

C₂H₃ 与 CH₃F 氢抽提反应机理与动力学性质

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Mechanism and Kinetics of the Hydrogen Abstraction Reaction of C₂H₃ with CH₃F

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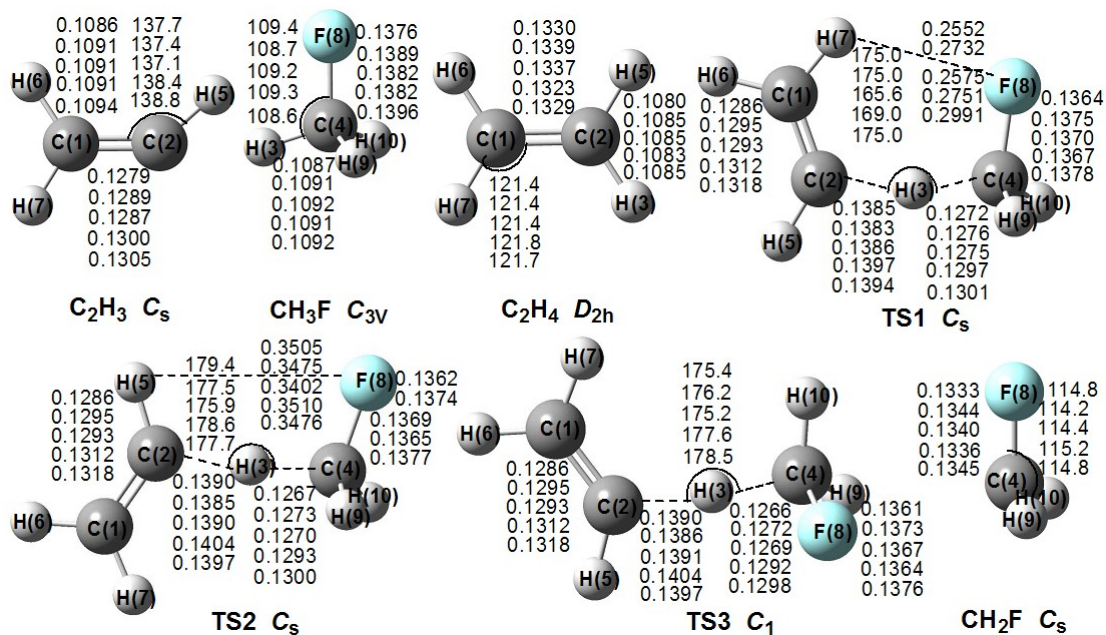


Fig.S1 The geometries of the reactants, products, and the transition states for the title reaction

optimized at different levels in the following order from the top: (1) MP2/6-311G(2df, 2p), (2) MP2/6-311+G(d, p), (3) MP2/6-311G(d, p), (4) B3LYP/6-311G(2df, 2p), (5) B3LYP/6-311+G(d, p). Bond lengths are in nm and bond angles are in degree.

Table S1 The harmonic vibrational frequencies (in cm^{-1}) for the reactants, products, and the transition states at different levels

