

Supplemental Material-II

Theoretical Kinetic and Mechanism Studies on the Reactions of CF₃CB₂H₂ (2-BTP) with OH and H Radicals

Huiting Bian¹, Lili Ye², Jinhua Sun^{1,*}

¹ *State Key Laboratory of Fire Science, University of Science and Technology of China, Hefei, Anhui 230026, P. R. China*

² *Key Laboratory for Power Machinery and Engineering of MOE, Shanghai Jiao Tong University, Shanghai 200240, P. R. China*

Index of supplemental material-II

Geometries and frequencies of all the species involved in the present work

- Geometries and frequencies of transition states, reactants, intermediates and products involved in the reactions of 2-BTP + OH calculated at B3LYP/aug-cc-pVTZ. 2
- Geometries and frequencies of transition states, reactants, intermediates and products involved in the reactions of 2-BTP + H calculated at B3LYP/aug-cc-pVTZ. 19

- **Geometries and frequencies of major species involved in the present work**
- Geometries and frequencies of transition states, reactants, intermediates and products involved in the reactions of 2-BTP + OH calculated at B3LYP/aug-cc-pVTZ.

TSa1

Cartessian coordinates:				Frequencies (cm-1):		
C	0.833621	-0.90039	-0.0097	-20.0752	20.3922	53.7807
C	-0.08845	0.072386	0.682234	73.4781	165.8377	185.2429
C	0.23856	0.710159	1.791895	225.2122	251.9462	326.6902
H	1.200707	0.540602	2.252882	336.4443	480.5961	482.4582
H	-0.43475	1.413365	2.257379	577.9922	616.717	690.9262
F	0.253545	-2.08986	-0.22484	730.3832	825.8335	978.9331
F	1.950856	-1.11559	0.703837	1092.542	1113.654	1172.012
F	1.225095	-0.42687	-1.22161	1270.072	1433.732	1689.027
Br	-1.7515	0.32919	-0.20149	3165.938	3256.234	3685.689
O	2.659834	2.301418	-0.55718			
H	2.490152	1.510926	-1.10387			

TSa2

Cartessian coordinates:				Frequencies (cm-1):		
C	1.250571	-0.43354	-0.0157	-277.069	66.7584	137.1088
C	0.070942	0.425026	0.411068	149.0496	190.118	243.4862
C	0.196386	1.382845	1.353868	299.834	324.6533	337.7329
H	1.176548	1.688304	1.68996	434.8619	479.665	570.284
H	-0.66924	1.885567	1.75317	578.9215	652.6766	690.4043
F	1.339248	-1.52186	0.775872	733.9596	832.0904	913.6741
F	2.408372	0.249332	0.119411	1089.367	1129.787	1192.055
F	1.169698	-0.85803	-1.27532	1253.612	1418.755	1574.768
Br	-1.62139	-0.29607	-0.03434	3167.91	3269.919	3723.716
O	0.21622	1.938862	-1.0417			
H	1.148388	2.20686	-0.98273			

TSa3

Cartessian coordinates:				Frequencies (cm-1):		
C	-1.59573	-0.2041	0.091669	-320.004	34.4739	50.7604
C	-0.53486	0.793953	-0.21954	104.9979	115.9783	156.0603
C	-0.65177	2.048761	-0.56918	220.9991	255.2096	375.0053
H	-1.62849	2.509622	-0.68639	441.6907	458.7604	544.8195
H	0.214243	2.671875	-0.75505	563.0267	591.1172	678.8675

F	-1.8104	-1.06221	-0.91977	797.5079	961.3706	1025.957
F	-2.78332	0.404812	0.344534	1106.227	1125.803	1136.416
F	-1.29295	-0.93334	1.184283	1200.132	1420.815	1721.716
Br	1.716887	0.149873	0.236501	3104.576	3186.888	3745.634
O	1.169999	-1.24097	-0.94279			
H	1.63731	-2.01432	-0.59287			

TSa4

Cartessian coordinates:				Frequencies (cm-1):		
C	1.557324	0.270994	0.000001	-1488.75	42.766	79.3938
C	0.055081	0.474778	-1.5E-05	87.1898	152.5268	160.3614
C	-0.50238	1.660596	-5.5E-05	245.0627	259.1051	323.0485
H	0.00467	2.615571	-8.3E-05	472.9277	480.788	564.1789
H	-1.75595	1.811841	-6.5E-05	568.747	633.5091	635.2012
F	1.960908	-0.41257	1.08377	700.3918	752.6917	879.2827
F	2.202958	1.450051	-3.5E-05	889.3118	1100.939	1145.156
F	1.960924	-0.41264	-1.08371	1165.706	1236.911	1439.097
Br	-0.94508	-1.14596	0.000028	1685.109	3200.82	3731.065
O	-2.97217	1.84098	-0.00007			
H	-3.17695	0.891527	-3.8E-05			

TSa5

Cartessian coordinates:				Frequencies (cm-1):		
C	-0.65969	1.000279	-1.5E-05	-1470.88	34.9827	64.3259
C	-0.08686	-0.39736	-3.1E-05	120.9887	147.4138	164.4461
C	-0.77018	-1.51522	-9.2E-05	227.9802	262.9523	316.3203
H	-2.02177	-1.57191	-0.0002	455.5382	479.297	560.6133
H	-0.36842	-2.51844	-7.1E-05	575.0765	623.2139	650.8562
F	-0.27099	1.691226	1.083353	686.3676	771.4101	872.7665
F	-2.00828	0.982593	0.000005	896.7934	1088.037	1150.414
F	-0.27101	1.691244	-1.08338	1154.362	1257.991	1445.622
Br	1.827916	-0.43983	0.000018	1689.797	3207.211	3748.906
O	-3.25173	-1.69554	0			
H	-3.52012	-0.76292	0.000665			

TSa6

Cartessian coordinates:				Frequencies (cm-1):		
C	-1.04081	-0.13546	-0.50495	-441.989	52.1951	81.7137
C	0.07722	0.719314	-0.06507	162.5493	188.7056	234.5716
C	-0.10774	2.00493	0.205809	294.0852	334.7305	371.9124

H	-1.10174	2.425912	0.163732	403.6496	452.1123	517.937
H	0.71523	2.641839	0.491159	544.5442	623.1918	667.2312
F	-0.77765	-1.24541	-1.12776	709.8703	753.4077	859.7015
F	-1.99553	0.45246	-1.17155	986.5465	1119.262	1247.581
F	-2.3217	0.248062	1.070601	1336.9	1429.069	1652.576
Br	1.778171	-0.11326	0.035663	3166.851	3262.282	3758.679
O	-1.08029	-1.35965	1.169699			
H	-0.92534	-0.85522	1.982956			

TSa7

Cartessian coordinates:				Frequencies (cm-1):		
C	1.050923	0.161178	0.380886	-459.759	50.505	73.72
C	-0.20178	0.767543	-0.13336	170.9345	195.8694	250.288
C	-0.20066	1.964443	-0.70468	325.4278	351.6112	372.0157
H	0.719311	2.521287	-0.80824	394.8509	458.028	524.6907
H	-1.10881	2.400554	-1.09052	546.4883	619.7329	650.2797
F	0.981967	-0.76561	1.281987	726.884	758.8316	845.7446
F	1.911841	1.081877	0.725437	977.1258	1112.532	1249.863
F	2.714752	-0.60194	-0.55903	1342.765	1428.557	1655.156
Br	-1.78023	-0.25885	0.068849	3167.246	3260.023	3741.324
O	0.883052	-1.0893	-1.23171			
H	1.265042	-1.93581	-0.94996			

TSa8

Cartessian coordinates:				Frequencies (cm-1):		
C	-0.61754	0.921634	-0.43845	-526.967	38.9003	60.7364
C	0.449791	0.698984	0.451189	78.9952	110.0266	126.0035
C	0.554868	1.313866	1.652574	180.8771	189.049	216.6746
H	-0.18437	2.041497	1.953957	321.3569	364.9165	410.6534
H	1.361001	1.08388	2.329597	523.4045	533.7231	602.2729
F	-0.59464	0.556463	-1.69519	647.4553	847.3294	853.5597
F	-1.45314	1.915372	-0.23552	1117.25	1206.863	1313.361
F	-1.96592	-0.67983	0.248788	1349.407	1438.834	1522.912
Br	1.728372	-0.60355	-0.09519	3167.859	3268.221	3743.85
O	-3.12735	-1.67485	0.538425			
H	-2.8503	-2.33749	-0.11382			

M1-TSa1

Cartessian coordinates:				Frequencies (cm-1):		
C	1.439914	-0.11938	-0.02159	-647.804	44.7981	737.4005

C	0.043434	0.420355	-0.03987	158.4876	179.0608	199.634
C	-0.20172	1.745984	-0.03902	326.4054	351.3925	376.3796
H	0.621366	2.436047	-0.16078	401.4213	442.6223	483.8233
H	0.156046	2.084615	1.893863	534.1515	610.1244	686.0973
F	1.699134	-0.83077	1.092857	715.9782	934.4841	1152.99
F	2.350937	0.877691	-0.0774	1119.741	1123.608	1127.474
F	1.680482	-0.93511	-1.0675	1253.409	1303.236	1353.064
Br	-1.3417	-0.85299	0.015832	1651.93	3188.325	3824.618
O	-1.45484	2.231767	-0.14191			
H	-1.44384	3.191875	-0.08074			

