On-the-fly dynamics of OH radical- and Cl atom-initiated reaction of glyoxal: Atmospheric chemistry of the HC(O)CO radical

Supplementary Material

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Optimized geometries[a] of the isolated A" HC(O)CO, A' HC(O)CO and C-C fission TS

	MPWB1K/6-31+G(d,p)			B3LYP/6-311G(d,p)			BH&HLYP/cc-pvDZ		
	A"	A'	TS	A"	A'	TS	A"	A'	TS
R (O_1C_2)	1.149	1.171	1.138	1.155	1.176	1.143	1.147	1.168	1.138
R (C_2C_3)	1.382	1.553	2.034	1.391	1.592	2.023	1.384	1.557	1.966
R (C_3O_4)	1.244	1.186	1.172	1.251	1.188	1.177	1.243	1.183	1.169
R (C_3H_5)	1.090	1.102	1.104	1.098	1.112	1.112	1.098	1.109	1.112
θ ($O_1C_2C_3$)	179.3	122.1	122.7	177.1	121.0	124.6	179.7	122.5	124.0
θ ($C_2C_3O_4$)	120.5	122.5	118.6	119.8	123.3	119.1	121.4	122.8	120.0
θ ($C_2C_3H_5$)	114.7	113.6	107.0	114.9	112.1	105.9	113.5	112.8	107.0
τ ($O_4C_3C_2O_1$)	0.0	180.0	79.4	0.0	180.0	82.0	180.0	180.0	86.3
τ ($H_5C_3C_2O_4$)	180.0	180.0	152.0	180.0	180.0	151.0	180.0	180.0	155.1

[a] Bond Length R in angstrom, and bond angles θ and dihedral angles τ in degrees.