Supporting Information (SI) for

A Mechanistic and Kinetic Study on the Formation of PBDD/Fs from PBDEs

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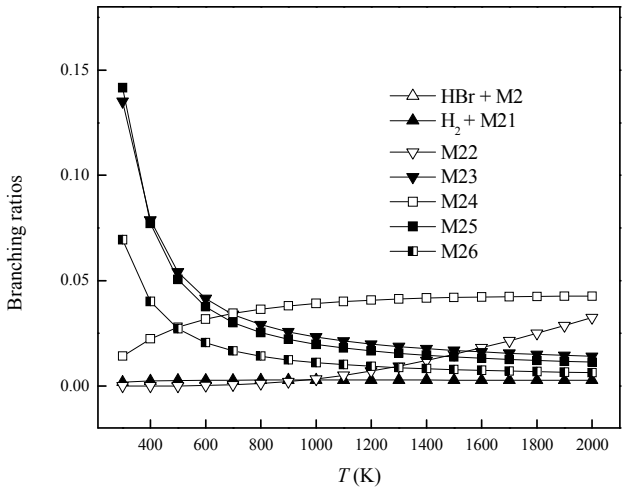


Figure S1. A smaller scale of Figure 2a.

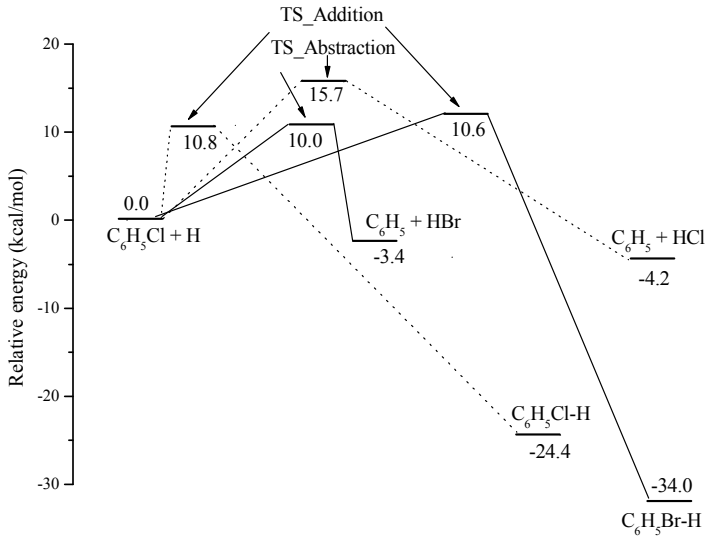
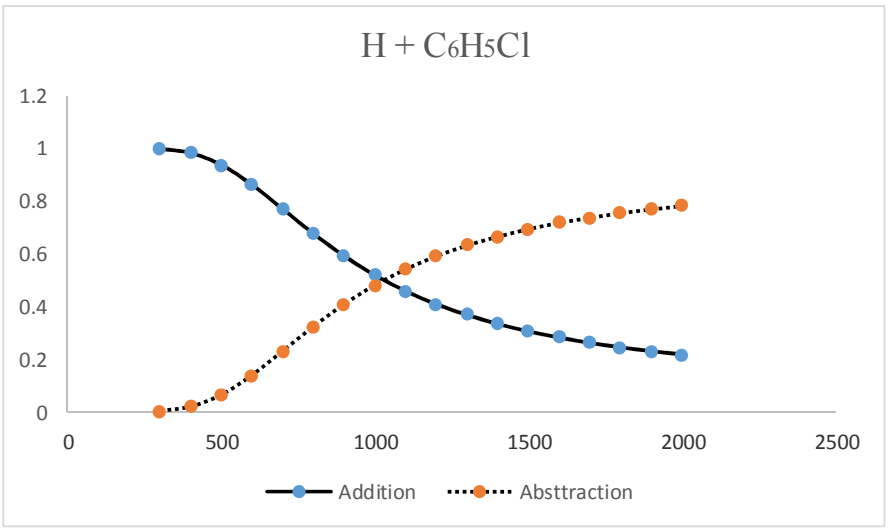
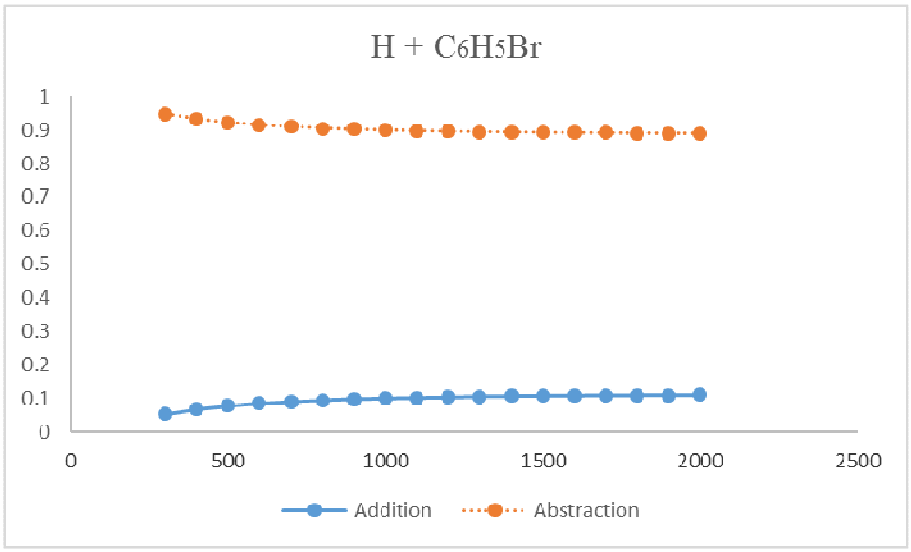


Figure S2. Reaction coordinates for the two systems of H + chlorobenzene and H + bromobenzene. Values (kcal/mol) in bold and italic are reaction and activation zero point energies; respectively (at 0K). Values are calculated at the M05-2X/GTLarge//M05-2X/6-311+G(d,p) level of theory.