M1-TSa2

Cartessian coordinates:				Frequencies (cm-1):		
C	1.434094	-0.17436	0.018622	-1895.78	50.9864	118.6402
C	0.079319	0.414396	0.305771	151.348	156.7786	216.3849
C	-0.06264	1.834478	-0.02227	295.2799	366.9096	374.4352
H	0.689739	2.343702	-0.61927	470.4358	486.0489	575.128
H	0.255005	1.366912	1.187634	613.4435	697.6425	824.8385
F	2.413315	0.683104	0.404006	906.5889	1074.457	1086.491
F	1.629204	-0.41001	-1.30005	1153.961	1218.295	1242.022
F	1.639255	-1.33103	0.660272	1247.243	1302.629	1427.989
Br	-1.39587	-0.81845	-0.00516	2101.377	3090.662	3807.413
O	-1.3292	2.338583	-0.0094			
H	-1.29632	3.300783	-0.00335			

M1-TSa3

Cartessian coordinates:				Frequencies (cm-1):		
C	1.288806	-0.440376	-0.379141	-209.0883	70.1039	117.3477
C	0.214317	0.275103	0.069445	142.9361	160.6693	193.2738
C	0.292378	1.734429	0.421077	255.4849	313.3167	327.5318
H	1.333983	2.005229	0.571267	371.9347	456.6298	515.0172
H	-0.236718	1.884159	1.362915	591.4087	658.4083	895.1229
F	1.062999	-0.449901	1.780392	1029.5607	1057.3564	1140.2765
F	2.480899	0.064739	-0.487613	1224.9201	1357.6917	1363.904
F	1.244093	-1.67221	-0.777948	1396.3118	1488.5685	1646.3261
Br	-1.490017	-0.50785	-0.047147	3059.3642	3131.981	3801.0232
O	-0.205719	2.561707	-0.617296			
H	-1.165841	2.493123	-0.647436			

M1-TSa4

Cartessian coordinates:				Frequencies (cm-1):		
C	1.539897	-0.1639	-0.00034	-1036.79	54.8333	113.3527
C	0.290431	0.395245	-0.00012	165.8204	171.4605	198.3956
C	0.070904	1.763729	-0.00019	219.6859	250.9124	348.6525
H	2.645781	0.574462	0.000259	375.1757	446.604	536.8474
F	1.816049	-1.45234	0.000011	578.5611	611.1245	660.3914
F	-1.19341	-0.79604	0.000023	952.1716	1027.893	1106.533
F	0.900632	2.454996	-0.00062	1197.855	1247.004	1351.264
Br	-1.19196	2.264005	0.000142	1363.076	1451.547	1567.236
H	-1.15929	3.224717	0.000106	1897.69	3004.341	3825.091
O	1.539897	-0.1639	-0.00034			
H	0.290431	0.395245	-0.00012			

M1-TSa5

Cartessian coordinates:				Frequencies (cm-1):		
C	1.219798	-0.57037	-0.01733	-2003.6	54.4169	121.0425
C	0.104006	0.457634	-0.03152	151.8084	206.248	289.9963
C	0.336839	1.755926	0.689627	314.3429	379.6929	448.387
H	1.241091	1.791457	1.29616	545.5947	581.7314	673.0145
H	-0.52327	2.129565	1.240914	805.1037	838.3107	944.8863
F	1.258713	-1.23336	1.157474	969.563	1091.851	1122.839
F	2.411719	0.030286	-0.17635	1144.989	1157.238	1185.503
F	1.083688	-1.47921	-0.99172	1290.792	1317.173	1515.565
Br	-1.65166	-0.29086	-0.01476	1968.609	3060.909	3117.157
O	0.509813	2.410364	-0.5859			
H	0.260697	1.257594	-1.0827			

M1-TSa6

Cartessian coordinates:				Frequencies (cm-1):		
C	0.790241	-0.88318	-0.35169	-1572.84	75.9679	96.0759
C	0.00378	0.242956	-0.39256	149.4011	176.2983	207.7018
C	0.622981	1.58956	-0.59894	246.095	318.7898	363.6553
H	-0.11438	2.368901	-0.35233	459.8469	534.5496	611.2849
H	0.78364	1.711766	-1.69159	628.656	720.1693	830.3512
F	1.816896	-0.08267	1.498463	1008.919	1104.427	1146.949
F	1.948849	-0.94991	-0.92323	1176.933	1211.32	1289.991
F	0.370654	-2.04243	0.032325	1374.945	1381.047	1571.889
Br	-1.79183	0.082201	0.092681	1607.966	2834.535	2945.409
O	1.801397	1.765899	0.06548			

H	1.904148	0.894203	0.867387
---	----------	----------	----------

M2-TSa1

Cartessian coordinates:

Frequencies (cm-1):

C	1.136083	-0.76035	0.098168	-912.536	53.0559	75.8137
C	0.387223	0.205463	0.80812	113.9411	156.9778	242.2872
C	0.49315	1.574208	0.454692	306.7494	334.168	424.7715
H	-0.2138	2.283754	0.879063	493.677	553.4748	623.0001
H	0.053426	-0.06607	1.796698	745.4965	796.5184	827.0615
F	2.82023	0.167991	-0.14295	936.7184	1022.376	1106.797
F	1.01625	-0.92765	-1.17781	1266.668	1313.857	1379.095
F	1.512279	-1.8444	0.68897	1399.052	1510.7	1634.687
Br	-2.10179	-0.06246	-0.07132	1679.03	3133.689	3225.57
O	1.405722	2.016523	-0.28966			
H	2.239541	1.156899	-0.34196			

M2-TSa2

Cartessian coordinates:

Frequencies (cm-1):

C	1.5004	-0.67173	0.00118	-303.955	13.3319	64.5665
C	-0.34579	0.725182	0.472989	92.5662	127.6765	145.4781
C	-0.12249	1.83865	-0.2597	216.1857	275.89	355.967
H	-0.5692	1.988332	-1.23352	377.1557	501.0847	506.6442
H	-0.04222	0.651227	1.504835	628.9543	750.6994	790.2182
F	1.486645	-1.75947	0.771534	903.9628	984.1415	1142.882
F	2.603134	0.036869	0.247509	1160.491	1176.615	1184.188
F	1.475584	-1.02612	-1.28184	1290.162	1320.186	1604.279
Br	-1.78696	-0.42634	-0.00591	3180.911	3213.635	3828.315
O	0.74523	2.779252	0.188698			
H	0.912353	3.434085	-0.4956			

M2-TSa3

Cartessian coordinates:

Frequencies (cm-1):

C	-1.44317	-0.12326	0.008971	-722.872	54.1537	155.0362
C	-0.05398	0.434896	-0.16735	174.1938	175.8543	320.2491
C	0.162281	1.755179	-0.00798	325.4211	378.9705	397.668
H	-0.67619	2.438928	0.003238	402.0191	454.2564	503.1832
H	-0.14536	0.350397	-2.14347	530.1266	598.245	614.2131
F	-1.68163	-1.19	-0.76399	718.3332	874.9197	942.1077
F	-2.37698	0.81012	-0.28211	1114.251	1146.324	1185.743

F	-1.66231	-0.51016	1.285546	1264.02	1299.643	1344.767
Br	1.365242	-0.81789	0.011844	1669.821	3182.376	3823.932
O	1.397591	2.276195	0.059149			
H	1.354781	3.236795	0.095602			

M2-TSa4

Cartessian coordinates:				Frequencies (cm-1):		
C	-0.40248	-0.97653	0.053685	-671.778	91.6788	110.5523
C	-0.97171	0.226085	-0.46484	145.9082	179.4334	202.4095
C	-1.32302	1.282173	0.352788	216.3871	262.8994	343.0825
H	-1.23453	1.231353	1.428395	399.4824	422.8379	474.3003
H	-1.00194	0.31777	-1.5376	490.8394	634.484	812.4055
F	-0.06146	-1.9552	-0.70384	909.7139	924.8786	1154.234
F	-2.37452	-1.14426	-0.25221	1225.935	1318.854	1324.167
F	-0.40675	-1.26455	1.310125	1420.801	1501.824	1653.587
Br	1.728923	0.355115	-0.04344	3205.233	3251.748	3799.509
O	-1.8106	2.382277	-0.20778			
H	-2.02334	3.04939	0.455321			

M3-TSa1

Cartessian coordinates:				Frequencies (cm-1):		
C	1.543728	-0.23647	-0.12007	-177.887	85.4295	99.2201
C	0.557247	0.651944	0.249049	110.3734	146.4693	195.7303
C	0.157194	1.82503	-0.6163	258.3442	297.341	341.1579
H	0.112651	1.504423	-1.65407	389.016	449.8149	508.448
H	0.957617	2.572154	-0.51943	621.6773	774.8387	956.4545
F	0.479402	0.897556	1.565966	1070.476	1110.151	1226.758
F	1.836692	-0.47773	-1.37014	1258.856	1361.634	1366.885
F	2.149898	-1.03169	0.713676	1422.686	1479.235	1609.15
Br	-1.28551	-0.96134	-0.04023	2965.358	3122.144	3804.434
O	-1.08905	2.377143	-0.29028			
H	-1.10797	2.616847	0.642282			

M3-TSa2

Cartessian coordinates:				Frequencies (cm-1):		
C	1.378743	-0.63485	-0.24524	-498.104	41.5819	80.0239
C	0.331397	-0.21938	0.506004	-498.104	41.5819	80.0239
C	0.228389	2.134308	0.440566	221.2699	290.2714	300.6903
H	1.249084	2.358796	0.714162	334.8278	350.0687	440.8061

H	-0.54023	2.194028	1.201984	334.8278	350.0687	440.8061
F	0.488508	-0.21395	1.842873	874.3377	976.7971	1076.402
F	2.624932	-0.57657	0.193508	1142.379	1193.091	1301.697
F	1.319057	-0.83052	-1.54716	1368.331	1488.847	1637.897
Br	-1.44517	-0.5824	-0.08572	3103.71	3234.735	3790.95
O	-0.08006	2.545273	-0.81588			
H	-1.01122	2.377809	-0.99995			

