Experimental and computational study of the ultraviolet photolysis of vinylacetylene

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Supporting Information

1. Table S1. Reactions used in the simulations.....page 2

Table S1. Reactions used in the simulations.[a,b]

			DFT			CCSD(T)			G2M			
Rxn	Reactant	Product	E_R	E_P	E_{TS}	E_R	E_P	E_{TS}	E_R	E_P	E_{TS}	Comment
R1	1	3	0.0	22.1	66.2	0.0	23.9	66.2	0.0	23.5	66.0	formally TS(6,3)
R2	1	10	0.0	54.5	67.8	0.0	59.7	70.3	0.0	55.8	70.3	
R2	4	3	35.7	22.1	95.5	36.0	23.9	97.9	35.2	23.5	97.1	formally TS(4,6)
R2	10	4	54.5	35.7	96.2	59.7	36.0	96.8	55.8	35.2	95.0	
R3	10	DP1	54.5	N/A	97.6	59.7	N/A	106.4	55.8	N/A	105.8	
R7	1	27b	0.0	80.2	79.8	0.0	79.3	79.2	0.0	80.1	79.2	
R9	1	14b	0.0	62.1	79.9	0.0	70.0	86.0	0.0	69.7	84.8	
R9	14b	2	62.1	2.8	74.8	70.0	11.0	80.4	69.7	7.4	80.1	
R10	1	2	0.0	2.8	89.9	0.0	11.0	90.8	0.0	7.4	90.2	
R10	2	13	2.8	56.8	71.1	11.0	54.0	69.7	7.4	54.0	68.8	
R11	1	22	0.0	72.3	92.3	0.0	76.4	97.6	0.0	77.3	98.7	
R11	22	DP2	72.3	N/A	76.4	76.4	N/A	81.1	77.3	N/A	82.0	
R12	22	24	72.3	75.1	77.7	76.4	79.2	80.7	77.3	80.1	81.2	
R12	24	5	75.1	39.2	77.7	79.2	33.8	81.3	80.1	33.7	82.4	
R13	1	DP5	0.0	N/A	93.0	0.0	N/A	94.9	0.0	N/A	94.8	
R14	1	DP4	0.0	N/A	102.5	0.0	N/A	102.4	0.0	N/A	102.6	
R15	1	DP6	0.0	N/A	89.8	0.0	N/A	97.8	0.0	N/A	101.0	
R17	2	DP1	2.8	N/A	88.2	11.0	N/A	90.3	7.4	N/A	89.8	
R18	2	DP3	2.8	N/A	89.6	11.0	N/A	97.0	7.4	N/A	96.5	
R19	2	DP6	2.8	N/A	83.9	11.0	N/A	91.0	7.4	N/A	95.1	
R21	3	14b	22.1	62.1	61.9	23.9	70.0	69.0	23.5	69.7	68.4	
R22	3	DP4	22.1	N/A	85.0	23.9	N/A	85.2	23.5	N/A	85.5	
R23	29	DP2	88.8	N/A	91.9	90.6	N/A	93.9	90.0	N/A	92.7	
R24a	1	DP8a	0.0	N/A	107.7	0.0	N/A	109.5	0.0	N/A	112.4	
R24b	1	DP8b	0.0	N/A	107.9	0.0	N/A	109.8	0.0	N/A	112.7	
R26	1	4	0.0	35.7	96.2	0.0	36.0	99.2	0.0	35.2	97.9	
R27	1	33	0.0	67.7	89.7	0.0	71.7	95.9	0.0	69.1	94.0	
R27	9	15	54.9	62.4	95.9	51.6	60.9	92.2	50.8	59.2	91.0	
R27	33	9	67.7	54.9	76.9	71.7	51.6	78.3	69.1	50.8	76.8	
R28	1	9	0.0	54.9	67.0	0.0	51.6	65.3	0.0	50.8	64.6	
R29	2	3	2.8	22.1	85.2	11.0	23.9	85.6	7.4	23.5	84.9	formally TS(28,3)
R30	29	12	88.8	55.8	91.1	90.6	53.9	90.2	90.0	52.6	92.7	
R31	12	15	55.8	62.4	91.1	53.9	60.9	91.9	52.6	59.2	91.0	
R32	12	5	55.8	39.2	66.5	53.9	33.8	69.5	52.6	33.7	67.8	

[a] Zero point corrected energies in kcal/mol for reactants (R), products (P), and transition states (TS), relative to **1**, calculated in Paper I.[23] N/A: dissociation product energies did not factor into the simulations.

[b] These reactions were chosen from those of Paper I[23] by two criteria: all reactions under 100 kcal/mol, and all dissociations of vinylacetylene under 120 kcal/mol.