(a)



(b)

Figure S3. Branching ratios (Y-axis) for addition and abstraction pathways in the two systems of H + chlorobenzene (a) and H + bromobenzene (b).

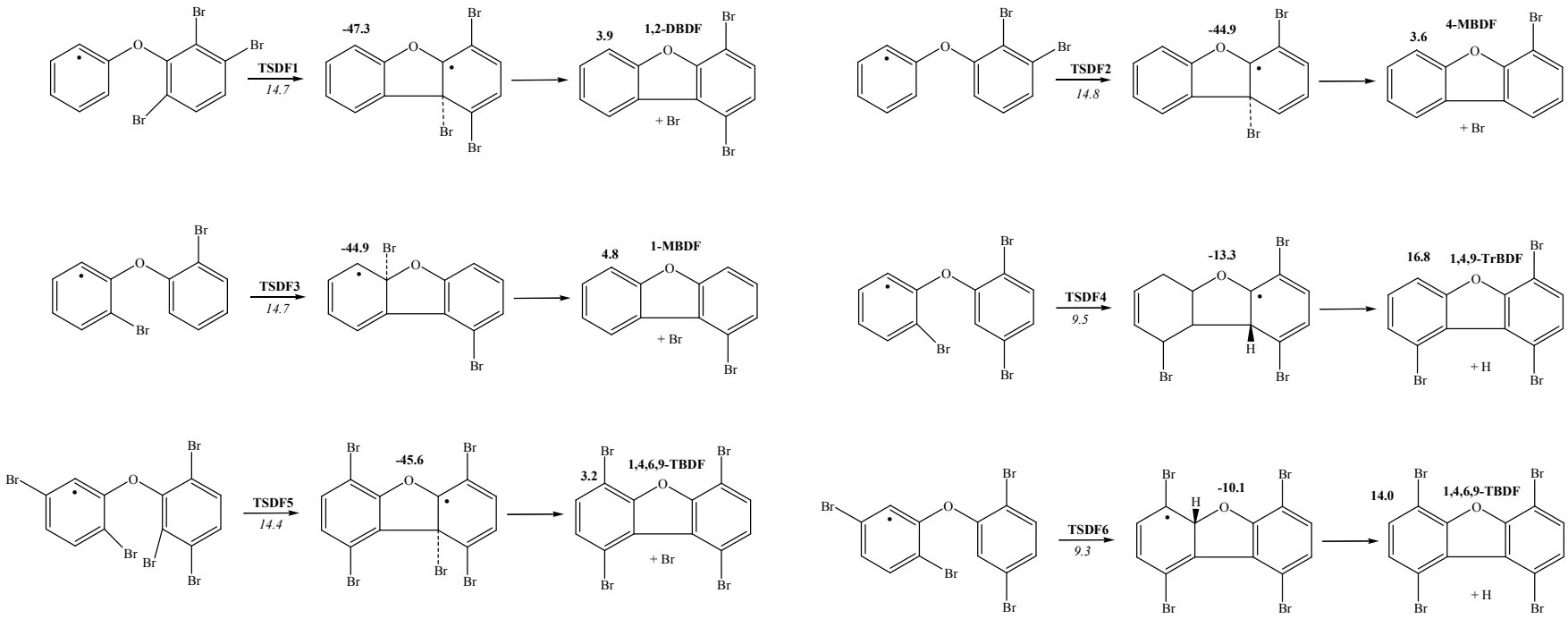


Figure S4: Pathways for formation of Different isomers of PBDFs. Values (kcal/mol) in bold and italic are reaction and activation energies, respectively, at 0 K. Values are calculated at the M052X/GTLarge//M052X/6-311+G(d,p) level of theory.

Table S1: Reactions rate parameters for abstraction and addition channels in the reactions H + chlorobenzene and H + bromobenzene .

Reaction	*A* (cm^3 $molecule^{-1}$ s^{-1})	*n*	*E*a/R (1/K)
H + C_6H_5Cl → C_6H_5Cl-H	6.31×10^{-16}	1.40	5 500
H + C_6H_5Cl → C_6H_5 + HCl	2.75×10^{-15}	1.54	8 000
H + C_6H_5Br → C_6H_5 Br -H	6.41×10^{-16}	1.39	5 500
H + C_6H_5 Br → C_6H_5 Br -H	1.86×10^{-15}	1.51	5 200

Vibrational Frequencies (in cm^{-1}) and Cartesian coordinates (in Å) for all structures

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M1

Atom	X	Y	Z
C	2.3378	-0.7569	-1.6545
C	3.7218	-0.6555	-1.5756
C	4.3280	-0.2663	-0.3872
C	3.5608	0.0166	0.7359
C	2.1857	-0.0957	0.6447
C	1.5637	-0.4731	-0.5433
H	4.3246	-0.8805	-2.4437
H	5.4039	-0.1871	-0.3275
C	-0.5942	0.4771	-0.4906
C	-0.1304	1.7651	-0.7243
C	-1.9326	0.2760	-0.1673
C	-1.0009	2.8420	-0.6224
C	-2.8005	1.3513	-0.0704
C	-2.3344	2.6402	-0.2959
H	-3.8343	1.1707	0.1855
H	-3.0127	3.4772	-0.2149
H	1.8366	-1.0586	-2.5632
O	1.3234	0.1450	1.7128
H	-0.6296	3.8409	-0.8027
H	4.0056	0.3102	1.6738
H	0.9073	1.9192	-0.9853
O	1.9073	0.5434	2.8019
O	0.2031	-0.6350	-0.6028
Br	-2.5685	-1.4784	0.1454