M4-TSa1

Cartessian coordinates:				Frequencies (cm-1):		
C	-0.24259	0.791732	0.117439	-233.382	28.792	106.5698
C	1.086248	0.199609	0.47397	178.9955	244.5897	278.2408
C	2.225045	0.531888	-0.25992	318.6596	332.4156	373.1168
H	2.268603	1.361108	-0.95402	408.2299	542.0942	587.2763
H	1.16261	-0.14962	1.490643	787.1067	860.4136	881.2443
F	-0.17196	1.529051	-1.01412	958.5714	965.5952	1073.561
F	1.439876	-1.74401	0.227835	1165.759	1211.721	1290.518
F	-0.6472	1.624696	1.10767	1350.553	1389.165	1598.387
Br	-1.61918	-0.58001	-0.12105	2995.413	3195.329	3218.988
O	3.290921	-0.20661	-0.16765			
H	2.914159	-1.08544	0.160117			

M4-TSa2

Cartessian coordinates:				Frequencies (cm-1):		
C	-0.20929	-0.44548	0.391056	-285.415	18.4767	61.1452
C	1.586993	0.863364	-0.39207	89.3371	132.7289	195.1059
C	2.665741	0.150157	-0.00845	235.1665	296.9907	306.5002
H	3.15077	0.334277	0.94108	329.6729	333.2941	519.3708
H	1.152718	0.823901	-1.37931	559.9747	622.8543	778.4663
F	-0.16899	-0.31976	1.714278	898.3968	1085.151	1098.45
F	1.262363	1.966894	0.31566	1140.454	1181.796	1223.994
F	0.061728	-1.71011	0.076261	1301.183	1348.977	1651.143
Br	-1.9332	0.122772	-0.33784	3182.343	3211.854	3836.654
O	3.120813	-0.86046	-0.79191			
H	3.735549	-1.41288	-0.30116			

M4-TSa3

Cartessian coordinates:				Frequencies (cm-1):		
C	-0.20482	0.735589	0.091874	-599.049	62.2054	141.9055

C	1.191476	0.224242	-0.13921	172.0229	247.744	282.5063
C	1.624034	-1.02493	0.099312	293.2509	316.3831	333.9981
H	0.916188	-1.82745	0.234737	356.7628	387.8253	410.1583
H	0.984727	0.045241	-2.16352	462.4054	611.583	641.2
F	-0.50329	1.717791	-0.77338	777.4462	858.2861	929.8723
F	2.077937	1.23413	-0.22628	1043.667	1099.15	1188.051
F	-0.30677	1.274225	1.331322	1247.87	1304.988	1361.709
Br	-1.58801	-0.66187	-0.06597	1717.498	3220.816	3831.387
O	2.94054	-1.30557	0.094093			
H	3.080047	-2.25245	0.188222			

M4-TSa4

Cartessian coordinates:				Frequencies (cm-1):		
C	0.14439	-0.69423	0.159494	-666.316	26.7941	82.4191
C	-1.0788	0.045729	-0.2286	118.662	155.7436	173.855
C	-1.36572	1.307518	0.144352	282.6971	295.0503	345.9322
H	-0.5902	1.97643	0.503755	388.1883	438.1465	490.5782
H	-1.9052	-0.60547	-0.73821	577.8624	634.7935	669.7867
F	0.294143	-1.81085	-0.56208	954.6031	962.6644	1110.02
F	-2.93649	-1.34238	-0.3441	1149.205	1179.376	1272.707
F	0.164849	-1.05102	1.459497	1301.004	1346.462	1658.681
Br	1.770028	0.437846	-0.16231	1952.359	3145.573	3802.983
O	-2.59317	1.80629	0.026559			
H	-2.61197	2.738171	0.271496			

M5-TSa1

Cartessian coordinates:				Frequencies (cm-1):		
C	1.100949	-0.70427	-0.00257	-687.495	66.5122	88.9654
C	0.116216	0.334973	-0.54238	155.3913	176.6316	224.4872
C	0.451025	1.789665	-0.17587	298.5385	333.1031	379.6552
H	-0.37488	1.766407	1.55012	392.98	511.8796	519.4024
H	-0.38778	2.486954	-0.34664	839.3873	948.0617	1014.158
F	1.238534	-0.63553	1.327477	1122.067	1154.775	1189.802
F	2.307042	-0.51948	-0.56261	1246.76	1324.25	1393.8
F	0.706821	-1.95274	-0.31142	1716.683	2930.225	3093.806
Br	-1.72085	-0.0689	0.005855	-687.495	66.5122	88.9654
O	1.574031	2.169135	0.058015			
H	0.119446	0.252768	-1.62866			

M5-TSa2

Cartessian coordinates:				Frequencies (cm-1):		
C	0.976807	-0.86848	-0.00254	-431.383	31.7325	82.8439
C	0.071247	0.229916	-0.51396	133.4322	151.12	192.9254
C	0.764848	2.023371	0.282484	277.1866	311.4034	402.2345
H	0.652812	1.675728	1.32096	515.1684	557.9271	606.6994
H	-0.09436	2.579116	-0.12281	676.3534	731.6413	854.3531
F	1.044733	-0.89624	1.337697	880.4197	1101.302	1123.492
F	2.214018	-0.71286	-0.48555	1146.108	1228.734	1236.113
F	0.535203	-2.08061	-0.40708	1299.62	1436.231	1580.888
Br	-1.74077	0.084824	-0.0132	2916.895	2984.51	3198.761
O	1.8926	2.152023	-0.22206			
H	0.204733	0.458705	-1.56128			

M5-TSa3

Cartessian coordinates:				Frequencies (cm-1):		
C	-1.44458	-0.40238	-0.00268	-554.309	59.4925	117.6331
C	0.306212	0.65501	0.602068	141.7035	261.5611	294.6988
C	-0.18407	1.892969	-0.0294	341.9743	358.6878	487.6005
H	0.202132	2.041255	-1.04154	523.2753	561.757	664.2571
H	-0.01192	2.788794	0.574037	713.7844	858.0722	917.9839
F	-0.96948	-1.48497	0.67696	1016.644	1042.543	1074.849
F	-1.25062	-0.61725	-1.29695	1148.749	1183.995	1203.345
F	-2.74323	-0.40803	0.278211	1255.764	1343.176	1509.635
Br	1.84387	-0.22287	-0.04585	3009.586	3052.384	3199.934
O	-1.53655	1.518626	0.00762			
H	0.171378	0.540018	1.667266			

Ma1

Cartessian coordinates:				Frequencies (cm-1):		
C	1.429408	-0.1514	-0.04357	17.5621	39.7177	126.856
C	0.036019	0.382414	0.030396	172.2197	177.7481	248.7508
C	-0.2365	1.786065	0.442946	313.9544	343.2575	417.3095
H	0.701174	2.347231	0.410068	520.8726	558.5096	612.0288
H	-0.60235	1.797327	1.478007	697.0492	873.0353	1009.634
F	1.914985	-0.47819	1.185455	1044.742	1074.642	1115.382
F	2.269872	0.777861	-0.54867	1174.274	1218.483	1273.042
F	1.532722	-1.24914	-0.80512	1325.679	1438.181	1492.745
Br	-1.36289	-0.84849	0.01442	2966.977	3039.051	3822.183
O	-1.20562	2.357687	-0.43103			

H	-1.58436	3.13396	-0.0081			
<hr/>						
Ma2						
Cartessian coordinates:				Frequencies (cm-1):		
C	-1.38492	-0.36633	-0.03159	61.7537	110.4965	137.8845
C	-0.19817	0.507372	-0.40812	176.8366	202.2206	256.2911
C	-0.13162	1.733451	0.317302	369.5204	389.346	409.8392
H	-0.38384	1.799337	1.369898	477.0864	544.0457	583.0582
H	-0.12067	0.61979	-1.48704	628.8829	686.3065	860.8485
F	-2.5349	0.23674	-0.44123	1057.905	1100.407	1126.967
F	-1.48632	-0.54322	1.305764	1159.868	1250.357	1275.063
F	-1.35181	-1.57598	-0.61451	1284.344	1355.281	1547.722
Br	1.555959	-0.63864	0.012156	3185.875	3219.499	3834.147
O	0.508623	2.766054	-0.27142			
H	0.622454	3.499992	0.3472			
<hr/>						
Ma3						
Cartessian coordinates:				Frequencies (cm-1):		
C	1.478294	-0.41079	-0.36294	53.8645	107.1046	154.4144
C	0.271473	0.33152	0.133061	165.9696	231.7516	279.5071
C	0.095193	1.686102	-0.55479	308.7305	314.0813	373.7198
H	-0.03419	1.529748	-1.62355	392.5372	570.3285	606.8638
H	1.020392	2.248997	-0.3935	718.3118	831.3299	956.4836
F	0.393743	0.563221	1.500777	1028.897	1069.687	1122.026
F	2.59494	0.31619	-0.44533	1218.658	1240.9	1322.077
F	1.732511	-1.58636	0.184587	1386.182	1418.856	1489.487
Br	-1.29703	-0.82156	-0.12951	3016.476	3113.862	3802.713
O	-1.02863	2.389744	-0.09341			
H	-0.92159	2.579276	0.844879			
<hr/>						
Ma4						
Cartessian coordinates:				Frequencies (cm-1):		
C	0.185708	-0.74676	0.105297	62.91	79.5082	164.9603
C	-1.17702	-0.24728	-0.38467	200.4263	275.0545	286.8151
C	-1.73157	0.825644	0.441514	308.2044	315.5435	362.5271
H	-1.71821	0.799733	1.52046	391.5149	458.7533	545.488
H	-1.08222	0.068028	-1.42311	600.6979	812.224	897.806
F	0.581585	-1.81781	-0.59705	924.9593	1067.392	1113.437
F	-2.02018	-1.39207	-0.38982	1210.14	1235.078	1247.716