Species	Methods	Frequencies											
C_2H_3	MP2/6-311G(2df, 2p)	737	993	1064	1089	1430	1918	3146	3246	3319			
	MP2/6-311+G(d, p)	738	971	1040	1083	1426	1854	3138	3241	3308			
	MP2/6-311G(d, p)	766	976	1055	1116	1458	1863	3194	3303	3357			
	B3LYP/6-311G(2df, 2p)	715	826	929	1052	1398	1656	3042	3135	3237			
	B3LYP/6-311+G(d, p)	707	818	923	1042	1390	1644	3039	3136	3240			
CH_3F	MP2/6-311G(2df, 2p)	1115	1222	1222	1521	1526	1526	3096	3192	3192			
	MP2/6-311+G(d, p)	1076	1216	1216	1517	1522	1522	3093	3198	3198			
	MP2/6-311G(d, p)	1106	1224	1224	1519	1519	1537	3087	3186	3186			
	B3LYP/6-311G(2df, 2p)	1075	1198	1198	1494	1497	1497	3028	3100	3100			
	B3LYP/6-311+G(d, p)	1033	1184	1184	1480	1489	1489	3033	3118	3118			
C_2H_4	MP2/6-311G(2df, 2p)	831	968	987	1084	1250	1387	1486	1687	3187	3204	3275	3301
	MP2/6-311+G(d, p)	829	889	966	1061	1237	1382	1481	1675	3175	3193	3266	3292
	MP2/6-311G(d, p)	828	914	971	1073	1236	1384	1481	1681	3178	3195	3268	3294
	B3LYP/6-311G(2df, 2p)	837	980	984	1073	1247	1384	1481	1697	3127	3141	3194	3222
	B3LYP/6-311+G(d, p)	835	974	977	1058	1238	1378	1471	1684	3122	3137	3194	3223
CH_2F	MP2/6-311G(2df, 2p)	639	1204	1226	1512	3209	3369						
	MP2/6-311+G(d, p)	698	1182	1202	1503	3197	3359						
	MP2/6-311G(d, p)	713	1206	1212	1520	3193	3351						
	B3LYP/6-311G(2df, 2p)	509	1172	1199	1473	3128	3282						
	B3LYP/6-311+G(d, p)	488	1160	1162	1455	3132	3295						
TS1	MP2/6-311G(2df, 2p)	66	120	257	287	568	589	875	1077	1115	1128	1211	1223
		1229	1384	1447	1487	1541	1999	3119	3166	3226	3248	3259	2027i
	MP2/6-311+G(d, p)	46	95	248	284	555	578	877	1044	1087	1093	1208	1219
		1236	1370	1446	1486	1538	1942	3118	3156	3226	3237	3251	2012i
	MP2/6-311G(d, p)	67	120	251	288	560	590	875	1054	1097	1117	1204	1227
		1236	1371	1444	1494	1557	1947	3113	3158	3220	3239	3255	2001i
	B3LYP/6-311G(2df, 2p)	62	93	255	283	518	534	866	926	972	1097	1183	1196
		1199	1316	1404	1447	1496	1663	3049	3084	3144	3160	3173	1612i
	B3LYP/6-311+G(d, p)	41	74	254	278	518	518	866	916	962	1061	1178	1189
		1192	1317	1398	1442	1486	1651	3054	3081	3155	3160	3172	1599i
TS2	MP2/6-311G(2df, 2p)	11	77	204	245	566	588	878	1086	1106	1137	1205	1225
		1247	1396	1453	1474	1520	1996	3119	3164	3223	3243	3261	2020i
	MP2/6-311+G(d, p)	7	96	193	266	551	592	881	1043	1084	1098	1203	1220
		1250	1378	1450	1482	1529	1941	3118	3156	3225	3239	3251	2012i
	MP2/6-311G(d, p)	19	73	209	236	547	595	879	1054	1094	1124	1201	1227
		1252	1373	1450	1481	1538	1944	3112	3156	3217	3239	3252	1997i
	B3LYP/6-311G(2df, 2p)	26	90	203	242	518	540	869	932	966	1105	1174	1202
		1213	1327	1411	1435	1489	1661	3048	3083	3141	3152	3177	1599i
	B3LYP/6-311+G(d, p)	25	101	205	249	520	543	869	922	959	1064	1167	1191
		1206	1320	1405	1436	1484	1650	3055	3081	3154	3156	3178	1597i
TS3	MP2/6-311G(2df, 2p)	20	103	142	352	535	582	885	1083	1105	1138	1203	1225
		1241	1403	1453	1479	1508	1994	3117	3165	3219	3245	3259	2011i
	MP2/6-311+G(d, p)	19	108	141	354	528	588	887	1043	1082	1100	1201	1222
		1238	1392	1450	1480	1511	1939	3116	3157	3222	3239	3249	2002i
	MP2/6-311G(d, p)	22	94	139	347	528	583	885	1054	1091	1126	1196	1228
		1244	1381	1450	1484	1520	1943	3109	3158	3212	3239	3250	1987i

