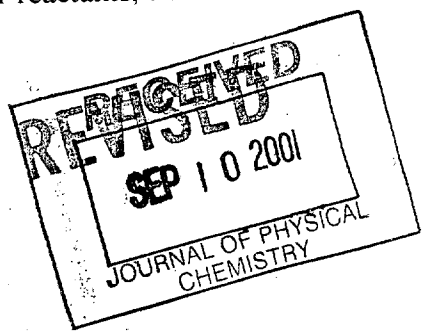
Table 1S. Cartesian coordinates (in 10^{-10} m), rotational constants (GHz) and unscaled harmonic frequencies (in cm^{-1}) obtained at the HF/6-31G(d) level of theory, for reactants, transition states and products in the H + C_4F_6 reaction.



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cis-C_4F_6

	X	Y	Z
C	-1.557103	-0.370296	0.190813
C	-0.716825	0.580661	-0.132982
C	0.716836	0.580662	0.132978
C	1.557106	-0.370292	-0.190839
F	-1.214451	-1.455483	0.814476
F	-2.820558	-0.351571	-0.087003
F	-1.183857	1.666826	-0.741862
F	1.183878	1.666814	0.741874
F	2.820550	-0.351594	0.087002
F	1.214430	-1.455482	-0.814467

B (GHz) 2.0227902 0.9538966 0.7385992

51.4804	105.4243	120.1161
205.8558	228.1561	278.3045
321.4019	407.1096	452.3289
517.5618	588.8472	615.9975
681.1642	692.8889	735.4795
779.3557	1078.1961	1263.5369
1335.7024	1493.8523	1508.0943
1547.3727	2024.9801	2048.8877

CF2H-CF• -CF=CF2

	X	Y	Z
C	1.391353	-0.562255	-0.000354
C	0.718371	0.628534	0.000083
C	-0.661913	0.828168	0.000139
C	-1.762703	-0.182605	0.000279
F	0.802874	-1.720424	-0.000397
F	2.687134	-0.639581	0.000081
F	1.476439	1.714583	0.000197
F	-1.080690	2.085709	-0.000282
F	-1.687472	-0.975122	-1.076980
F	-1.686756	-0.975486	1.077208
H	-2.714406	0.321825	0.000664

B (GHz) 1.6847155 1.1366917 0.7699003

35.6182	64.4480	91.5006
132.2270	136.2430	166.2630
221.7707	327.1237	365.3922
426.8006	473.0656	508.8041
556.8697	623.4781	700.3782

798.8195	1082.8103	1247.8429
1251.4853	1315.8321	1387.8851
1513.1072	1528.3108	1553.8619
1610.6609	1718.5987	3351.6356

•CF2-CFH -CF=CF2

	X	Y	Z
C	1.584249	-0.291914	-0.251261
C	0.724000	0.447279	0.398383
C	-0.683418	0.056525	0.731572
C	-1.583707	-0.006785	-0.474616
F	1.291445	-1.460144	-0.734904
F	2.811428	0.040366	-0.490978
F	1.105680	1.639703	0.848837
F	-0.721611	-1.168031	1.321503
F	-2.808971	-0.383854	-0.198562
F	-1.586217	1.107585	-1.174119
H	-1.072528	0.788732	1.429545

B (GHz) 2.0200085 0.8589519 0.7974869

10.1953	66.0457	109.1667
151.0913	204.3665	292.4235
308.2943	386.5786	433.2503
470.9142	553.3388	581.3756
635.4366	715.4624	730.3473
870.5226	1116.6212	1227.1403
1294.6510	1332.4614	1379.3402
1403.8680	1498.2513	1526.3773
1570.4015	2043.6127	3263.3990

•CFH-CF2 -CF=CF2

	X	Y	Z
C	1.719787	0.149895	-0.109958
C	0.574053	-0.462995	0.052441
C	-0.791720	0.131896	0.217250
C	-1.727788	-0.317595	-0.857958
F	1.887246	1.430531	-0.164773
F	2.841380	-0.483640	-0.244325
F	0.564562	-1.792984	0.073215
F	-0.700008	1.471275	0.230263
F	-2.994438	-0.025994	-0.622554
H	-1.437812	-0.258408	-1.889499
F	-1.288539	-0.237943	1.403602

B (GHz) 2.3884548 0.8655998 0.7496639

37.5186	77.7021	118.4667
188.8849	216.9737	269.7849
301.4615	365.0162	380.9018

435.8900	535.8548	601.0055
619.2169	711.3533	733.3334
784.2865	877.7855	1069.5744
1282.2816	1287.2400	1315.6243
1377.6530	1462.4619	1537.1681
1566.4605	2040.7777	3398.3365