F	0.138034	-1.10604	1.402097	1319.978	1341.778	1499.159
Br	1.552537	0.663528	-0.1044	3096.665	3205.855	3820.201
O	-2.56742	1.682598	-0.19767			
H	-2.95678	2.301639	0.428067			

Ma5

Cartessian coordinates:				Frequencies (cm-1):		
C	1.024985	-0.79019	-0.00659	50.9552	105.944	152.3862
C	0.159877	0.398765	-0.41572	185.8396	223.1784	300.0136
C	0.574919	1.709693	0.27325	338.3453	434.6866	526.054
H	0.653775	1.582719	1.364719	558.9932	576.4312	682.3103
H	-0.23478	2.4516	0.153321	771.1392	830.14	1027.3
F	0.964487	-1.03402	1.31493	1065.193	1090.935	1131.636
F	2.31371	-0.53782	-0.30845	1176.433	1204.406	1249.965
F	0.674404	-1.9142	-0.64972	1322.769	1364.071	1385.154
Br	-1.72538	0.019959	-0.01598	2912.26	2949.918	3131.327
O	1.701018	2.278295	-0.22266			
H	0.228968	0.505533	-1.49402			

CF₃CBr=CH₂

Cartessian coordinates:				Frequencies (cm-1):		
C	1.539897	-0.1639	-0.00034	45.1484	138.4317	149.8831
C	0.290431	0.395245	-0.00012	166.3446	175.26	302.357
C	0.070904	1.763729	-0.00019	350.3164	425.9534	433.4728
H	2.645781	0.574462	0.000259	566.8506	602.4441	629.1592
H	1.816049	-1.45234	0.000011	972.5421	1118.501	1248.787
F	-1.19341	-0.79604	0.000023	1278.403	1300.82	1523.364
F	0.900632	2.454996	-0.00062	1548.647	3197.516	3837.486
F	-1.19196	2.264005	0.000142	45.1484	138.4317	149.8831
Br	-1.15929	3.224717	0.000106			

CF₂CFCH₂OH

Cartessian coordinates:				Frequencies (cm-1):		
C	-1.04398	-0.16332	-0.00555	80.613	138.3389	209.3683
C	0.180935	0.294758	0.201108	250.6092	302.934	357.6819
C	1.405792	-0.49875	0.484022	250.6092	302.934	357.6819
H	1.139373	-1.54508	0.61156	656.7693	784.7321	937.8697
H	1.850075	-0.14307	1.42039	1029.65	1115.695	1226.384
F	0.373657	1.63608	0.138867	1256.363	1304.627	1368.748

F	-1.36252	-1.44675	0.017692	1414.864	1484.908	1831.994
F	-2.09706	0.590037	-0.25001	3002.778	3120.661	3810.276
O	2.357385	-0.44755	-0.57447			
H	2.668322	0.458143	-0.67267			

CF₂CBrCHOH

Cartesian coordinates:				Frequencies (cm-1):		
C	0.947325	0.964388	0.000121	65.334	169.4045	182.0441
C	0.295064	-0.23641	-8.5E-05	204.5475	241.5056	298.9344
C	0.857176	-1.50673	-1.6E-05	350.8811	381.0417	441.703
H	0.23329	-2.38602	-0.00018	524.48	580.1381	733.5709
F	2.262901	1.089812	-0.00033	963.0423	1110.557	1240.603
F	0.354722	2.144885	0.000252	1282.543	1300.29	1502.46
Br	-1.61385	-0.17546	-2.8E-05	1554.194	3217.696	3834.494
O	2.208804	-1.66401	0.000188			
H	2.424923	-2.60075	0.000253			

CF₂=CFBr

Cartesian coordinates:				Frequencies (cm-1):		
C	-1.323	0.526546	0	155.7051	161.2933	313.9796
C	0	0.590286	0	361.6703	363.8344	510.8666
F	0.612576	1.775739	0	575.2614	669.4799	1025.942
F	-2.10105	1.590964	0	1189.808	1312.428	1818.717
F	-2.01407	-0.59317	0			
Br	1.127454	-0.90465	0			

CH₂OH

Cartesian coordinates:				Frequencies (cm-1):		
C	0.684488	0.027498	0.056724	407.0037	520.1112	1052.192
H	1.237275	-0.88499	-0.09256	1198.606	1356.178	1482.022
H	1.117083	0.996573	-0.14708	3134.488	3274.465	3823.177
O	-0.66976	-0.12583	-0.01882			
H	-1.10321	0.730053	0.049817			

CF₃CHCHOH

Cartesian coordinates:				Frequencies (cm-1):		
C	0.851929	-0.03163	0.000035	85.8215	190.2474	200.3249
C	-0.53703	-0.54954	-0.00015	363.8575	397.1649	409.439
C	-1.59332	0.254981	-5.1E-05	418.5294	553.311	574.9449

H	-1.48862	1.332577	0.000218	689.2092	852.5275	873.7715
H	-0.64145	-1.62487	-0.00034	975.1948	1083.944	1098.984
F	1.549848	-0.45717	-1.08201	1168.801	1233.966	1280.702
F	1.54989	-0.45779	1.081615	1359.96	1386.693	1754.138
F	0.916173	1.319132	0.000456	3176.749	3204.002	3838.962
O	-2.85617	-0.23418	0.000444			
H	-3.49329	0.485297	-0.003			

CHBr=CHOH

Cartesian coordinates:				Frequencies (cm-1):		
C	-0.3381	0.75546	0	186.7358	241.8043	292.0473
C	0.835541	1.43306	0	380.432	778.2381	790.7629
C	1.762188	0.89806	0	934.9846	1139.408	1169.589
H	-1.26474	1.29046	0	1298.003	1346.406	1710.213
H	-0.3381	-1.15454	0	3171.279	3226.118	3845.071
F	0.835541	2.73436	0			
F	1.666926	3.21436	0			

CF₃CBrCHOH

Cartesian coordinates:				Frequencies (cm-1):		
C	-1.43963	-0.0986	0.000073	45.1731	157.4651	163.4398
C	-0.04706	0.449077	0.000171	179.8801	322.1437	327.9829
C	0.190805	1.759085	0.000042	398.1035	411.968	479.0246
H	-0.63775	2.45481	0.000557	529.9147	606.0013	610.5548
F	-1.68755	-0.86405	-1.08161	715.4981	906.0356	944.7942
F	-2.35917	0.894241	0.000307	1118.952	1125.559	1185.487
F	-1.68789	-0.86496	1.080978	1118.952	1125.559	1185.487
Br	1.346829	-0.82923	-7E-06	1118.952	1125.559	1185.487
O	1.435917	2.273656	0.000527			
H	1.398075	3.234534	-0.00327			

CF₂BrCFCHOH

Cartesian coordinates:				Frequencies (cm-1):		
C	-0.56319	0.410227	0.000156	50.3604	145.7951	165.7014
C	0.514972	-0.35705	0.000001	251.7876	280.9168	297.5974
C	0.430171	-1.43621	-0.00016	313.0403	318.9049	400.2178
H	-0.57748	1.489215	0.000302	436.2026	624.4495	632.9413
F	-1.79496	-0.15457	-5.4E-05	781.3029	880.1614	937.9186
F	1.770429	0.190903	-0.00026	1044.066	1079.475	1180.863

F	2.427819	-0.50813	0.001455	1249.441	1315.648	1369.569
Br	-0.56319	0.410227	0.000156	1783.765	3224.605	3839.7
O	0.514972	-0.35705	0.000001			
H	0.430171	-1.43621	-0.00016			

CHF=CHOH

Cartessian coordinates:				Frequencies (cm-1):		
C	-0.56319	0.410227	0.000156	45.3766	138.4117	149.8244
C	0.514972	-0.35705	0.000001	166.3424	175.2553	302.2411
H	0.430171	-1.43621	-0.00016	350.3071	425.9688	433.4725
H	-0.57748	1.489215	0.000302	566.8421	602.4306	629.1523
F	-1.79496	-0.15457	-5.4E-05	972.5443	1118.499	1248.795
O	1.770429	0.190903	-0.00026			
H	2.427819	-0.50813	0.001455			

CF₂BrCCHOH

Cartessian coordinates:				Frequencies (cm-1):		
C	0.105712	0.875029	-2.2E-05	91.53	103.2599	154.306
C	-1.28353	0.514012	0.000205	271.8045	280.0914	285.8816
C	-2.0911	-0.51696	0.000066	373.2464	409.3383	528.0406
H	-1.68435	-1.52673	-0.00016	610.2231	633.7328	860.8122
F	0.47335	1.591119	1.082744	861.784	1088.466	1089.27
F	0.47344	1.590867	-1.08281	1237.885	1257.288	1377.858
Br	1.261392	-0.79606	0.00001	1796.402	3095.191	3826.96
O	-3.44107	-0.40086	-0.00047			
H	-3.84344	-1.27462	0.002601			

CF₂CBrCH₂O

Cartessian coordinates:				Frequencies (cm-1):		
C	-1.36354	-0.5579	-0.00128	56.6278	135.1066	163.9589
C	-0.33242	0.258623	0.150287	199.061	275.3872	366.5076
C	-0.48289	1.734336	0.405403	449.7131	577.7914	606.7667
H	0.057235	2.020377	1.327266	628.7629	683.9713	952.8937
H	-1.53294	1.985633	0.62136	1037.713	1128.367	1166.703
F	-2.62726	-0.16205	0.065991	1278.341	1326.042	1374.716
F	-1.30437	-1.85058	-0.22977	1772.483	2896.566	2954.308
Br	1.429692	-0.42728	0.022834			
O	-0.01323	2.556508	-0.57503			

