, Figure 4(b).

		Collision Energy, kJ mol^{-1}						
From	To	0	5	10	15	20	26.4	30
i4$_{2b}$	**i5$_{2b}$**	3.10E+11	3.45E+11	3.82E+11	4.21E+11	4.60E+11	5.20E+11	5.53E+11
i5$_{2b}$	**i4$_{2b}$**	3.60E+10	4.05E+10	4.50E+10	4.99E+10	5.52E+10	6.24E+10	6.66E+10
i4$_{2b}$	**i6$_{2b}$**	1.93E+08	2.55E+08	3.30E+08	4.22E+08	5.33E+08	7.06E+08	8.21E+08
i6$_{2b}$	**i4$_{2b}$**	1.14E+09	1.45E+09	1.82E+09	2.26E+09	2.76E+09	3.52E+09	4.01E+09
i5$_{2b}$	**i9$_{2b}$**	0.00E+00	0.00E+00	2.06E+00	8.38E+00	2.86E+01	1.11E+02	2.18E+02
i9$_{2b}$	**i5$_{2b}$**	0.00E+00	0.00E+00	8.37E-05	3.83E-04	1.47E-03	6.58E-03	1.40E-02
i5$_{2b}$	**i10$_{2b}$**	2.81E+07	3.57E+07	4.49E+07	5.59E+07	6.88E+07	8.86E+07	1.01E+08
i10$_{2b}$	**i5$_{2b}$**	4.51E+02	6.55E+02	9.39E+02	1.33E+03	1.85E+03	2.77E+03	3.46E+03
i5$_{2b}$	**p2$_{2b}$**	5.60E+06	1.02E+07	1.78E+07	2.96E+07	4.75E+07	8.32E+07	1.12E+08
i6$_{2b}$	**i7$_{2b}$**	4.83E+08	6.43E+08	8.42E+08	1.08E+09	1.37E+09	1.83E+09	2.12E+09
i7$_{2b}$	**i6$_{2b}$**	1.09E+06	1.56E+06	2.20E+06	3.02E+06	4.10E+06	5.91E+06	7.19E+06
i7$_{2b}$	**i8$_{2b}$**	4.66E+09	5.39E+09	6.19E+09	7.07E+09	8.03E+09	9.39E+09	1.02E+10
i8$_{2b}$	**i7$_{2b}$**	1.08E+09	1.26E+09	1.47E+09	1.69E+09	1.94E+09	2.31E+09	2.53E+09
i8$_{2b}$	**p1$_{2b}$**	5.73E+11	6.54E+11	7.44E+11	8.42E+11	9.49E+11	1.10E+12	1.19E+12
i9$_{2b}$	**p3$_{2b}$**	3.99E+09	4.75E+09	5.62E+09	6.61E+09	7.75E+09	9.44E+09	1.05E+10

i9$_{2b}$	**p5$_{2b}$**	5.73E+08	7.22E+08	9.04E+08	1.12E+09	1.39E+09	1.80E+09	2.07E+09
i10$_{2b}$	**p3$_{2b}$**	5.37E+07	6.78E+07	8.48E+07	1.05E+08	1.30E+08	1.69E+08	1.95E+08
i10$_{2b}$	**p4$_{2b}$**	6.52E+10	7.57E+10	8.74E+10	1.01E+11	1.15E+11	1.37E+11	1.50E+11

(c) $C_2(X^1\Sigma_g^+)$ + 1-butyne, Figure 5(a).

		Collision Energy, kJ mol^{-1}					
From	To	0	4.18	8.37	12.55	16.74	22.00
i2$_{1b}$	**i3$_{1b}$**	6.22E+10	6.69E+10	7.18E+10	7.69E+10	8.24E+10	8.95E+10
i3$_{1b}$	**i2$_{1b}$**	5.87E+04	6.91E+04	8.19E+04	9.62E+04	1.13E+05	1.35E+05
i3$_{1b}$	**p2$_{1b}$**	1.59E+10	1.69E+10	1.80E+10	1.91E+10	2.02E+10	2.16E+10
i3$_{1b}$	**p1$_{1b}$**	9.55E+08	1.04E+09	1.14E+09	1.24E+09	1.35E+09	1.50E+09
i3$_{1b}$	**p3$_{1b}$**	1.13E+07	1.31E+07	1.50E+07	1.73E+07	1.99E+07	2.35E+08

(d) $C_2(a^3\Pi_u)$ + 1-butyne, Figure 5(b).

