

Supporting Information

Characterization of the 1,1-HF Elimination Reaction from the Competition between the 1,1- HF and 1,2-DF Unimolecular Elimination Reactions of $\text{CD}_3\text{CD}_2\text{CHF}_2$.

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Table S1. Calculated frequencies for gauche and anti conformations of CH₃CH₂CHF₂, the 1,1 HF elimination transition state, the 1,2 HF trans elimination transition state, and the 1,2 HF cis elimination transition state. All computations were with B3PW91/cc-pvDZ.

	G1 (Gauche)	G3 (Anti)	1,1 HF	1,2 HF trans	1,2 HF cis
	104.53	112.91*	-	-	-
	213.26	219.35	38.15*	132.41	128.42
	244.31	239.60	157.63	183.04	171.32
	384.08	433.80	207.16	263.66	241.02
	499.67	465.85	251.34	305.23	279.05
Frequencies (cm ⁻¹)	677.34	572.41	294.84	473.53	513.28
	783.04	785.59	547.99	544.24	611.38
	878.64	893.90	750.87	639.54	645.04
	993.32	996.57	892.57	750.25	768.68
	1008.08	1074.47	904.00	930.48	931.85
	1114.46	1128.82	1007.31	1014.12	1002.21
	1149.06	1151.69	1067.13	1049.54	1036.87
	1160.58	1164.11	1122.54	1109.62	1057.36
	1281.37	1275.13	1158.07	1220.70	1155.76
	1362.43	1318.30	1231.82	1238.69	1241.11
	1382.87	1377.25	1287.74	1261.47	1270.12
	1384.43	1399.82	1369.64	1310.78	1371.27
	1405.55	1421.49	1385.85	1401.50	1418.67
	1445.26	1450.81	1403.57	1457.16	1460.21
	1464.57	1469.09	1465.50	1474.46	1468.06
	1483.87	1482.22	1479.71	1581.30	1565.56
	3053.50	3050.20	1912.08	1688.35	1686.22
	3060.99	3056.59	2997.30	3039.48	3045.02
	3073.14	3061.92	3065.86	3114.94	3122.11
	3103.95	3110.88	3126.95	3136.23	3148.31
	3148.43	3133.98	3157.33	3168.22	3166.88
	3153.15	3150.38	3164.23	3209.90	3224.61

I _x (amu Å ²)	72.80	58.02	90.42	74.48	80.01
I _y	123.82	141.34	143.30	147.01	133.24
I _z	149.34	182.95	156.04	200.46	176.00

I _{red} (amu Å ²)	16.38	15.02	19.22
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*Frequencies replaced with I_{red} values: G3 as a hindered rotor; 1,1 HF as a free rotor

¹ G1 was 0.13 kcal/mol higher energy than G3

² 1,2 HF trans was 0.42 kcal/mol higher than 1,2 HF cis

Table S2. Calculated frequencies for anti conformation of CD₃CD₂CHF₂, the 1,1 HF elimination transition state, and the 1,2 DF trans elimination transition states; calculated with B3PW91/cc-pvDZ.

	G3 (Anti)	1,1 HF	1,2 DF trans	1,2 DF cis
	97.40*	-	-	-
	165.15	33.94*	107.19	97.57
	215.37	131.94	147.28	146.67
	408.87	180.31	245.26	219.66
	413.44	218.56	292.43	276.06
Frequencies (cm ⁻¹)	542.94	275.88	423.59	482.34
	608.56	472.94	521.03	505.29
	722.75	594.85	572.20	611.80
	798.04	687.03	626.46	632.22
	901.88	810.11	730.33	791.35
	970.12	832.80	812.70	817.19
	1003.29	908.47	871.63	858.92
	1050.46	951.78	923.69	902.46
	1054.43	1025.24	1018.76	966.73
	1061.54	1042.84	1022.06	1011.18
	1115.46	1053.61	1048.73	1051.57
	1118.24	1063.55	1060.22	1056.18
	1163.37	1091.62	1158.73	1096.64
	1233.97	1156.71	1225.46	1229.10
	1374.34	1251.90	1230.69	1241.18
	1401.58	1291.10	1293.30	1350.08
	2194.35	1911.72	1559.04	1544.81
	2230.15	2187.27	2186.99	2191.57
	2306.18	2203.28	2306.99	2310.70
	2320.46	2308.76	2322.75	2330.89
	2334.33	2340.47	2336.02	2337.22
	3058.03	2344.61	3209.70	3223.34
I _x (amu Å ²)	66.38	101.66	81.44	88.44
I _y	147.89	163.99	170.82	153.87
I _z	206.67	205.82	223.51	196.48
I _{red} (amu Å ²)	19.60	25.10		

*Frequencies replaced with I_{red} values: G3 as a hindered rotor; 1,1 HF as a free rotor

Figure S1. Newman projection confirmations and barrier height to internal rotation for $\text{CH}_3\text{CH}_2\text{CHF}_2$ calculated with B3PW91/cc-pvDZ.