Moment of Inertia (AMU): 2732.1648 6811.1945 7459.5286

Frequencies (cm**-1):

19 27 52 70 123 133 177 209 265 277 320 335
391 431 451 502 517 532 570 598 609 652 693 722
746 755 780 797 846 868 871 937 951 973 982 1020
1028 1042 1080 1118 1134 1143 1159 1206 1217 1251 1255 1267
1285 1298 1438 1453 1476 1484 1601 1607 1616 1630 3112 3118
3121 3129 3129 3137 3138 3155

TS5

Atom	X	Y	Z
C	2.6114	-1.0558	-1.2197

C	3.9648	-0.9848	-0.9423
C	4.4175	-0.2250	0.1357
C	3.5113	0.4405	0.9406
C	2.1485	0.3537	0.6739
C	1.6950	-0.3785	-0.4228
H	4.6676	-1.5168	-1.5672
H	5.4740	-0.1616	0.3528
C	-0.4729	0.5053	-0.3579
C	-0.2063	1.8497	-0.7629
C	-1.8415	0.1381	-0.1636
C	-1.2019	2.7919	-0.7355
C	-2.8267	1.0959	-0.1316
C	-2.5123	2.4277	-0.4041
H	-3.8424	0.8031	0.0895
H	-3.2938	3.1729	-0.3816
H	2.2289	-1.6271	-2.0537
O	1.3055	1.0571	1.4885
H	-0.9769	3.8157	-0.9976
H	3.8254	1.0254	1.7937
H	0.8054	2.1024	-1.0481
O	0.0336	0.5344	1.4406
O	0.3696	-0.4950	-0.7642
Br	-2.2366	-1.6611	0.1953

Moment of Inertia (AMU): 2453.9455 5915.6936 7243.6615

Frequencies (cm**-1):

49 62 99 132 146 194 239 279 311 346 357 420
434 454 470 482 534 568 588 624 639 680 710 726
735 751 817 831 849 865 934 940 965 971 971 1010
1022 1028 1098 1113 1131 1134 1186 1202 1238 1249 1259 1276
1311 1411 1427 1455 1486 1527 1563 1610 1628 3114 3117 3123
3126 3130 3133 3137 3141

Imaginary Frequency (cm**-1): -640i

M4

Atom	X	Y	Z
C	2.5941	-0.6669	-1.4432
C	3.9379	-0.7286	-1.1014
C	4.3803	-0.2296	0.1198
C	3.4729	0.3232	1.0134
C	2.1365	0.3888	0.6609
C	1.6887	-0.0930	-0.5634
H	4.6414	-1.1715	-1.7919
H	5.4266	-0.2828	0.3836
C	-0.4813	0.6524	0.0072

C	-0.4808	2.1199	-0.2823
C	-1.8438	0.0399	-0.0715
C	-1.6228	2.8099	-0.5076
C	-2.9645	0.7740	-0.2921
C	-2.8820	2.1643	-0.5003
H	-3.9231	0.2766	-0.3207
H	-3.7842	2.7300	-0.6738
H	2.2262	-1.0485	-2.3850
O	1.2430	0.9953	1.5171
H	-1.5731	3.8712	-0.7066
H	3.7767	0.7043	1.9781
H	0.4878	2.5976	-0.3005
O	-0.0306	0.3764	1.3378
O	0.3692	-0.0294	-0.9135
Br	-1.9298	-1.8212	0.1729

Moment of Inertia (AMU): 2516.1332 5726.1286 7067.5786

Frequencies (cm**-1):

25 46 107 135 150 215 234 275 295 354 380 416
439 454 475 518 539 555 576 603 612 699 704 716
745 750 794 817 846 856 908 933 945 957 966 970
979 986 1023 1067 1088 1097 1124 1135 1193 1227 1251 1264
1276 1300 1356 1388 1458 1491 1505 1569 1620 1628 3115 3116
3124 3127 3132 3136 3138 3145

TS7

Atom	X	Y	Z
C	2.4482	-0.4049	-1.3334
C	3.4587	0.2268	-0.6627
C	3.4331	0.4252	0.7404
C	2.4282	-0.1385	1.5177
C	1.3965	-0.7605	0.8543
C	1.2870	-0.8071	-0.5998
H	4.2965	0.6159	-1.2246
H	4.2557	0.9396	1.2145
C	-1.0780	-0.6266	-0.6482
C	-1.5499	0.5325	-0.0468
C	-1.8567	-1.7717	-0.6679
C	-2.7995	0.5487	0.5558
C	-3.1074	-1.7575	-0.0696
H	-1.4507	-2.6568	-1.1333
C	-3.5762	-0.6014	0.5437
H	-3.7141	-2.6517	-0.0786
H	-4.5503	-0.5895	1.0117
H	2.4306	-0.4875	-2.4098
O	0.6420	-1.7806	1.2751

H	-3.1543	1.4569	1.0203
H	2.4910	-0.1897	2.5946
O	0.9324	-2.5260	0.0407
O	0.1401	-0.6140	-1.3066
Br	-0.4921	2.1068	-0.0620