		Collision Energy, kJ mol^{-1}					
From	To	0	4.18	8.37	12.55	16.74	22.00
i8$_{1b}$	**i11$_{1b}$**	4.39E+07	5.09E+07	5.87E+07	6.73E+07	7.69E+07	9.03E+07
i11$_{1b}$	**i8$_{1b}$**	1.49E+04	1.85E+04	2.28E+04	2.78E+04	3.39E+04	4.30E+04
i8$_{1b}$	**i6$_{1b}$**	9.91E+02	1.55E+03	2.32E+03	3.40E+03	4.87E+03	7.45E+03
i11$_{1b}$	**i12$_{1b}$**	2.96E+09	3.06E+09	3.16E+09	3.26E+09	3.36E+09	3.49E+09
i12$_{1b}$	**i11$_{1b}$**	7.34E+10	7.93E+10	8.55E+10	9.21E+10	9.90E+10	1.08E+11
i11$_{1b}$	**i10$_{1b}$**	2.86E+12	2.87E+12	2.88E+12	2.89E+12	2.91E+12	2.91E+12
i10$_{1b}$	**i11$_{1b}$**	5.19E+12	5.21E+12	5.23E+12	5.25E+12	5.27E+12	5.29E+12
i12$_{1b}$	**i16$_{1b}$**	1.70E+09	1.87E+09	2.05E+09	2.24E+09	2.47E+09	2.74E+09
i16$_{1b}$	**i12$_{1b}$**	3.75E+06	4.30E+06	4.91E+06	5.61E+06	6.38E+06	7.48E+06
i16$_{1b}$	**i17$_{1b}$**	3.47E+09	3.70E+09	3.95E+09	4.21E+09	4.48E+09	4.84E+09
i17$_{1b}$	**i16$_{1b}$**	2.83E+09	3.02E+09	3.23E+09	3.45E+09	3.68E+09	3.99E+09
i16$_{1b}$	**p5$_{1b}$**	1.56E+11	1.63E+11	1.70E+11	1.77E+11	1.84E+11	1.93E+11
i17$_{1b}$	**i18$_{1b}$**	1.82E+13	1.81E+13	1.80E+13	1.79E+13	2.11E+13	2.21E+13
i18$_{1b}$	**i17$_{1b}$**	4.84E+10	4.99E+10	5.17E+10	5.34E+10	5.51E+10	5.73E+10
i17$_{1b}$	**p5$_{1b}$**	1.66E+11	1.73E+11	1.81E+11	1.88E+11	1.96E+11	2.06E+11
i18$_{1b}$	**i19$_{1b}$**	5.88E+08	6.04E+08	6.20E+08	6.36E+08	6.53E+08	6.73E+08
i19$_{1b}$	**i18$_{1b}$**	4.15E+12	4.20E+12	4.25E+12	4.30E+12	4.34E+12	4.40E+12
i18$_{1b}$	**p5$_{1b}$**	2.07E+08	2.16E+08	2.25E+08	2.35E+08	2.44E+08	2.57E+08
i19$_{1b}$	**p6$_{1b}$**	3.55E+06	4.45E+06	5.55E+06	6.88E+06	8.49E+06	1.10E+07
i10$_{1b}$	**i9$_{1b}$**	1.82E+12	1.83E+12	1.83E+12	1.83E+12	1.84E+12	1.84E+12
i9$_{1b}$	**i10$_{1b}$**	3.12E+12	3.13E+12	3.14E+12	3.15E+12	3.16E+12	3.18E+12
i9$_{1b}$	**i7$_{1b}$**	2.78E+08	3.06E+08	3.36E+08	3.68E+08	4.03E+08	4.49E+08
i7$_{1b}$	**i9$_{1b}$**	5.40E+11	5.49E+11	5.59E+11	5.68E+11	5.78E+11	5.89E+11
i9$_{1b}$	**i13$_{1b}$**	3.26E+07	3.87E+07	4.58E+07	5.39E+07	6.32E+07	7.66E+07