CF₂CHBrCHO

Cartessian coordinates:

C	-1.1542	-0.7947	-0.04571
C	-0.25712	0.397535	-0.42706
C	-0.61806	1.516463	0.335595
H	0.09951	1.977739	0.981519
H	-0.3813	0.619215	-1.46645
F	-0.77977	-1.63129	0.945459
F	-2.31503	-1.00324	-0.70258
Br	1.569103	-0.04451	-0.08411
O	-1.82591	1.994479	0.258223

Frequencies (cm-1):

52.1761	66.522	152.0553
200.0489	251.063	305.6448
437.3467	537.7201	572.1457
704.0946	856.4276	1012.785
1014.963	1146.423	1184.21
1271.433	1322.489	1401.729
1798.806	2959.121	3149.479

CF₂BrCH=CHO

Cartessian coordinates:

C	0.016785	0.762764	-0.03904
C	1.251649	0.151773	-0.55432
C	2.299323	-0.34947	0.282966
H	2.172833	-0.24541	1.370284
H	1.329587	0.035076	-1.62594
F	-0.43808	1.750217	-0.83048
F	0.139072	1.253078	1.206378
Br	-1.39071	-0.66493	0.007013
O	3.307116	-0.86715	-0.18882

Frequencies (cm-1):

58.4258	131.9985	187.8718
260.6586	284.9218	299.9715
401.0355	475.8345	590.2953
676.4868	753.3796	900.9328
977.1824	1105.692	1142.717
1236.735	1335.396	1446.112
1578.158	2987.537	3208.418

CF₃CHBrCHO

Cartessian coordinates:

C	-1.53992	-0.16387	-0.00046
C	-0.29044	0.395239	-0.00013
C	-0.07092	1.763748	-0.00016
H	-0.90067	2.454984	-0.00075
F	-2.64582	0.574414	0.000248
F	-1.81603	-1.45237	0.000109
F	1.193433	-0.79603	0.000011
Br	1.191934	2.264013	0.000208
O	1.159277	3.224721	0.000031
H	-1.53992	-0.16387	-0.00046

Frequencies (cm-1):

71.5559	90.0298	145.494
176.777	249.4239	299.9904
328.1763	507.2021	517.7896
572.6975	674.9294	756.0676
851.7371	937.4115	1030.257
1120.817	1147.163	1188.375
1261.944	1348.665	1422.871
1815.879	2935.837	3105.808

CF₃CHBr

Cartessian coordinates:

Frequencies (cm-1):

C	1.314649	-0.02321	-0.0046	32.2057	152.3264	214.6461
C	0.061944	-0.81929	-0.02854	319.2675	403.7047	519.0662
F	1.375245	0.887972	-0.99695	561.2973	640.4064	770.0341
F	2.373377	-0.8474	-0.13842	890.9571	1092.007	1111.741
F	1.480599	0.660035	1.152173	1220.116	1322.979	3248.014
Br	-1.58337	0.01835	0.000248			
H	0.095422	-1.89271	0.038936			

CH₂O

Cartessian coordinates:				Frequencies (cm-1):		
C	0	0	-0.527	1198.207	1263.298	1530.126
H	0	0.938574	-1.11187	1813.364	2884.677	2939.649
H	0	-0.93857	-1.11187			
O	0	0	0.673215			

cCH₂CHBrO

Cartessian coordinates:				Frequencies (cm-1):		
C	-0.83967	0.173163	0.533439	291.0316	327.477	551.332
C	-1.88	-0.67714	-0.02759	814.4449	911.3898	1008.073
H	-2.7626	-0.91036	0.556465	1088.287	1155.183	1167.035
H	-1.61791	-1.37132	-0.81561	1271.811	1326.998	1517.02
Br	1.012398	-0.02898	-0.03703	3104.323	3166.372	3200.781
O	-1.73377	0.720202	-0.37792			
H	-0.86527	0.558248	1.543537			

CF₃COHCH₂

Cartessian coordinates:				Frequencies (cm-1):		
C	0.589626	0.021278	-5.2E-05	60.8991	246.9012	252.4536
C	-0.92303	0.05206	-3.5E-05	362.8843	380.454	419.1826
C	-1.62337	1.177985	-4.7E-05	500.6948	575.3026	602.2785
H	-1.12681	2.133108	-0.00014	690.7431	729.8111	785.3396
H	-2.70461	1.164216	0.000048	879.7083	979.1683	1127.113
F	1.064247	-0.62108	1.084509	1136.362	1168.927	1239.923
F	1.114096	1.258037	-0.00061	1407.812	1454.757	1724.478
F	1.064271	-0.62207	-1.08393	3163.244	3267.883	3806.796
O	-1.40538	-1.21704	0.000089			
H	-2.36848	-1.20293	0.000452			

CF₃CCH₂

Cartessian coordinates:				Frequencies (cm-1):		
C	0.371451	-0.04135	0.00001	95.3878	192.6705	322.8984
C	-1.01134	-0.55388	0.000054	416.2248	480.5134	545.3308
C	-2.21503	-0.06272	-2.5E-05	591.9791	638.8924	796.9205
H	-3.09446	-0.69612	0.000134	942.4897	997.8817	1104.513
H	-2.38292	1.013779	-7.5E-05	1133.182	1206.942	1412.228
F	0.405267	1.314097	-0.00015	1763.048	3070.057	3169.6
F	1.053309	-0.4555	-1.08514			
F	1.0533	-0.45526	1.085248			

CF₃CBrOH

Cartessian coordinates:				Frequencies (cm-1):		
C	-1.32493	-0.15453	-2.6E-05	49.6551	153.8375	219.225
C	-0.11508	0.752558	-0.00015	289.5565	296.7943	466.4046
C	-0.15298	2.041263	-0.00033	475.5963	573.4199	627.477
H	0.455624	2.924716	-0.00073	655.7091	714.8985	727.8069
H	-1.34325	-0.94932	-1.08353	859.1136	1144.42	1166.672
F	-2.45898	0.562627	-0.00018	1230.296	1697.829	3309.808
F	-1.34338	-0.94911	1.083476			
F	1.583221	-0.19252	0.000167			

CF₂OHCB₂CH₂

Cartessian coordinates:				Frequencies (cm-1):		
C	-1.29442	-0.22746	0.00185	51.8169	169.3982	173.6756
C	-0.09456	0.705419	0.007144	235.3719	326.8959	342.464
C	-0.18126	2.024067	0.03423	475.6619	486.804	573.2723
H	-1.15082	2.500354	0.033768	618.3488	686.2747	735.1748
H	0.698439	2.649137	0.050489	820.354	969.7458	1047.344
F	-1.296	-0.9975	-1.10753	1061.694	1154.285	1233.733
F	-2.43703	0.533003	-0.0591	1349.519	1428.067	1685.327
Br	1.58725	-0.19129	-0.00638	3163.676	3253.346	3808.375
O	-1.36292	-1.08461	1.062343			
H	-1.17934	-0.60928	1.880583			

CF₂CBrCH₂

Cartessian coordinates:				Frequencies (cm-1):		
C	1.34496	0.419686	0	114.1086	176.5014	263.3053
C	0	0.693263	0	311.5836	362.5801	460.0463
C	-0.53314	1.962889	0	492.8729	521.7527	644.3169

H	0.120721	2.822075	0	735.0065	855.6574	1110.307
H	-1.59881	2.116217	0	1268.754	1305.909	1480.257
F	1.89353	-0.7743	0	1535.019	3169.586	3274.453
F	2.260699	1.373903	0			
Br	-1.16517	-0.82256	0			

- Geometries and frequencies of transition states, reactants, intermediates and products involved in the reactions of 2-BTP + OH calculated at B3LYP/aug-cc-pVTZ.

TSb1

Cartessian coordinates:				Frequencies (cm-1):		
C	1.332089	-0.17479	-5.6E-05	-883.076	50.0794	139.2077
C	0.081133	0.683216	-1.9E-05	162.5195	224.0962	239.0487
C	0.112024	1.987532	-4.7E-05	319.7066	370.2755	478.7585
H	0.946053	2.670197	-9.9E-05	480.075	578.6518	615.3961
H	-1.1756	2.725494	-6E-06	683.8848	732.9088	809.1408
F	1.389569	-0.96671	1.083819	890.2355	966.152	1054.744
F	2.439183	0.590487	-0.00013	1144.322	1159.426	1228.337
F	1.38947	-0.96676	-1.0839	1640.34	2372.674	3239.667
Br	-1.5422	-0.32658	0.000075			
H	-1.90892	3.145503	0.000017			

TSb2

Cartessian coordinates:				Frequencies (cm-1):		
C	1.25222	-0.33117	-1E-06	-953.934	46.1554	161.0389
C	0.12894	0.681411	-5E-06	162.4946	227.3298	271.728
C	0.261709	1.978525	-6E-06	309.5077	387.2133	475.1856
H	1.576643	2.601527	0.000007	481.4867	577.4302	634.1555
H	-0.48547	2.754904	-4E-06	698.5986	746.1799	824.1796
F	1.195296	-1.12466	1.083985	914.337	945.5542	1105.483
F	2.453071	0.267396	-2.1E-05	1143.288	1165.681	1243.355
F	1.19528	-1.1247	-1.08396	1658.131	2211.418	3244.447
Br	-1.6245	-0.12933	0			
H	2.316278	3.035305	0.000016			