Moment of Inertia (AMU): 2852.4537 4356.8564 6036.7784

Frequencies (cm**-1):

31 46 73 129 139 177 217 248 259 296 344 400
432 440 492 504 530 561 569 616 648 681 704 724
738 766 792 829 852 857 862 902 941 966 981 986
1017 1035 1094 1109 1129 1142 1180 1190 1224 1246 1265 1277
1334 1403 1430 1439 1471 1525 1569 1604 1609 3115 3115 3127
3129 3137 3140 3143 3149

Imaginary Frequency (cm**-1): -428i

M6

Atom	X	Y	Z
C	-2.5805	0.2007	-1.2863
C	-3.2656	-0.7693	-0.6157
C	-3.1121	-1.0186	0.7878
C	-2.3678	-0.1429	1.6014
C	-1.6298	0.7790	0.9155
C	-1.4780	0.8729	-0.5535
H	-3.9769	-1.3799	-1.1610
H	-3.6770	-1.8233	1.2417
C	0.9443	0.7093	-0.5711
C	1.6512	-0.3710	-0.0334
C	1.5244	1.9779	-0.5667
C	2.9154	-0.1816	0.5200
C	2.7844	2.1690	-0.0091
H	0.9699	2.7998	-0.9985
C	3.4789	1.0913	0.5366
H	3.2238	3.1595	-0.0068
H	4.4623	1.2342	0.9688
H	-2.6993	0.3783	-2.3475
O	-1.3141	2.0914	1.1535
H	3.4511	-1.0283	0.9294
O	-1.4493	2.3572	-0.3276
O	-0.2753	0.4905	-1.1931
Br	0.9097	-2.1321	-0.0777
H	-2.4720	-0.1293	2.6791

Moment of Inertia (AMU): 3066.7452 4412.0505 6368.2857

Frequencies (cm**-1):

26 43 70 106 132 186 199 211 265 297 337 378
416 437 479 504 505 513 557 609 634 648 671 701
705 739 748 766 786 819 829 838 881 925 931 939
955 997 1009 1021 1072 1095 1111 1135 1142 1177 1211 1230
1259 1293 1339 1360 1408 1436 1485 1530 1545 1554 3044 3047
3060 3061 3071 3074 3076 3089

TS6

Atom	X	Y	Z
C	-1.2395	1.0238	1.1848
C	-2.4050	1.1823	1.9383
C	-3.6624	0.8215	1.4223
C	-3.7558	0.2876	0.1574
C	-2.5834	0.0743	-0.6220
C	-1.3093	0.4902	-0.0940
H	-2.3325	1.5991	2.9360
H	-4.5543	0.9705	2.0185
C	1.0015	0.7682	-0.5558
C	1.3599	2.0813	-0.8514
C	1.9338	-0.1025	0.0116
C	2.6457	2.5319	-0.5706
C	3.2227	0.3499	0.2906
C	3.5759	1.6652	0.0012
H	3.9419	-0.3309	0.7273
H	4.5809	2.0072	0.2181
H	-0.2831	1.3261	1.5908
O	-2.6973	-0.2748	-1.9369
H	2.9211	3.5529	-0.8059
H	0.6225	2.7291	-1.3102
O	-2.5400	-1.5601	-1.2444
O	-0.2546	0.3160	-0.9248
H	-4.6996	-0.0010	-0.2869
Br	1.4581	-1.9070	0.3968

Moment of Inertia (AMU): 2870.5633 6003.8359 7179.5957

Frequencies (cm**-1):

18 29 68 111 132 148 172 220 248 257 307 398
431 450 452 457 503 523 560 602 644 662 691 719
724 762 781 814 831 843 870 906 926 941 958 999
1003 1021 1083 1094 1125 1135 1160 1201 1216 1231 1250 1261
1275 1393 1408 1418 1440 1498 1530 1548 1556 3049 3051 3060
3064 3069 3076 3076 3084

Imaginary Frequency (cm**-1): -432i

M8

Atom	X	Y	Z
C	-1.2826	0.8250	1.2889
C	-2.4478	0.8616	2.0732
C	-3.6911	0.4329	1.5458
C	-3.7867	-0.0211	0.2636
C	-2.6109	-0.0732	-0.6134
C	-1.3307	0.3720	-0.0088
H	-2.3875	1.2156	3.0948
H	-4.5743	0.4659	2.1732
C	0.9569	0.7842	-0.4807
C	1.2177	2.1384	-0.6769
C	1.9611	-0.0602	-0.0041
C	2.4770	2.6535	-0.3873
C	3.2238	0.4560	0.2830
C	3.4789	1.8115	0.0934
H	3.9986	-0.2055	0.6485
H	4.4638	2.2045	0.3162
H	-0.3384	1.1478	1.7089
O	-2.8227	0.2599	-1.9801
H	2.6762	3.7066	-0.5452
H	0.4261	2.7674	-1.0661
O	-2.5513	-1.1385	-1.5438
O	-0.2736	0.2718	-0.8521
H	-4.7179	-0.3571	-0.1745
Br	1.6183	-1.9193	0.2455

Moment of Inertia (AMU): 2861.2283 6197.0389 7253.0315

Frequencies (cm**-1):

12 27 67 83 130 147 193 241 254 286 302 401
422 437 441 455 499 508 547 593 600 643 669 682
710 740 743 772 786 818 842 872 877 925 931 956
978 1002 1020 1072 1094 1111 1135 1141 1195 1200 1231 1239
1261 1287 1375 1386 1409 1439 1478 1530 1548 1556 3048 3049
3060 3062 3070 3073 3076 3079