i13$_{1b}$	**i9$_{1b}$**	6.23E+04	7.79E+04	9.69E+04	1.20E+05	1.48E+05	1.90E+05
i9$_{1b}$	**p3$_{1b}$**	5.84E+08	7.18E+08	8.77E+08	1.07E+09	1.29E+09	1.62E+09
i7$_{1b}$	**i6$_{1b}$**	2.08E+03	3.18E+03	4.73E+03	6.86E+03	9.70E+03	1.47E+04
i6$_{1b}$	**i7$_{1b}$**	3.09E+06	4.35E+06	5.96E+06	8.02E+06	1.06E+07	1.46E+07
i7$_{1b}$	**p2$_{1b}$**	2.30E+12	2.49E+12	2.67E+12	2.86E+12	3.06E+12	3.33E+12
i7$_{1b}$	**p1$_{1b}$**	2.54E+11	2.84E+11	3.15E+11	3.49E+11	3.86E+11	4.35E+11
i6$_{1b}$	**i5$_{1b}$**	2.11E+10	2.53E+10	3.00E+10	3.52E+10	4.10E+10	4.91E+10
i5$_{1b}$	**i6$_{1b}$**	5.56E+07	7.06E+07	9.11E+07	1.15E+08	1.43E+08	1.85E+08
i5$_{1b}$	**i4$_{1b}$**	3.52E+10	3.88E+10	4.26E+10	4.67E+10	5.09E+10	5.66E+10
i4$_{1b}$	**i5$_{1b}$**	6.04E+10	6.70E+10	7.33E+10	8.03E+10	8.77E+10	9.76E+10
i13$_{1b}$	**i4$_{1b}$**	1.63E+12	1.63E+12	1.63E+12	1.63E+12	1.63E+12	1.63E+12
i14$_{1b}$	**i13$_{1b}$**	2.57E+12	2.58E+12	2.58E+12	2.59E+12	2.60E+12	2.60E+12
i13$_{1b}$	**p8$_{1b}$**	6.85E+06	8.17E+06	9.70E+06	1.15E+07	1.35E+07	1.68E+07
i13$_{1b}$	**p10$_{1b}$**	3.82E+07	4.42E+07	5.10E+07	5.88E+07	6.73E+07	7.97E+07
i14$_{1b}$	**i15$_{1b}$**	3.95E+11	4.04E+11	4.13E+11	4.23E+11	4.32E+11	4.44E+11
i15$_{1b}$	**i14$_{1b}$**	3.67E+11	3.76E+11	3.84E+11	3.94E+11	4.03E+11	4.14E+11
i15$_{1b}$	**p7$_{1b}$**	3.44E+07	3.99E+07	4.62E+07	5.33E+07	6.13E+07	7.29E+07
i15$_{1b}$	**p9$_{1b}$**	8.39E+06	9.98E+06	1.19E+07	1.41E+07	1.66E+07	2.03E+07

(e) $C_2(X^1\Sigma_g^+)$ + 1,2-butadiene, Figure 6(a).