TSb3

Cartessian coordinates:				Frequencies (cm-1):		
C	1.351848	-0.23394	0.003978	-493.942	51.4587	143.7141
C	0.206743	0.740265	-0.00361	163.4259	198.7626	258.8422
C	0.32651	2.051231	0.025089	308.2024	351.8751	475.8892
H	1.306983	2.509783	0.037947	488.5279	571.6679	600.0906
H	-0.53705	2.6998	0.03189	689.6304	716.6866	819.831
F	1.315267	-1.03577	1.083942	974.5086	1071.305	1141.733
F	2.538881	0.406124	0.019521	1149.493	1149.493	1149.493
F	1.339405	-1.02582	-1.08385	1695.392	3145.941	3235.622
Br	-1.59046	-0.13455	-0.02884			
H	-3.15634	-0.94647	0.610402			

TSb4

Cartessian coordinates:				Frequencies (cm-1):		
C	1.29509	-0.22143	0.004599	-828.093	61.3182	160.8394
C	0.09084	0.697887	-0.11667	258.8471	318.7982	322.8317
C	0.192085	2.017962	0.070481	388.4003	462.321	476.0892
H	1.165436	2.486484	0.094079	504.2696	578.7277	605.772
H	-0.68302	2.644563	0.141635	671.4393	692.4651	823.3318
F	1.405532	-0.68368	1.266366	933.7951	1088.118	1136.637
F	2.431365	0.441678	-0.28004	1176.835	1253.546	1418.772
F	1.231248	-1.28732	-0.80266	1602.814	3163.063	3258.398
Br	-1.59256	-0.19849	0.012527			
H	0.175698	0.613433	-2.07761			

TSb5

Cartessian coordinates:				Frequencies (cm-1):		
C	-1.28496	-0.24751	0.000519	-332.931	51.4149	157.446
C	-0.0896	0.666664	-0.1187	165.2418	178.9859	254.4695
C	-0.19189	1.980841	-0.27302	327.1724	341.2093	480.702
H	-1.16428	2.440735	-0.36902	484.872	578.7347	627.1819
H	0.681946	2.603874	-0.38174	692.2849	763.4933	829.0026
F	-1.29085	-1.1874	-0.96225	964.6729	1093.44	1140.751
F	-2.43656	0.44201	-0.1042	1159.531	1264.547	1427.42
F	-1.3064	-0.88691	1.184436	1654.39	3167.467	3259.189
Br	1.583229	-0.21797	0.006032			
H	-0.22775	2.875063	1.824962			

TSb6

Cartessian coordinates:				Frequencies (cm-1):		
C	1.301037	-0.13564	-0.35206	-717.739	78.6221	142.7806
C	0.041274	0.735253	-0.10559	220.3865	227.2196	304.2494
C	0.146832	2.061447	-0.06151	346.6106	376.6324	438.2485
H	1.104644	2.541017	-0.20559	491.1489	591.8468	629.4411
H	-0.70604	2.67319	0.186872	699.3222	904.7148	1061.278
F	1.160736	-0.5157	1.435886	1089.591	1152.874	1172.937
F	2.53254	0.366905	-0.1767	1236.798	1384.298	1548.83
F	1.269481	-1.43892	-0.65237	1800.063	3161.64	3258.191
Br	-1.57504	-0.20484	-0.02425			
H	1.127984	0.278173	-1.47895			

TSb7

Cartessian coordinates:				Frequencies (cm-1):		
C	-1.23986	-0.07564	-0.21433	-1530.76	57.1724	155.4488
C	-0.04036	0.74062	0.003127	197.1766	271.5111	318.9702
C	-0.09445	2.046827	0.246219	329.0556	348.1664	426.7255
H	-1.04569	2.559278	0.249743	429.255	536.561	560.2379
H	0.797135	2.620443	0.444489	654.6539	688.3744	812.1653
F	-1.15452	-1.04982	-1.09646	942.1762	970.2378	1114.087
F	-2.35737	0.606712	-0.3963	1259.98	1320.897	1431.131
F	-1.54343	-0.89772	1.188516	1638.69	3165.469	3258.65
Br	1.598463	-0.22096	-0.01014			
H	-1.95166	-1.64964	2.188652			

TSb8

Cartessian coordinates:				Frequencies (cm-1):		
C	1.15655	-0.33378	0.000005	-1480.25	35.1006	157.7604
C	0.067329	0.669865	0	221.5927	224.0569	272.7556
C	0.23616	1.979587	0.000007	334.6157	386.5033	419.4654
H	1.233198	2.393364	0.00001	467.1594	522.5731	597.1784
H	-0.60698	2.653385	0.000011	621.4347	737.0361	774.6177
F	1.228998	-1.08933	1.079926	983.6575	983.8931	1111.658
F	2.625436	0.463588	-3.5E-05	1231.214	1287.978	1434.3
F	1.228966	-1.08938	-1.07988	1696.718	3168.818	3261.108
Br	-1.68477	-0.12676	-4E-06			
H	3.829916	0.931922	-7.3E-05			

M1-TSb1

Cartessian coordinates:	Frequencies (cm-1):
-------------------------	---------------------

C	-1.28683	-0.25173	-0.01513	-1915.88	55.3431	156.5222
C	-0.10013	0.640679	-0.23759	204.7925	271.5642	300.0365
C	-0.24901	2.074011	0.049213	359.1825	439.6081	488.6971
H	-0.30589	1.513096	-1.15375	569.5716	615.7528	682.5837
H	0.640137	2.680204	0.081693	761.564	828.0228	1054.915
F	-1.19137	-1.41705	-0.67067	1091.493	1160.647	1171.355
F	-2.41592	0.36391	-0.4388	1223.263	1325.192	1426.791
F	-1.47178	-0.5458	1.292972	2192.453	3158.392	3281.937
Br	1.610697	-0.20094	0.005743			
H	-1.18115	2.452138	0.440535			

M1-TSb2

Cartessian coordinates:				Frequencies (cm-1):		
C	1.247882	-0.42647	-0.27381	-235.618	136.4251	145.7032
C	0.226028	0.479901	-0.20206	173.9763	189.7956	258.4718
C	0.394003	1.922634	-0.51613	285.5734	334.3853	372.6324
H	1.444794	2.199346	-0.48668	508.5766	530.7914	645.0296
H	-0.14322	2.513123	0.222817	902.5816	1044.809	1132.472
F	0.941549	0.467365	1.698366	1159.39	1355.651	1418.526
F	2.479303	-0.08416	-0.52934	1466.417	1477.206	1653.691
F	1.122828	-1.70681	-0.10897	3040.677	3110.292	3142.287
Br	-1.52535	-0.19437	-0.05203			
H	-0.01486	2.146446	-1.50344			

M1-TSb3

Cartessian coordinates:				Frequencies (cm-1):		
C	1.086219	-0.68932	-0.22006	-921.114	62.7487	100.0948
C	0.155341	0.283847	-0.46541	162.0934	179.4107	284.2359
C	0.574803	1.611386	-0.86656	341.7492	370.5447	393.291
H	1.094706	1.909674	0.136945	517.3767	558.4218	644.6838
H	-0.2374	2.27949	-1.12658	759.4218	912.2383	1127.74
F	1.659147	1.214366	1.390279	1169.029	1254.839	1357.718
F	2.315963	-0.60407	-0.62664	1370.045	1471.314	1598.918
F	0.83211	-1.84143	0.321114	2026.289	3083.94	3175.157
Br	-1.61124	-0.05593	0.061315			
H	1.372995	1.613232	-1.60706			

M2-TSb1

Cartessian coordinates:				Frequencies (cm-1):		
C	1.406437	-0.21429	-0.01376	-163.202	54.9751	124.8977

C	0.385413	0.757647	-0.56742	202.9182	247.1334	391.2222
C	0.214983	1.986286	0.024487	427.4542	497.8811	540.1798
H	-0.33067	2.765325	-0.48517	601.9612	633.366	805.7232
H	0.540031	2.167442	1.038361	895.6449	968.798	1028.11
F	1.43971	-0.22646	1.326416	1108.128	1189.302	1250.484
F	2.635743	0.168853	-0.44217	1272.153	1444.119	1544.964
F	1.217369	-1.46582	-0.44488	3163.603	3201.051	3264.314
Br	-1.71728	-0.2011	0.013168			
H	0.219057	0.638744	-1.62816			

M2-TSb2

Cartessian coordinates:				Frequencies (cm-1):		
C	1.570701	-0.21532	0.004101	-372.296	23.5249	83.3835
C	-0.34267	0.937174	-0.52356	112.1707	158.2566	238.4325
C	-0.20029	2.110182	0.126266	352.8293	485.3377	509.7131
H	0.459045	2.865285	-0.28053	512.9461	591.0124	662.5849
H	-0.66475	2.298929	1.082303	862.0581	921.0037	1002.575
F	2.580283	0.56557	-0.37401	1025.273	1191.734	1212.844
F	1.614619	-1.36507	-0.66028	1258.243	1361.653	1528.2
F	1.625366	-0.43237	1.309393	3146.665	3195.715	3243.861
Br	-1.6658	-0.339	0.018034			
H	-0.04022	0.795304	-1.54982			

M2-TSb3

Cartessian coordinates:				Frequencies (cm-1):		
C	0.861343	-0.50762	0.082894	-676.676	123.0718	128.688
C	0.873433	0.799734	-0.5104	173.9695	230.3196	238.4478
C	0.653226	1.956602	0.230078	287.8885	351.2298	457.3102
H	0.562665	2.903136	-0.27682	471.6598	506.7037	597.3649
H	0.611771	1.929043	1.306832	814.5389	839.9806	990.7671
F	0.988562	-0.7005	1.344846	1056.749	1248.345	1327.093
F	2.639764	0.236509	-0.33253	1433.958	1497.31	1569.164
F	0.930539	-1.58271	-0.61094	3180.721	3245.067	3289.136
Br	-1.63887	-0.02014	-0.05346			
H	0.828186	0.800722	-1.58667			

M3-TSb1

Cartessian coordinates:				Frequencies (cm-1):		
C	1.40932	-0.40004	-0.06635	-213.395	106.1708	109.5722