TS8

Atom	X	Y	Z
C	2.3446	0.5296	1.3981
C	3.6482	0.6983	0.9691

C	4.1379	0.0533	-0.1840
C	3.3212	-0.7741	-0.9137
C	2.0161	-1.0411	-0.4403
C	1.5181	-0.3379	0.6910
H	4.3027	1.3593	1.5202
H	5.1575	0.2251	-0.4977
C	-0.7607	-0.8250	-0.0098
C	-1.4052	-2.1208	0.3752
C	-1.7266	0.3245	-0.0340
C	-2.7432	-2.2430	0.5143
C	-3.0728	0.1496	0.0989
C	-3.6008	-1.1220	0.3627
H	-3.7256	1.0073	0.0261
H	-4.6682	-1.2398	0.4699
H	1.9494	1.0539	2.2559
O	1.2155	-1.8863	-0.9955
H	-3.1723	-3.2076	0.7469
H	3.6537	-1.2814	-1.8080
H	-0.7267	-2.9544	0.4779
O	-0.2306	-0.8320	-1.2585
O	0.2455	-0.5224	1.0428
Br	-0.9907	2.0347	-0.2990

Moment of Inertia (AMU): 2603.2756 5058.0128 6681.5659

Frequencies (cm**-1):

37 43 98 137 165 189 222 253 308 342 381 387
422 453 466 485 527 546 557 597 604 668 675 719
745 757 795 804 851 861 877 906 946 964 972 974
980 1002 1070 1094 1102 1117 1147 1196 1221 1254 1259 1297
1321 1341 1378 1415 1457 1489 1550 1570 1592 3112 3115 3125
3126 3136 3140 3141 3145

Imaginary Frequency (cm**-1): -811i

TS9

Atom	X	Y	Z
C	2.5902	-1.6735	-0.5115
C	3.9595	-1.6036	-0.2938
C	4.5374	-0.4290	0.1902
C	3.7474	0.6730	0.4496
C	2.3477	0.6139	0.3011
C	1.7904	-0.5850	-0.2177
H	4.5776	-2.4623	-0.5137
H	5.6048	-0.3765	0.3505
C	-0.3177	0.3880	-0.1669

C	0.1456	1.6875	-0.6833
C	-1.7537	0.2186	0.1768
C	-0.7304	2.7563	-0.6189
C	-2.6441	1.3744	0.0238
C	-2.0957	2.5874	-0.2426
H	-3.7056	1.2383	0.1616
H	-2.7437	3.4520	-0.2899
H	2.1218	-2.5628	-0.9088
O	1.5989	1.6344	0.6522
H	-0.4141	3.7152	-1.0022
H	4.1623	1.5996	0.8206
H	0.9102	1.6883	-1.4464
O	-0.7621	0.3770	1.1683
O	0.4517	-0.6942	-0.5251
Br	-2.5794	-1.5108	0.0578

Moment of Inertia (AMU): 2300.3956 6084.5327 7965.6025

Frequencies (cm**-1):

52 85 93 150 175 232 252 278 331 347 374 434
448 466 475 509 546 571 582 629 688 715 718 745
751 775 804 836 845 850 858 938 954 964 968 970
1007 1022 1076 1093 1099 1139 1155 1174 1190 1211 1256 1280
1348 1372 1409 1425 1445 1451 1559 1562 1600 3112 3113 3121
3123 3130 3133 3136 3147

Imaginary Frequency (cm**-1): -1037i

M9

Atom	X	Y	Z
C	2.5730	-1.7900	-0.2940
C	3.9405	-1.6879	-0.0915
C	4.5100	-0.4526	0.2026
C	3.7147	0.6801	0.2772
C	2.3465	0.5858	0.0643
C	1.7768	-0.6597	-0.2061
H	4.5581	-2.5720	-0.1559
H	5.5745	-0.3696	0.3688
C	-0.3002	0.2979	-0.0366
C	0.3352	1.5747	-0.5193
C	-1.7395	0.2395	0.1923
C	-0.5238	2.7700	-0.3105
C	-2.5494	1.4505	-0.0223
C	-1.8912	2.6639	-0.1724
H	-3.6225	1.3802	0.0452
H	-2.4820	3.5700	-0.1726
H	2.0950	-2.7355	-0.5074

O	1.5876	1.7273	0.1432
H	-0.0389	3.7325	-0.3738
H	4.1290	1.6545	0.4947
H	0.5321	1.4460	-1.5927
O	-0.8176	0.3093	1.2782
O	0.4121	-0.8166	-0.3969
Br	-2.6674	-1.4257	-0.0229

Moment of Inertia (AMU): 2245.0935 6037.6719 7991.8918

Frequencies (cm**-1):

50 78 100 148 199 234 261 290 317 357 376 453
468 478 489 541 554 585 593 627 649 696 724 740
766 779 811 855 868 874 925 956 957 989 1008 1047
1051 1060 1099 1120 1154 1155 1160 1207 1217 1284 1291 1315
1336 1359 1387 1428 1478 1490 1515 1524 1647 1668 2970 3174
3179 3188 3196 3202 3203 3226