	B3LYP/6-311G(2df, 2p)	13	112	146	321	497	547	878	931	966	1105	1168	1197
		1212	1336	1409	1437	1481	1661	3047	3084	3139	3154	3175	1591i
	B3LYP/6-311+G(d, p)	11	116	147	328	496	549	876	920	957	1065	1164	1188
		1203	1336	1403	1431	1473	1650	3054	3082	3152	3157	3175	1589i
TS4	B3LYP/6-311G(d, p)	11	106	144	320	494	546	875	921	959	1087	1159	1191
		1209	1324	1405	1432	1481	1657	3042	3080	3138	3153	3173	1557i

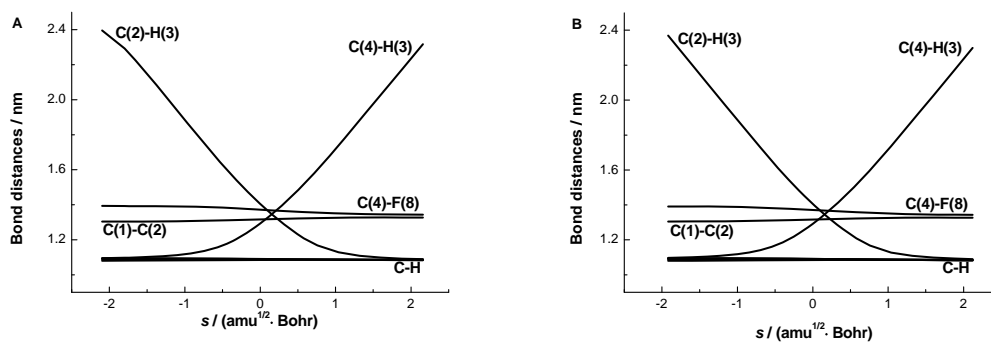


Fig.S2 The variations of bond distances as functions of $s \text{ amu}^{1/2} \cdot \text{Bohr}$ at the B3LYP/6-311G(d, p) level
(A) reaction R2, and (B) reaction R3.

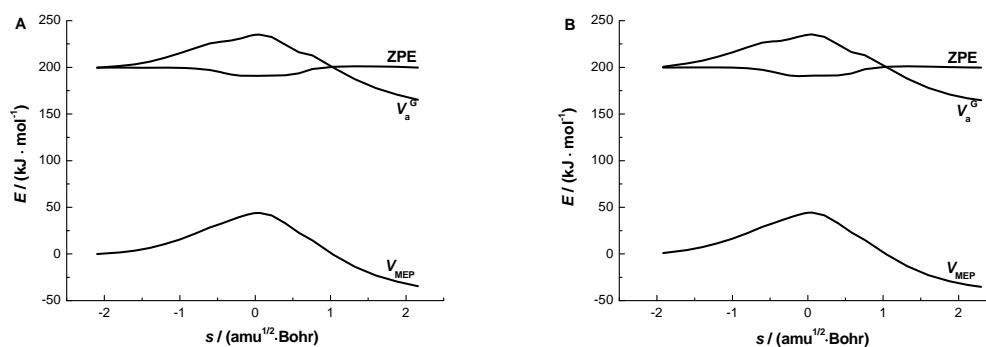


Fig.S3 The classical potential energy curve (V_{MEP}), the ground state vibrational adiabatic potential energy (V_a^G) and the zero-point energy curve (ZPE) as functions of $s \text{ amu}^{1/2} \cdot \text{Bohr}$ at the QCISD(T)/6-311++G(d, p)//B3LYP/6-311G(d, p) level
(A) reaction R2, and (B) reaction R3.