CF2H-CF2-C•=CF2

	X	Y	Z
C	1.828467	-0.174158	-0.174129
C	0.610628	-0.045144	-0.644026
C	-0.632829	0.602046	-0.169402
C	-1.718661	-0.369204	0.266784
F	2.775647	-0.813888	-0.789197
F	2.255386	0.310967	0.953301
F	-0.370600	1.400520	0.874660
F	-2.014068	-1.171687	-0.755822
F	-1.257539	-1.113639	1.271402
H	-2.603789	0.158649	0.582550
F	-1.157920	1.361073	-1.138555

B (GHz) 1.9466700 0.8616334 0.8247450

19.5648	79.5152	92.7943
139.1468	227.6567	275.1767
355.5503	386.8646	414.0576
551.4391	589.1106	607.6031
633.6469	687.5135	774.0321
871.9579	1108.3198	1253.8292
1292.6416	1314.8604	1330.8871
1446.6450	1460.4790	1543.2909
1589.5238	1861.5624	3349.9472

CF3-CH• -CF=CF2

	X	Y	Z
C	-1.551755	-0.446937	0.000029
C	-0.909585	0.766205	-0.000007
C	0.447221	1.050635	-0.000020
C	1.547213	0.039283	0.000000
F	-0.934922	-1.589312	-0.000016
F	-2.844094	-0.561594	0.000001
F	-1.731612	1.811888	-0.000003
F	1.512698	-0.744748	-1.064229
F	1.512752	-0.744644	1.064308
H	0.738225	2.081619	-0.000029
F	2.714424	0.657661	-0.000059

B (GHz) 2.3432449 0.8901797 0.7247381

58.2515	78.2676	131.3280

151.2597	188.2550	227.4114
349.0481	366.7662	435.0520
450.9202	524.5659	576.3090
586.7880	654.1810	690.2262
765.3987	831.5186	981.3648
1237.6583	1299.5890	1351.7761
1415.4728	1421.1044	1520.8093
1612.1975	1708.8042	3422.8543

H...CF2-CF•-CF=CF2
alpha-TS

	X	Y	Z
C	1.593602	-0.405648	-0.139464
C	0.742001	0.603401	0.060160
C	-0.680428	0.595660	-0.154660
C	-1.575482	-0.375496	0.211646
F	1.243051	-1.569521	-0.592948
F	2.859920	-0.334525	0.123194
F	1.255994	1.767740	0.437518
F	-1.199596	1.759165	-0.514419
F	-2.802227	-0.362475	-0.221882
F	-1.182289	-1.572643	0.545511
H	-2.051835	0.302834	2.141142

B (GHz) 1.9679447 0.9675263 0.6985708

-682.1364	57.8956	106.7584
122.8957	188.4923	210.8205
277.8152	303.1661	337.5729
367.5639	396.2194	412.1953
470.5775	519.1762	528.2566
600.2869	622.7052	661.2234
740.3146	1041.4200	1222.7237
1349.7638	1481.4376	1504.1395
1536.4891	1672.8996	1806.9389

•CF2-CF(...H)-CF=CF2
beta-TS

	X	Y	Z
C	1.867713	-0.072709	-0.054216
C	0.617363	0.394267	0.062301
C	-0.592414	-0.381434	0.169687
C	-1.851850	0.072428	-0.223106
F	2.185171	-1.325915	-0.150156
F	2.904861	0.706689	-0.076341
F	0.470156	1.709437	0.146586
F	-0.431058	-1.694685	0.104246
F	-2.885677	-0.709903	-0.089363
F	-2.172659	1.332116	-0.143707
H	-0.882012	-0.234961	2.150620

B (GHz)2.4368348 0.8331792 0.6322971

-700.4144	38.9026	106.0271
133.9552	165.5872	228.6811
286.5309	305.6805	336.4712
367.2572	393.3403	410.6521
464.2317	519.0342	563.1942
621.7143	629.6646	658.2820
750.5272	998.0073	1270.8820
1343.8919	1463.5988	1500.4175
1547.9148	1660.0673	1778.5980

Adduct isomerization 1,2 H shift TS

	X	Y	Z
C	-0.356978	0.614548	0.331432
C	-1.812954	0.606263	0.190260
C	0.425477	-0.598076	0.196967
F	0.280632	1.749280	0.062315
H	-1.191465	0.487640	1.428933
F	-2.388138	-0.285734	-0.595224
F	-2.338526	1.802502	0.031602
C	1.716528	-0.706571	-0.115745
F	-0.228751	-1.709796	0.517378
F	2.481330	0.288358	-0.444958
F	2.344454	-1.842901	-0.131826

B (GHZ)2.3954671 0.8314345 0.6486146

-2576.369	50.3540	79.3300
119.6703	153.0954	217.0034
298.1035	308.9904	375.8316
390.1525	451.6529	495.5780
566.1945	609.5575	653.2419
711.0749	802.1749	1007.9623
1182.5208	1246.7190	1326.6430
1410.2106	1481.3286	1537.3686
1574.2535	1753.8689	1840.6669