TS11

Atom	X	Y	Z
C	2.4153	-1.8320	-0.1931
C	3.8003	-1.7597	-0.1405
C	4.4375	-0.5241	-0.0768
C	3.6905	0.6450	-0.0680
C	2.3096	0.5661	-0.1351
C	1.6707	-0.6649	-0.1975
H	4.3824	-2.6700	-0.1423
H	5.5156	-0.4700	-0.0293
C	-0.3818	0.3070	0.3424
C	0.2702	1.6775	0.2504
C	-1.8158	0.2713	-0.0881
C	-0.5299	2.8316	-0.1449
C	-2.4914	1.3822	-0.3891
C	-1.8357	2.6815	-0.4104
H	-3.5422	1.3242	-0.6327
H	-2.4349	3.5434	-0.6686
H	1.8912	-2.7759	-0.2382
O	1.5818	1.7322	-0.1844
H	-0.0303	3.7889	-0.1859
H	4.1531	1.6205	-0.0200
H	0.2743	1.5856	1.5171
O	-0.2272	0.2708	1.7337
O	0.3074	-0.7301	-0.3110
Br	-2.6498	-1.4177	-0.0572

Moment of Inertia (AMU): 2352.1549 5884.9278 7797.5034

Frequencies (cm**-1):

48 59 101 146 193 203 229 279 301 334 384 423
448 459 479 535 556 565 595 612 643 689 713 740
752 780 811 849 861 876 893 937 969 969 996 1001
1022 1049 1079 1096 1132 1138 1147 1189 1213 1258 1264 1296
1309 1338 1397 1461 1493 1564 1623 1630 1661 1904 3115 3116
3124 3130 3132 3136 3138

Imaginary Frequency (cm**-1): -1682i

M10

Atom	X	Y	Z
C	2.4434	-1.7258	-0.5800
C	3.8188	-1.6865	-0.3975
C	4.4333	-0.5177	0.0404
C	3.6759	0.6198	0.2795
C	2.3071	0.5803	0.0769
C	1.6851	-0.5918	-0.3392
H	4.4083	-2.5717	-0.5881
H	5.5026	-0.4888	0.1925
C	-0.3651	0.3216	0.2831
C	0.2484	1.6741	0.0689
C	-1.8082	0.3155	-0.1119
C	-0.4604	2.7825	-0.2695
C	-2.4968	1.4333	-0.4363
C	-1.8407	2.6861	-0.5060
H	-3.5539	1.3650	-0.6487
H	-2.4051	3.5651	-0.7741
H	1.9353	-2.6225	-0.9056
O	1.5872	1.7399	0.2623
H	0.0651	3.7202	-0.3791
H	4.1229	1.5464	0.6105
H	-0.5723	-0.8672	1.7904
O	-0.1754	-0.0015	1.6357
O	0.3257	-0.6345	-0.5250
Br	-2.6642	-1.3665	0.0305

Moment of Inertia (AMU): 2286.0711 5941.9386 7727.3991

Frequencies (cm**-1):

51 67 103 161 179 224 246 264 290 311 323 385
435 448 463 480 514 544 560 587 608 658 681 714
721 740 751 809 848 858 884 885 905 934 967 987
1008 1025 1051 1092 1095 1133 1143 1181 1203 1259 1261 1285
1295 1306 1347 1400 1460 1494 1518 1573 1621 1635 3114 3124

3126 3130 3131 3137 3149 3669

TS12

Atom	X	Y	Z
C	2.4832	-1.4915	-0.8819
C	3.8680	-1.4927	-0.8202
C	4.5249	-0.4869	-0.1222
C	3.7877	0.5001	0.5131
C	2.3971	0.5116	0.4672
C	1.7414	-0.4999	-0.2543
H	4.4262	-2.2730	-1.3176
H	5.6043	-0.4703	-0.0686
C	-0.4180	0.4244	0.1426
C	0.0059	1.7637	-0.3717
C	-1.8754	0.1873	-0.1929
C	-0.8134	2.8023	-0.6744
C	-2.7024	1.1985	-0.5856
C	-2.1669	2.4779	-0.8262
H	-3.7612	1.0253	-0.7018
H	-2.8470	3.2500	-1.1676
H	1.9412	-2.2555	-1.4217
O	1.7447	1.5270	1.1097
H	-0.4455	3.7943	-0.8938
H	4.2663	1.2934	1.0703
H	0.8793	1.1312	1.5527
O	-0.4109	0.5084	1.4797
O	0.3690	-0.6052	-0.4174
Br	-2.5337	-1.4945	0.2060

Moment of Inertia (AMU): 2373.2112 6229.0648 7780.8319

Frequencies (cm**-1):

42 78 93 125 157 180 267 283 300 335 366 402
424 450 468 483 527 552 560 592 611 678 705 725
749 754 804 847 850 858 929 936 965 1000 1022 1029
1033 1069 1084 1098 1133 1148 1169 1196 1245 1253 1274 1287
1317 1347 1417 1463 1489 1504 1571 1601 1625 2117 3098 3109
3118 3125 3126 3133 3143

Imaginary Frequency (cm**-1): -205i

M11

Atom	X	Y	Z

C	-2.1945	0.8603	-0.9721
C	-3.5507	1.0399	-1.2286
C	-4.4926	0.2869	-0.5411
C	-4.0948	-0.6485	0.4070
C	-2.7476	-0.8297	0.6745
C	-1.8104	-0.0639	-0.0177
H	-3.8612	1.7602	-1.9712
H	-5.5456	0.4228	-0.7433
C	0.4200	0.6457	0.0557
C	0.2704	1.9388	0.6967
C	1.8370	0.2612	-0.2443
C	1.2501	2.7879	0.9597
C	2.9197	1.1747	0.1541
C	2.6246	2.3780	0.6694
H	3.9386	0.8394	0.0329
H	3.4227	3.0584	0.9341
H	-1.4483	1.4209	-1.5179
O	-2.3545	-1.7394	1.5998
H	1.0706	3.7474	1.4260
H	-4.8120	-1.2452	0.9524
H	-1.3928	-1.7346	1.6469
O	0.9533	0.6671	-1.2626
O	-0.4894	-0.3360	0.3224
Br	2.3190	-1.5997	-0.2776

