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SUPPLEMENTARY MATERIAL - Table 4

Results of Intrinsic Reaction Coordinate calculations of $CH_3COCl \longrightarrow CH_2CO + HCl$.

reaction coordinate	energy kcal mol^{-1}	R_{CCl}	R_{CO}	R_{CC}	R_{CH_1}	RC_{CH}	⟨ClCO	⟨ClCC	⟨CCH_1	⟨CCH
-2.49	-35.52	2.091	1.139	1.494	1.073	1.084	116.7	108.0	111.2	107.1
-2.39	-33.03	2.142	1.136	1.493	1.073	1.084	116.1	106.8	111.0	107.0
-2.29	-30.57	2.193	1.132	1.491	1.072	1.084	115.5	105.7	110.8	106.9
-2.19	-28.15	2.245	1.128	1.490	1.072	1.084	114.9	104.5	110.6	106.8
-2.09	-25.80	2.296	1.125	1.488	1.072	1.084	114.2	103.3	110.4	106.7
-1.99	-23.54	2.347	1.122	1.487	1.072	1.084	113.6	102.1	110.1	106.6
-1.89	-21.37	2.398	1.119	1.485	1.072	1.084	112.9	100.8	109.9	106.5
-1.79	-19.31	2.449	1.117	1.484	1.073	1.084	112.2	99.5	109.6	106.5
-1.69	-17.36	2.500	1.114	1.482	1.073	1.084	111.5	98.1	109.3	106.4
-1.59	-15.51	2.551	1.112	1.481	1.073	1.084	110.8	96.7	109.0	106.4
-1.49	-13.78	2.601	1.110	1.479	1.074	1.084	110.2	95.2	108.6	106.4
-1.39	-12.16	2.652	1.108	1.478	1.075	1.084	109.6	93.7	108.2	106.4
-1.29	-10.65	2.702	1.106	1.476	1.076	1.084	109.0	92.2	107.8	106.4
-1.19	-9.24	2.753	1.104	1.474	1.078	1.084	108.5	90.6	107.3	106.5
-1.09	-7.94	2.803	1.103	1.473	1.080	1.084	108.1	89.0	106.8	106.5
-0.99	-6.74	2.853	1.102	1.471	1.082	1.084	107.8	87.2	106.3	106.6
-0.89	-5.63	2.903	1.101	1.469	1.084	1.083	107.5	85.5	105.7	106.7
-0.79	-4.62	2.952	1.100	1.466	1.088	1.083	107.5	83.6	105.2	106.8
-0.69	-3.70	3.001	1.099	1.464	1.091	1.083	107.5	81.7	104.6	107.0
-0.59	-2.87	3.050	1.099	1.460	1.096	1.083	107.7	79.7	104.0	107.2
-0.49	-2.13	3.098	1.099	1.456	1.103	1.083	108.0	77.6	103.3	107.4
-0.39	-1.49	3.145	1.099	1.451	1.110	1.083	108.4	75.4	102.7	107.7
-0.29	-0.93	3.190	1.099	1.445	1.121	1.083	108.9	73.1	102.0	108.1
-0.19	-0.48	3.231	1.100	1.436	1.138	1.082	109.5	70.5	101.1	108.63
-0.09	-0.14	3.263	1.102	1.424	1.164	1.082	110.2	67.8	100.2	109.28
0.00	-0.00	3.284	1.104	1.410	1.199	1.081	110.8	65.1	99.4	109.98
0.39	-3.60	3.320	1.118	1.363	1.382	1.079	113.1	59.0	98.9	112.4
0.79	-10.70	3.365	1.128	1.335	1.576	1.076	114.1	59.7	98.6	114.8
1.19	-17.31	3.459	1.134	1.319	1.801	1.074	112.6	63.4	95.8	117.2
1.59	-20.35	3.556	1.137	1.315	1.975	1.072	110.9	66.4	93.3	118.2
1.99	-22.01	3.673	1.139	1.313	2.144	1.072	109.5	68.6	91.5	118.7
2.39	-22.81	3.815	1.139	1.312	2.296	1.072	109.3	69.3	91.1	118.8
2.49	-22.94	3.855	1.140	1.311	2.329	1.072	109.6	69.1	91.3	118.8

Supplementary Material: Table 5

Results of B3LYP/6-311++G(d,p) calculations for the Intrinsic Reaction Coordinate of $CH_3CO^{\cdot} + Cl^{\cdot} \longrightarrow CH_3Cl + CO$.

reaction coordinate	energy kcal mol^{-1}	R_{CO}	R_{CC}	R_{CH}	R_{CCl}	⟨CCO + 90°	⟨CCH	⟨ClCH
-.749	-5.96	1.137	1.465	1.097	2.626	114.8	105.1	69.8
-.699	-5.30	1.137	1.477	1.097	2.616	116.0	104.5	69.4
-.649	-4.69	1.136	1.489	1.096	2.605	117.3	103.9	69.3
-.599	-4.12	1.136	1.503	1.095	2.594	118.5	103.4	69.4
-.549	-3.57	1.136	1.517	1.094	2.582	119.7	102.8	69.6
-.499	-3.04	1.136	1.533	1.093	2.570	120.8	102.2	69.9
-.449	-2.54	1.136	1.549	1.092	2.558	121.9	101.6	70.4
-.399	-2.06	1.136	1.565	1.092	2.547	122.9	101.0	70.9
-.349	-1.62	1.135	1.583	1.091	2.535	123.9	100.5	71.4
-.299	-1.22	1.135	1.601	1.090	2.523	124.8	99.9	72.0
-.249	-0.89	1.135	1.619	1.089	2.512	125.8	99.3	72.5
-.199	-0.56	1.135	1.637	1.088	2.500	126.6	98.7	73.1
-.149	-0.33	1.134	1.656	1.087	2.489	127.3	98.2	73.7
-.099	-0.14	1.134	1.675	1.086	2.477	128.1	97.6	74.3
-.050	-0.04	1.134	1.695	1.086	2.465	128.8	97.1	74.9
.000	0.00	1.133	1.714	1.085	2.454	129.4	96.5	75.5
.050	-0.04	1.133	1.734	1.084	2.442	130.0	96.0	76.2
.099	-0.14	1.133	1.754	1.084	2.430	130.6	95.4	76.8
.149	-0.34	1.132	1.774	1.083	2.418	131.1	94.8	77.4
.199	-0.60	1.132	1.794	1.082	2.406	131.6	94.3	78.1
.249	-0.94	1.131	1.814	1.082	2.394	132.1	93.7	78.7
.299	-1.37	1.131	1.834	1.081	2.381	132.5	93.2	79.3
.349	-1.86	1.131	1.853	1.081	2.369	132.9	92.6	79.9
.399	-2.43	1.131	1.873	1.080	2.356	133.3	92.0	80.6
.449	-3.07	1.130	1.893	1.080	2.343	133.7	91.5	81.2
.499	-3.77	1.130	1.913	1.080	2.331	134.1	90.9	81.8
.549	-4.54	1.130	1.932	1.079	2.317	134.4	90.3	82.4
.599	-5.37	1.130	1.952	1.079	2.304	134.7	89.7	83.1
.649	-6.26	1.129	1.971	1.079	2.290	135.1	89.2	83.7
.699	-7.19	1.129	1.990	1.078	2.276	135.3	88.6	84.4
.749	-8.18	1.129	2.009	1.078	2.263	135.6	88.0	85.0