		Collision Energy, kJ mol^{-1}					
From	To	0	4.18	8.37	12.55	16.74	22.00
i1$_{bd}$	**i2$_{bd}$**	3.88E+10	4.07E+10	4.25E+10	4.43E+10	4.62E+10	4.84E+10
i2$_{bd}$	**i1$_{bd}$**	3.90E+06	4.30E+06	4.74E+06	5.20E+06	5.71E+06	6.37E+06
i2$_{bd}$	**p1$_{bd}$**	3.13E+08	3.42E+08	3.73E+08	4.07E+08	4.43E+08	4.92E+08
i2$_{bd}$	**p2$_{bd}$**	4.24E+09	4.57E+09	4.92E+09	5.29E+09	5.68E+09	6.21E+09
i2$_{bd}$	**p3$_{bd}$**	4.09E+08	4.49E+08	4.92E+08	5.39E+08	5.90E+08	6.59E+08
i2$_{bd}$	**p4$_{bd}$**	4.70E+08	5.13E+08	5.60E+08	6.11E+08	6.65E+08	7.39E+08

(f) $C_2(a^3\Pi_u)$ + 1,2-butadiene, Figure 6(b).

		Collision Energy, kJ mol^{-1}					
From	To	0	4.18	8.37	12.55	16.74	22.00
i6$_{bd}$	**i8$_{bd}$**	5.16E+10	5.62E+10	6.09E+10	6.57E+10	7.07E+10	7.74E+10
i8$_{bd}$	**i6$_{bd}$**	3.95E+03	5.18E+03	6.73E+03	8.68E+03	1.11E+04	1.50E+04
i6$_{bd}$	**i5$_{bd}$**	1.73E+09	2.02E+09	2.34E+09	2.69E+09	3.06E+09	3.58E+09
i5$_{bd}$	**i6$_{bd}$**	2.48E+07	3.27E+07	4.25E+07	5.47E+07	6.96E+07	9.32E+07
i5$_{bd}$	**i17$_{bd}$**	4.34E+10	4.83E+10	5.36E+10	5.93E+10	6.52E+10	7.37E+10
i17$_{bd}$	**i5$_{bd}$**	1.60E+04	1.96E+04	2.39E+04	2.89E+04	3.48E+04	4.38E+04
i6$_{bd}$	**p6$_{bd}$**	4.75E+02	2.39E+03	8.71E+03	2.56E+04	6.48E+04	1.78E+05
i6$_{bd}$	**p5$_{bd}$**	2.60E+04	9.21E+04	2.66E+05	6.63E+05	1.49E+06	3.64E+06