Moment of Inertia (AMU): 2519.8863 6474.5702 7916.2446

Frequencies (cm**-1):

21 38 67 125 139 176 205 231 272 297 338 404
407 437 452 474 485 522 555 562 577 620 653 703
722 737 745 794 818 845 849 860 901 927 934 966
968 978 1031 1083 1089 1139 1154 1160 1206 1209 1271 1286
1297 1322 1340 1377 1466 1504 1565 1627 1630 1661 3104 3113
3116 3121 3130 3137 3141 3698

TS10

Atom	X	Y	Z
C	1.8053	-1.6718	0.0189
C	2.9831	-1.9626	-0.6567
C	3.9276	-0.9625	-0.8750
C	3.6967	0.3257	-0.4236
C	2.5379	0.6215	0.2981
C	1.5848	-0.3901	0.4912
H	3.1589	-2.9654	-1.0187
H	4.8413	-1.1878	-1.4067
C	-0.4648	0.7629	0.6942
C	0.0155	2.0382	0.1866

C	-1.7653	0.2878	0.0704
C	-0.6531	2.8062	-0.6694
C	-2.4123	1.1216	-0.9465
C	-1.9113	2.3346	-1.2327
H	-3.2708	0.7225	-1.4662
H	-2.4106	2.9638	-1.9569
H	1.0474	-2.4211	0.1962
O	2.3742	1.8471	0.8184
H	-0.2535	3.7542	-1.0031
H	4.4093	1.1226	-0.5821
H	1.3071	2.1859	0.6165
O	-1.6773	0.7734	1.3890
O	0.4309	-0.1409	1.2160
Br	-2.1119	-1.5966	-0.0714

Moment of Inertia (AMU): 2770.1814 5221.4769 7010.7166

Frequencies (cm**-1):

44 56 102 148 161 187 260 281 321 354 358 376
430 447 491 503 537 551 567 580 624 677 692 725
756 762 795 827 837 856 861 883 905 944 964 970
974 989 1024 1091 1107 1134 1160 1176 1189 1248 1253 1278
1284 1325 1380 1405 1453 1470 1560 1586 1613 1656 3108 3113
3118 3125 3133 3137 3139

Imaginary Frequency (cm**-1): -1994i

TS19

Atom	X	Y	Z
C	-2.6729	0.6771	-1.4328
C	-3.9817	0.4736	-1.0294
C	-4.2863	0.0009	0.2585
C	-3.2760	-0.2788	1.1480
C	-1.9319	-0.1752	0.7268
C	-1.6418	0.3572	-0.5573
H	-4.7863	0.7012	-1.7146
H	-5.3185	-0.1306	0.5499
C	0.6323	0.8487	0.1184
C	1.7654	-0.1321	-0.0440
C	1.0807	2.2709	-0.0257
C	3.0594	0.2664	-0.0233
C	2.3990	2.6231	0.0039
C	3.3969	1.6409	0.0351
H	2.6719	3.6684	-0.0240
H	4.4378	1.9253	0.0622
H	-2.4304	1.0719	-2.4087
O	-0.9355	-0.5351	1.4681

H	3.8429	-0.4750	-0.0829
H	-3.4659	-0.6383	2.1491
O	0.1082	0.9400	1.3684
O	-0.3658	0.5688	-0.9118
H	0.2774	2.9907	-0.0613
Br	1.3445	-1.9526	-0.2553

Moment of Inertia (AMU): 2526.9003 5393.5818 6773.2038

Frequencies (cm**-1):

24 53 95 144 152 198 221 245 312 343 361 382
419 451 465 516 533 546 561 585 621 673 693 721
750 755 800 811 851 866 907 919 944 948 973 975
995 1008 1072 1087 1100 1103 1130 1196 1220 1233 1268 1286
1312 1339 1378 1412 1455 1497 1552 1554 1592 3113 3117 3124
3126 3134 3139 3140 3148

Imaginary Frequency (cm**-1): -813i

M17

Atom	X	Y	Z
C	2.6087	-0.6396	-0.9365
C	3.8659	-0.3251	-0.2921
C	3.9245	0.0011	1.0310
C	2.7437	0.0379	1.8016
C	1.4988	-0.2497	1.2466
C	1.4155	-0.5736	-0.0920
H	4.7449	-0.3681	-0.9194
H	4.8718	0.2312	1.4981
C	-0.9282	-0.8390	-0.0650
C	-1.7574	-2.0830	-0.1380
C	-2.9774	0.4576	0.2400
C	-3.2111	-1.9549	-0.0555
C	-3.7619	-0.7602	0.2132
H	-3.8212	-2.8295	-0.2301
H	-4.8338	-0.6660	0.3182
H	-3.4900	1.4038	0.3369
H	2.7998	0.2950	2.8495
O	-1.0093	-1.6972	1.0353
O	0.2700	-0.8536	-0.7557
C	-1.6529	0.4445	0.0292
H	0.6144	-0.2177	1.8648
O	2.5360	-0.9501	-2.1313
H	-1.3174	-2.9239	-0.6562
Br	-0.7015	2.0568	-0.2327