C	0.64142	0.74189	0.137838	194.3027	216.8699	235.6854
C	0.551728	1.831206	-0.8785	330.8129	351.8219	444.2484
H	-0.32646	2.438036	-0.67747	511.0193	553.8033	736.6955
H	0.474389	1.417336	-1.87969	975.6541	1054.644	1170.817
F	0.630094	1.16066	1.411069	1258.121	1357.808	1420.428
F	1.646641	-0.87462	-1.26114	1467.506	1478.16	1588.887
F	1.723732	-1.23019	0.887178	3037.036	3122.854	3158.655
Br	-1.5203	-0.31016	-0.03207			
H	1.44361	2.458984	-0.81228			

M3-TSb2

Cartessian coordinates:				Frequencies (cm-1):		
C	1.317117	-0.56532	0.089959	-566.415	102.0516	104.6886
C	0.287746	0.282106	0.330377	111.3393	153.7052	168.7729
C	0.508952	1.906853	-1.3581	295.8089	305.8679	346.9476
H	0.354849	1.321897	-2.2524	441.3714	482.8166	493.2948
H	1.513082	2.236778	-1.13551	526.3868	652.477	836.8159
F	0.435971	1.171572	1.322614	991.3135	1159.03	1310.156
F	2.555737	-0.2879	0.449081	1416.945	1418.104	1639.751
F	1.259492	-1.55247	-0.77818	3095.786	3256.319	3262.369
Br	-1.5001	-0.28006	0.030984			
H	-0.30829	2.520773	-1.0116			

M3-TSb3

Cartessian coordinates:				Frequencies (cm-1):		
C	1.086383	-0.68899	-0.22021	-923.683	62.4812	100.0562
C	0.155398	0.284149	-0.4652	162.1403	179.4218	284.3604
C	0.574731	1.611836	-0.86574	342.1394	370.5448	393.2973
H	1.094826	1.908628	0.138158	517.3699	558.2696	644.6191
H	-0.23733	2.280385	-1.12493	758.6591	912.1537	1127.508
F	1.658336	1.213537	1.390342	1168.717	1254.548	1357.452
F	2.316058	-0.60359	-0.62699	1369.741	1471.283	1598.931
F	0.83248	-1.84108	0.321156	2025.309	3084.086	3175.468
Br	-1.61119	-0.05615	0.061115			
H	1.373151	1.614354	-1.60597			

M4-TSb1

Cartessian coordinates:				Frequencies (cm-1):		
C	-0.08738	0.643786	-0.1161	-406.403	31.3634	84.9645
C	-1.83767	-0.60763	0.500284	126.4804	202.8332	242.1752

C	-1.34315	-0.78799	1.44493	305.3155	315.2268	486.499
H	-2.885	0.227654	0.337768	491.0572	616.7013	657.1289
H	-3.09681	0.965266	1.095893	1103.361	1151.178	1171.234
F	-3.46035	0.230067	-0.57573	1285.527	1405.252	1558.902
F	-1.63507	-1.60866	-0.38367	3166.507	3183.398	3266.415
F	-0.29494	0.985388	-1.37951	-406.403	31.3634	84.9645
Br	-0.11581	1.737176	0.640328			
H	1.576372	-0.3433	0.108823			

M4-TSb2

Cartessian coordinates:				Frequencies (cm-1):		
C	0.294869	-0.52183	0.087698	-761.889	67.8435	179.1949
C	1.40259	0.507236	-0.08236	260.2809	293.4421	317.3377
C	1.071022	0.659282	-2.02798	323.8608	380.0696	418.9045
H	1.360405	1.802042	0.231338	458.831	558.5238	631.9975
H	0.419452	2.293606	0.408491	693.4455	712.9023	900.8877
F	2.273158	2.377872	0.243614	927.3428	945.144	1088.328
F	2.586172	-0.11966	-0.23142	1132.042	1282.964	1407.999
F	0.417357	-1.51092	-0.81004	1647.332	3181.44	3284.641
Br	0.407156	-1.08737	1.310698			
H	-1.50877	0.240173	-0.0705			

M4-TSb3

Cartessian coordinates:				Frequencies (cm-1):		
C	0.294869	-0.52183	0.087698	-420.464	27.7849	82.0719
C	1.40259	0.507236	-0.08236	144.2284	184.3178	262.9368
C	1.071022	0.659282	-2.02798	298.4673	308.0597	440.0211
H	1.360405	1.802042	0.231338	523.8476	588.2637	721.1259
H	0.419452	2.293606	0.408491	829.9734	890.808	987.2503
F	2.273158	2.377872	0.243614	1005.907	1140.63	1199.254
F	2.586172	-0.11966	-0.23142	1211.982	1420.803	1636.617
F	0.417357	-1.51092	-0.81004	2334.055	3142.58	3235.707
Br	0.407156	-1.08737	1.310698			
H	-1.50877	0.240173	-0.0705			

M4-TSb4

Cartessian coordinates:				Frequencies (cm-1):		
C	-0.24412	0.399078	0.199738	-1889.72	81.7649	161.7776
C	-1.42707	-0.40932	-0.05341	202.5638	253.3068	277.8622
C	-1.29072	0.210468	-1.18305	293.701	346.8488	349.5413

H	-1.42818	-1.82656	-0.24676	415.3202	519.5715	579.861
H	-0.56272	-2.32642	-0.64779	614.609	674.4299	903.1308
F	-2.3755	-2.33916	-0.20986	993.1499	1141.086	1231.766
F	-2.52723	0.094792	0.600326	1287.232	1388.318	1454.421
F	-0.41538	1.118949	-1.60289	1672.813	3182.288	3290.667
Br	-0.38859	1.504767	0.855513			
H	1.50874	-0.25688	0.113336			

Mb1

Cartessian coordinates:				Frequencies (cm-1):		
C	1.281902	-0.24657	-0.01891	33.607	107.8404	158.432
C	0.076265	0.620594	-0.17209	175.3019	284.0754	324.0187
C	0.153793	2.092685	-0.00605	417.6513	469.5745	561.8124
H	0.048314	2.383546	1.045933	571.5063	691.1312	847.0372
H	-0.64381	2.585019	-0.5609	1014.173	1058.623	1094.991
F	1.577073	-0.49578	1.285842	1127.829	1173.453	1317.877
F	2.369141	0.360581	-0.54503	1409.885	1467.364	1477.899
F	1.153827	-1.43936	-0.62057	2988.859	3074.494	3118.556
Br	-1.58543	-0.23035	-0.00065			
H	1.113359	2.464471	-0.36209			

Mb2

Cartessian coordinates:				Frequencies (cm-1):		
C	1.312663	-0.22204	-0.01381	65.3349	145.5176	231.2434
C	0.192703	0.684747	-0.50929	242.1728	250.266	327.1439
C	0.198754	2.017512	0.031108	428.3307	477.3781	545.6014
H	-0.28611	2.815247	-0.50853	601.5302	634.1351	714.0325
H	0.539399	2.199686	1.038677	802.0188	1011.644	1073.852
F	1.376943	-0.28231	1.325044	1123.078	1159.198	1204.146
F	2.495634	0.269125	-0.45157	1257.83	1400.74	1479.437
F	1.208264	-1.47176	-0.48433	3150.209	3165.416	3272.713
Br	-1.61009	-0.20469	0.014583			
H	0.147455	0.632527	-1.59086			

Mb3

Cartessian coordinates:				Frequencies (cm-1):		
C	1.296807	-0.4823	-0.37523	59.3913	157.0371	206.7985
C	0.307768	0.515493	0.161269	251.8442	279.6207	302.5013
C	0.427633	1.880075	-0.47088	305.6961	384.4436	533.5442
H	-0.33328	2.535537	-0.05524	579.6786	724.2037	795.7824

H	0.297223	1.816398	-1.54846	886.4754	1100.56	1117.849
F	0.473562	0.63056	1.531383	1139.209	1228.208	1331.737
F	2.545406	-0.02679	-0.49938	1418.044	1482.344	1486.274
F	1.296424	-1.68219	0.181487	3055.339	3128.156	3146.126
Br	-1.49742	-0.24041	-0.14164			
H	1.413889	2.288665	-0.25141			

Mb4

Cartessian coordinates:				Frequencies (cm-1):		
C	-0.24412	0.399078	0.199738	81.2379	98.7406	153.3499
C	-1.42707	-0.40932	-0.05341	245.6975	287.3567	295.5331
C	-1.29072	0.210468	-1.18305	314.6165	385.0759	491.1177
H	-1.42818	-1.82656	-0.24676	583.6767	623.833	739.9295
H	-0.56272	-2.32642	-0.64779	885.6755	946.7185	1016.866
F	-2.3755	-2.33916	-0.20986	1121.519	1160.48	1215.828
F	-2.52723	0.094792	0.600326	1329.054	1379.324	1466.184
F	-0.41538	1.118949	-1.60289	3098.16	3165.803	3278.249
Br	-0.38859	1.504767	0.855513			
H	1.50874	-0.25688	0.113336			

CF₃CBr=CH₂(2-BTP)

Cartessian coordinates:				Frequencies (cm-1):		
C	1.288871	-0.20737	0.000035	52.5298	166.1386	225.2337
C	0.090994	0.712111	-5.9E-05	326.333	336.7488	480.3144
C	0.188872	2.029236	-0.00016	480.4412	578.3881	617.8373
H	1.161187	2.499975	-0.0002	690.0438	731.4281	825.6787
H	-0.68638	2.660314	-0.00021	970.8079	1091.321	1143.19
F	1.304725	-1.00422	1.08397	1159.817	1268.217	1431.334
F	2.439764	0.492225	-6.7E-05	1691.658	3165.323	3255.501
F	1.304689	-1.00447	-1.08375			
Br	-1.58085	-0.19188	0.000003			
H	1.288871	-0.20737	0.000035			