i8$_{bd}$	**i11**$_{bd}$	5.45E+08	5.76E+08	6.09E+08	6.42E+08	6.77E+08	7.22E+08
i11$_{bd}$	**i8**$_{bd}$	3.81E+10	4.09E+10	4.39E+10	4.72E+10	5.05E+10	5.50E+10
i8$_{bd}$	**i14**$_{bd}$	1.75E+08	1.93E+08	2.11E+08	2.32E+08	2.54E+08	2.83E+08
i14$_{bd}$	**i8**$_{bd}$	4.63E+09	5.17E+09	5.74E+09	6.37E+09	7.06E+09	7.99E+09
i8$_{bd}$	**p10**$_{bd}$	2.41E+09	2.75E+09	3.12E+09	3.54E+09	3.99E+09	4.64E+09
i8$_{bd}$	**p8**$_{bd}$	5.62E+09	6.48E+09	7.45E+09	8.53E+09	9.74E+09	1.15E+10
i11$_{bd}$	**i12**$_{bd}$	2.01E+10	2.23E+10	2.46E+10	2.71E+10	2.98E+10	3.36E+09
i12$_{bd}$	**i11**$_{bd}$	1.75E+06	2.02E+06	2.32E+06	2.66E+06	3.04E+06	3.59E+06
i11$_{bd}$	**i10**$_{bd}$	2.81E+03	3.88E+03	5.25E+03	7.07E+03	9.41E+03	1.33E+04
i10$_{bd}$	**i11**$_{bd}$	3.62E+05	4.71E+05	6.07E+05	7.73E+05	9.79E+05	1.30E+06
i12$_{bd}$	**i15**$_{bd}$	3.59E+06	4.12E+06	4.71E+06	5.38E+06	6.12E+06	7.19E+06
i15$_{bd}$	**i12**$_{bd}$	2.40E+09	3.62E+09	3.98E+09	4.36E+09	4.76E+09	5.32E+09
i12$_{bd}$	**p11**$_{bd}$	3.10E+11	3.23E+11	3.36E+11	3.51E+11	3.64E+11	3.83E+11
i14$_{bd}$	**i16**$_{bd}$	3.81E+10	4.12E+10	4.44E+10	4.79E+10	5.16E+10	5.65E+10
i16$_{bd}$	**i14**$_{bd}$	3.23E+08	3.49E+08	3.78E+08	4.09E+08	4.41E+08	4.84E+08
i16$_{bd}$	**i15**$_{bd}$	2.06E+08	2.17E+08	2.30E+08	2.43E+08	2.56E+08	2.74E+08
i15$_{bd}$	**i16**$_{bd}$	8.57E+10	9.08E+10	9.61E+10	1.02E+11	1.07E+11	1.15E+11
i16$_{bd}$	**p4**$_{bd}$	9.21E+09	1.03E+10	1.16E+10	1.29E+10	1.44E+10	1.65E+10
i7$_{bd}$	**i4**$_{bd}$	9.74E+10	1.04E+11	1.10E+11	1.17E+11	1.23E+11	1.32E+11
i4$_{bd}$	**i7**$_{bd}$	3.61E+10	3.72E+10	3.83E+10	3.94E+10	4.05E+10	4.18E+10
i7$_{bd}$	**i10**$_{bd}$	6.15E+07	6.89E+07	7.70E+07	8.59E+07	9.57E+07	1.09E+08
i10$_{bd}$	**i7**$_{bd}$	1.09E+12	1.13E+12	1.17E+12	1.21E+12	1.25E+12	1.30E+12
i3$_{bd}$	**i4**$_{bd}$	1.02E+09	1.15E+09	1.30E+09	1.46E+09	1.63E+09	1.88E+09
i4$_{bd}$	**i3**$_{bd}$	5.74E+05	6.83E+05	8.09E+05	9.55E+05	1.12E+06	1.37E+06
i3$_{bd}$	**i13**$_{bd}$	2.78E+07	3.24E+07	3.76E+07	4.35E+07	5.00E+07	5.93E+07
i3$_{bd}$	**i5**$_{bd}$	9.08E+05	1.15E+06	1.43E+06	1.78E+06	2.17E+06	2.76E+06
i5$_{bd}$	**i3**$_{bd}$	1.29E+08	1.60E+08	1.97E+08	2.40E+08	2.91E+08	3.68E+08
i4$_{bd}$	**p9**$_{bd}$	4.76E+07	5.69E+07	6.79E+07	8.05E+07	9.54E+07	1.17E+08
i9$_{bd}$	**i13**$_{bd}$	8.82E+09	1.02E+10	1.16E+10	1.32E+10	1.50E+10	1.73E+10
i13$_{bd}$	**i9**$_{bd}$	2.85E+06	3.91E+06	5.29E+06	7.06E+06	9.30E+06	1.30E+07
i9$_{bd}$	**p7**$_{bd}$	1.16E+09	1.78E+09	2.64E+09	3.79E+09	5.30E+09	7.84E+09
i13$_{bd}$	**i17**$_{bd}$	1.06E+11	1.17E+11	1.28E+11	1.40E+11	1.52E+11	1.69E+11
i17$_{bd}$	**i13**$_{bd}$	3.90E+04	4.65E+04	5.52E+04	6.52E+04	7.68E+04	9.38E+04
i17$_{bd}$	**p1**$_{bd}$	2.46E+09	2.75E+09	3.06E+09	3.38E+09	3.75E+09	4.25E+09
i17$_{bd}$	**p2**$_{bd}$	4.90E+10	5.39E+10	5.92E+10	6.47E+10	7.09E+10	7.91E+10
i17$_{bd}$	**p3**$_{bd}$	4.06E+09	4.57E+09	5.12E+09	5.76E+09	6.40E+09	7.33E+09
i17$_{bd}$	**p4**$_{bd}$	3.53E+09	4.01E+09	4.57E+09	5.15E+09	5.82E+09	6.75E+09