Supporting Information

The Unimolecular Reactions of CF_3CHF_2 Studied by Chemical Activation: Assignment of Rate Constants and Threshold Energies to the 1,2-H-Atom Transfer, 1,1-HF Elimination and 1,2-HF Elimination Reactions and the Dependence of Threshold Energies on the Number of F-Atom Substituents in the Fluoroethane Molecules

Caleb A. Smith, Blanton R. Gillespie, George L. Heard, D. W. Setser[#] and Bert E. Holmes*

Department of Chemistry, University of N. Carolina – Asheville, One University Heights, Asheville, N. Carolina, 28804-8511, United States.
[#] Kansas State University, Manhattan, Kansas, 66506, United States.

TABLE S1. **Calculated frequencies for the ground state of CF_3CHF_2, the 1,1-HF elimination transition state, the 1,2-HF elimination transition state, the 1,2-H atom transfer transition state. All computations were with M06-2X/aug-cc-pvtz.**

	Ground	1,1 HF	1,2 HF	1,2 H-atom transfer	Post Transition State Complex
Frequencies (cm^{-1})	85*	-1145	-1817	-1407	28
	218	75*	114	37	49
	251	163	209	162	96
	368	245	262	166	145
	425	253	272	221	271
	528	311	323	282	351
	590	433	421	521	421
	595	544	521	525	541
	740	563	549	611	550
	892	691	641	664	700
	1183	840	721	784	724
	1198	919	815	1087	728
	1238	1047	1177	1207	882
	1272	1225	1221	1239	1230
	1347	1293	1312	1252	1299
	1387	1309	1501	1253	1304
	1479	1394	1610	1365	1399
	3158	2187	1765	2626	3703
I_X (amu-Å^2)	136	150	156	128	156
I_y (amu-Å^2)	207	213	236	273	354
I_z (amu-Å^2)	250	271	260	319	421
I_{red} (amu-Å^2)	*34	*42	N/A		-
Potential Energy Barrier (kcal/mol)				3.9 kcal/mol	

TABLE S2. **Calculated frequencies for the ground state of CF_3CHF_2, the 1,1-HF elimination transition state, the 1,2-HF elimination transition state, the 1,2-H atom transfer transition state. All computations were with B3PW91/cc-pvdz.**

	Ground	1,1 HF	1,2 HF	1,2 H-atom transfer	Post Transition State Complex
Frequencies (cm^{-1})	62	-632	-1722	-1230	14
	201	56	108	18	34
	235	138	191	129	57
	358	220	263	131	161
	410	236	265	215	256
	518	306	315	269	339
	576	419	415	505	405
	579	532	505	510	523
	720	544	553	587	537
	867	679	642	641	699
	1150	828	744	745	717
	1164	946	812	1065	717
	1208	1034	1146	1179	866
	1239	1176	1188	1216	1207
	1320	1270	1278	1223	1246
	1365	1288	1453	1233	1271
	1444	1355	1609	1365	1352
	3100	2119	1729	2840	3598
I_X (amu-Å^2)	138	155	158	131	153
I_y (amu-Å^2)	210	223	239	283	359
I_z (amu-Å^2)	254	285	263	330	421
See Table S1 for information about				internal rotation	