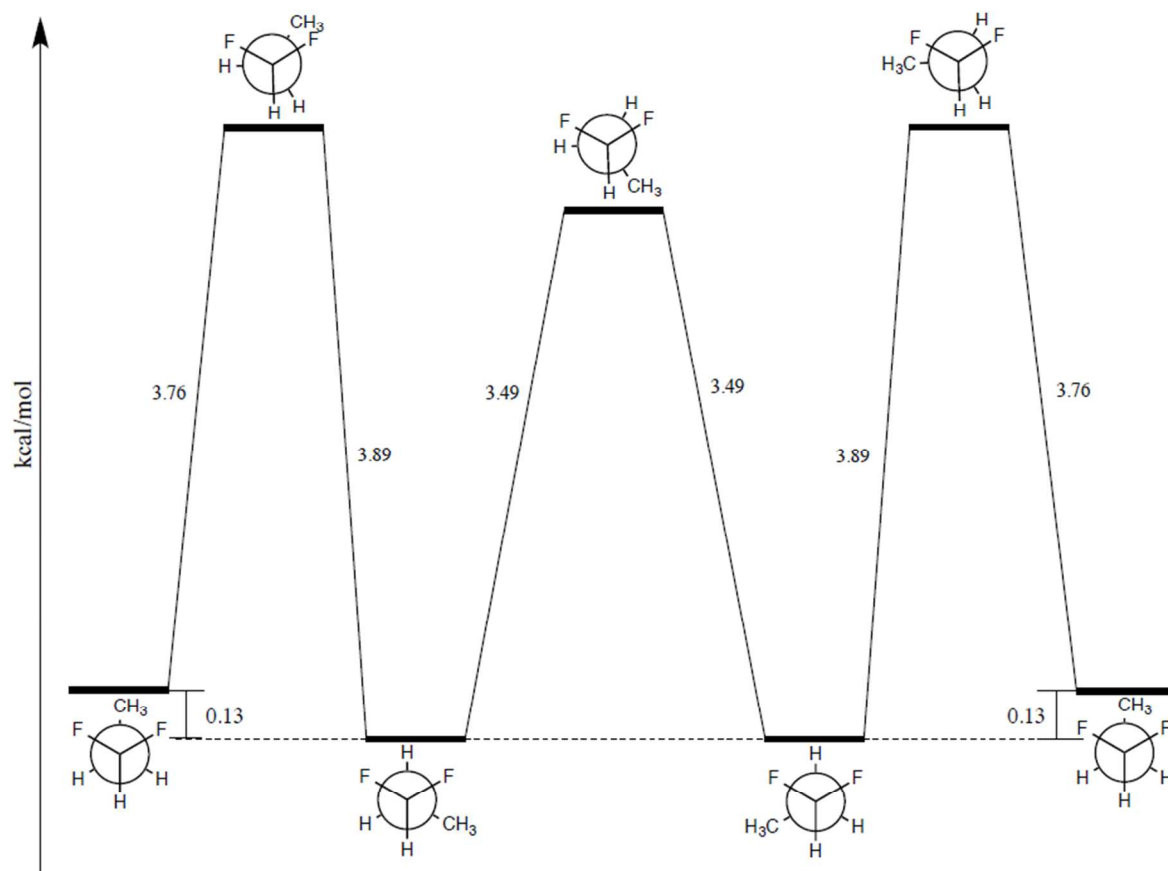


Table S3. Calculated frequencies for gauche and anti conformations of CHF₂CHF₂, the 1,1 HF elimination transition state, and the 1,2 HF elimination transition state. Frequencies were calculated with B3PW91/cc-pvDZ.

	G1 (Anti)	G3 (Gauche)	1,1 HF	1,2 HF
	75.02*	67.23	-	-
Frequencies (cm ⁻¹)	195.96	226.57	46.23*	118.55
	358.28	240.22	130.76	217.52
	401.95	404.17	228.17	257.00
	479.70	519.99	273.15	361.77
	541.37	599.76	416.75	433.01
	624.18	776.01	479.36	586.03
	1110.68	910.39	586.49	599.82
	1133.18	1128.49	856.47	637.55
	1144.68	1139.48	981.04	880.27
	1159.65	1155.04	1102.86	973.98
	1167.14	1218.20	1159.05	1150.10
	1302.07	1320.40	1184.85	1244.92
	1343.46	1376.17	1261.95	1258.78
	1370.74	1406.12	1333.56	1330.55
	1460.05	1437.33	1385.69	1588.68
	3088.38	3078.61	2092.19	1688.44
	3099.20	3087.90	3074.17	3234.82

I _x (amu Å ²)	99.14	96.77	117.13	114.81
I _y	160.91	181.35	177.01	186.44
I _z	245.67	382.39	279.26	236.05

I _{red} (amu Å ²)	26.14	-	31.78	
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*Frequencies replaced with I_{red} values: G1 as a hindered rotor; 1,1 HF as a free rotor