Br

Cartessian coordinates:				Frequencies (cm-1):		
Br	0	0	0			

CF₂=CFBr

Cartessian coordinates:				Frequencies (cm-1):		
C	-1.4004	-0.25642	-1E-06	155.8326	160.4704	314.1286

C	-0.3132	0.500281	-1E-06	361.546	363.9925	510.6695
C	-0.4238	1.830022	0	575.0139	669.2827	1025.455
H	-2.625	0.232355	0.000001	1190.422	1311.615	1818.024
H	-1.3913	-1.57226	0			
F	1.435501	-0.16783	0			
F	-1.4004	-0.25642	-1E-06			
F	-0.3132	0.500281	-1E-06			
Br	-0.4238	1.830022	0			
H	-2.625	0.232355	0.000001			

CF₂Br

Cartessian coordinates:				Frequencies (cm-1):		
C	-0.36179	-0.91727	0	304.0657	320.0833	577.2351
F	0.040957	-1.55795	1.082635	664.9574	1141.694	1193.649
F	0.040957	-1.55795	-1.08264			
Br	0.040957	0.958479	0			

CF₂BrCCH₂

Cartessian coordinates:				Frequencies (cm-1):		
C	-0.61293	0.586137	0.00005	115.899	149.9784	284.6481
C	-1.69916	-0.37555	0.000544	291.1211	366.6364	380.8994
C	-1.97094	-1.64505	0.000095	487.9781	618.2948	641.6007
H	-2.99325	-2.00592	0.00058	827.44	946.1145	982.5793
H	-1.18112	-2.39445	-0.00057	1108.134	1166.767	1411.956
F	-0.63991	1.382124	-1.08601	1785.152	3075.333	3167.935
F	-0.63925	1.382781	1.085619			
Br	1.182426	-0.33934	-1.8E-05			

CF₂BrCFCH₂

Cartessian coordinates:				Frequencies (cm-1):		
C	0.320991	-0.50893	-3.9E-05	53.5527	184.7316	242.5584
C	1.410074	0.537735	0.000228	302.0317	315.9306	325.3955
C	1.316143	1.851083	0.000102	394.3916	553.8073	669.0636
H	0.356032	2.336751	0.000392	698.8591	746.1112	933.8817
H	2.213661	2.451255	-0.00029	934.3514	950.5991	1097.578
F	2.610006	-0.07703	0.000071	1110.529	1290.694	1415.908
F	0.450704	-1.30205	-1.08373	1742.014	3182.016	3283.723

F	0.449796	-1.30211	1.083805
Br	-1.4985	0.230383	-0.00009

CF₂CFCH₃

Cartessian coordinates:				Frequencies (cm-1):		
C	0.678699	0.073007	0.00006	174.9983	185.7044	218.5461
C	-0.63325	-0.10236	-2.9E-05	354.759	372.4995	507.154
C	-1.68318	0.943232	0.000153	553.8718	585.502	752.3413
H	-2.31773	0.844623	-0.88273	980.4878	1068.863	1167.436
H	-1.23715	1.934808	0.000149	1253.524	1294.226	1425.901
F	-1.08871	-1.37859	-0.00016	1474.024	1488.181	1847.345
F	1.260827	1.265966	-0.00017	3031.143	3078.801	3132.943
F	1.572213	-0.8993	0.000164			
H	-2.31771	0.844601	0.882961			

CF₂HCBBrCH₂

Cartessian coordinates:				Frequencies (cm-1):		
C	-1.35942	-0.40275	0.327675	62.2961	178.1892	282.7359
C	-0.28508	0.590537	-0.0232	324.4077	364.5209	519.7342
C	-0.49982	1.85397	-0.34075	586.9459	691.5292	752.3134
H	-1.51135	2.23394	-0.36448	952.1142	964.5777	1060.621
H	0.308487	2.527856	-0.57944	1081.477	1167.923	1363.29
F	-1.4307	-1.38457	-0.62183	1390.71	1428.359	1695.392
F	-2.57977	0.209207	0.363727	3079.058	3161.195	3251.737
F	1.467282	-0.15857	0.062644			
Br	-1.1919	-0.88422	1.291958			
H	-1.35942	-0.40275	0.327675			

CF₃

Cartessian coordinates:				Frequencies (cm-1):		
C	0	0	0	-1138.21	464.3664	464.3718
F	0	1.315785	0	883.6017	1411.163	1411.185
F	-1.1395	-0.65789	0			
F	1.139503	-0.65789	0			

CF₃CBrCH

Cartessian coordinates:				Frequencies (cm-1):		
C	-1.32493	-0.15453	-2.6E-05	49.6551	153.8375	219.225
C	-0.11508	0.752558	-0.00015	289.5565	296.7943	466.4046
C	-0.15298	2.041263	-0.00033	475.5963	573.4199	627.477

H	0.455624	2.924716	-0.00073	655.7091	714.8985	727.8069
F	-1.34325	-0.94932	-1.08353	859.1136	1144.42	1166.672
F	-2.45898	0.562627	-0.00018	1230.296	1697.829	3309.808
F	-1.34338	-0.94911	1.083476			
Br	1.583221	-0.19252	0.000167			

CH₃CCH₂

Cartessian coordinates:				Frequencies (cm-1):		
C	0.371451	-0.04135	0.00001	95.3878	192.6705	322.8984
C	-1.01134	-0.55388	0.000054	416.2248	480.5134	545.3308
C	-2.21503	-0.06272	-2.5E-05	591.9791	638.8924	796.9205
H	-3.09446	-0.69612	0.000134	942.4897	997.8817	1104.513
H	-2.38292	1.013779	-7.5E-05	1133.182	1206.942	1412.228
F	0.405267	1.314097	-0.00015	1763.048	3070.057	3169.6
F	1.053309	-0.4555	-1.08514			
F	1.0533	-0.45526	1.085248			

CF₂CBrCH₂

Cartessian coordinates:				Frequencies (cm-1):		
C	1.382331	-0.27061	0	113.6777	178.014	263.3912
C	0.330721	0.611404	0	311.0458	360.7913	459.6009
C	0.464451	1.981896	0	491.9971	522.4834	642.7621
H	-0.40106	2.622399	0	735.3385	855.5404	1109.826
F	2.642271	0.129366	0	1268.592	1307.509	1480.454
F	1.29301	-1.58162	0	1535.11	3169.012	3273.584
Br	-1.41511	-0.16906	0			
H	1.447376	2.428871	0			

CF₃CHCH₂

Cartessian coordinates:				Frequencies (cm-1):		
C	0.370139	-0.01808	0.000039	94.7005	269.7114	318.5222
C	-0.98785	-0.64286	0.000062	427.988	511.4572	541.9365
C	-2.11377	0.05037	0.000006	630.46	719.4781	807.5328
H	-3.0712	-0.45064	0.000032	1006.342	1020.242	1025.848
H	-2.11599	1.131087	-0.00011	1116.12	1158.782	1279.851
F	0.338492	1.327066	-0.00053	1327.556	1461.076	1721.309
F	1.083484	-0.40244	-1.08434	3156.043	3185.543	3242.26
F	1.08324	-0.40156	1.084782			
H	-0.97087	-1.72465	0.00014			

CFBrCFCH₂

Cartessian coordinates:				Frequencies (cm-1):		
C	0.313224	0.469279	0	105.0218	187.2161	219.8365
C	1.457567	-0.32649	0	326.4989	354.9356	442.9456
C	1.544668	-1.68503	0	510.9269	607.203	671.2127
H	0.657897	-2.29518	0	764.9695	935.0022	1021.979
H	2.51524	-2.15425	0	1197.151	1347.749	1410.635
F	2.607562	0.388427	0	1511.47	3185.802	3287.209
F	0.426032	1.792662	0			
Br	-1.43909	-0.16934	0			

CH₃

Cartessian coordinates:				Frequencies (cm-1):		
C	0	0	0	542.0577	1407.588	1407.588
H	0	1.078065	0	3108.737	3283.534	3283.534
H	-0.93363	-0.53903	0			
H	0.933632	-0.53903	0			

CHBr=CH₂

Cartessian coordinates:				Frequencies (cm-1):		
C	-1.08924	0.522562	0	345.905	600.012	601.6452
C	-2.11157	-0.3114	0	941.4288	976.5493	1021.046
H	-3.11899	0.084314	-1E-06	1282.387	1408.424	1656.76
H	-1.98991	-1.38475	0	3143.637	3211.103	3234.42
Br	0.728362	-0.04469	0			
H	-1.17889	1.597586	0			

CFH=CH₂

Cartessian coordinates:				Frequencies (cm-1):		
C	-0.02217	0.434116	-5E-06	487.5799	729.3017	901.1633
H	0.11849	1.506069	0.000005	936.2071	967.2145	1163.256
C	-1.17729	-0.19918	0	1334.18	1415.353	1705.863
H	-2.09211	0.37291	0.000011	3165.179	3201.064	3258.105
H	-1.23437	-1.27772	-2E-06			
F	1.156081	-0.22343	0.000002			

F

Cartessian coordinates:				Frequencies (cm-1):		
F	0	0	0			

H

Cartessian coordinates:				Frequencies (cm-1):
H	0	0	0	

H₂

Cartessian coordinates:				Frequencies (cm-1):
H	0	0	0.371458	
H	0	0	-0.37146	

HBr

Cartessian coordinates:				Frequencies (cm-1):
Br	0	0	0.039555	2624.583
H	0	0	-1.38441	

HF

Cartessian coordinates:				Frequencies (cm-1):
F	0	0	0.092399	4071.909
H	0	0	-0.83159	