Moment of Inertia (AMU): 2691.7851 5486.0176 6736.2296

Frequencies (cm**-1):

27 52 60 121 139 179 207 243 258 276 308 388
428 465 479 489 510 535 547 561 622 674 701 717
751 761 792 834 841 867 899 915 929 962 965 975
992 1010 1019 1089 1105 1133 1160 1174 1217 1257 1263 1283
1345 1360 1385 1412 1431 1482 1526 1569 1574 1655 3106 3113
3114 3127 3128 3135 3135 3142

M18

Atom	X	Y	Z
C	2.7796	-0.8959	-1.0908
C	3.9560	-0.4952	-0.4765
C	3.9189	0.1416	0.7601
C	2.7019	0.3894	1.3756
C	1.5274	-0.0064	0.7582
C	1.5637	-0.6607	-0.4701
H	4.9024	-0.6835	-0.9628
H	4.8350	0.4513	1.2419
C	-0.6905	-1.0589	-0.2878
C	-0.7821	0.1490	0.6091
C	-1.9169	-1.7479	-0.6663
C	-2.0267	0.2415	1.3803
C	-3.1919	-1.2630	-0.1204
C	-3.1839	-0.3770	0.9398
H	-4.1144	-1.6758	-0.4973
H	-4.1127	-0.1474	1.4432
H	2.7761	-1.3974	-2.0480
O	0.3345	0.2630	1.4030
H	-2.0136	0.9097	2.2273
H	2.6343	0.8943	2.3286
O	-0.9894	-2.2659	0.3476
O	0.4130	-1.0727	-1.1088
Br	-0.8285	1.7736	-0.6729
H	-1.9066	-2.3203	-1.5828

Moment of Inertia (AMU): 2369.1372 4814.6157 5690.2227

Frequencies (cm**-1):

47 82 112 153 196 235 256 281 296 340 380 428
451 466 476 533 550 565 586 603 647 668 701 713
750 771 783 817 842 849 872 936 937 951 971 995
1026 1050 1065 1096 1124 1134 1136 1168 1190 1245 1264 1266
1295 1323 1353 1391 1458 1473 1482 1494 1621 1636 3115 3116
3117 3125 3132 3139 3144 3150

Zero-Point Energy (au): 0.1746481

Energies (au): -3261.8602232

Spin Multiplicity: 2

TS20

Atom	X	Y	Z
C	2.5567	-1.1150	-1.1007
C	3.7747	-0.7818	-0.5239
C	3.8206	-0.1677	0.7312
C	2.6517	0.1104	1.4062
C	1.3985	-0.2854	0.8871
C	1.3830	-0.8725	-0.4135
H	4.6902	-0.9842	-1.0613
H	4.7727	0.1011	1.1663
C	-0.9410	-0.9357	-0.3259
C	-1.1096	0.4099	0.2748
C	-2.1604	-1.7528	-0.5959
C	-2.3308	0.7085	0.8584
C	-3.4445	-1.2109	-0.1627
C	-3.4670	-0.1202	0.6519
H	-4.3564	-1.7104	-0.4543
H	-4.4109	0.2235	1.0523
H	2.4965	-1.5532	-2.0867
O	0.3085	-0.1211	1.5761
H	-2.4622	1.6790	1.3126
H	2.6481	0.5892	2.3752
O	-1.2558	-1.9864	0.5148
O	0.2049	-1.1256	-1.0754
Br	-0.2320	1.8887	-0.5480
H	-2.1101	-2.5054	-1.3705

Moment of Inertia (AMU): 2389.8602 4679.3795 5767.3840

Frequencies (cm**-1):

51 99 120 142 188 247 253 288 313 341 375 414
440 471 490 508 541 557 580 624 661 713 714 745
750 775 817 844 845 853 931 934 952 961 966 980
1015 1018 1035 1082 1094 1135 1152 1189 1221 1242 1260 1285
1335 1351 1382 1413 1438 1449 1551 1554 1597 3108 3112 3114
3122 3131 3134 3136 3139

Imaginary Frequency (cm**-1): -1032i

M19

Atom	X	Y	Z
C	2.4317	-1.3729	-0.2013
C	3.6391	-0.7473	0.0824
C	3.6852	0.6282	0.2811
C	2.5256	1.3875	0.1948
C	1.3272	0.7607	-0.0971
C	1.2805	-0.6130	-0.2978
H	4.5422	-1.3364	0.1527
H	4.6240	1.1132	0.5065
C	-1.0059	-0.5889	-0.0403
C	-1.0075	0.8870	-0.0983
C	-2.3064	-1.2863	-0.0390
C	-2.1581	1.5696	-0.0368
C	-3.5232	-0.4683	-0.0822
C	-3.4276	0.8709	-0.0277
H	-4.4806	-0.9602	-0.1746
H	-4.3263	1.4726	-0.0284
H	2.3619	-2.4395	-0.3596
O	0.1897	1.5241	-0.2272
H	-2.1314	2.6495	-0.0531
H	2.5292	2.4578	0.3441
O	-1.4686	-1.1730	1.1436
O	0.0840	-1.2044	-0.6390
H	-2.3225	-2.2933	-0.4338

Moment of Inertia (AMU): 1031.1926 3982.8318 4782.7918

Frequencies (cm**-1):

55 96 179 229 267 280 305 377 413 440 449 508
545 555 566 599 627 647 684 709 714 751 795 827
845 852 863 880 935 944 964 970 973 1017 1022 1082
1095 1135 1140 1166 1184 1227 1258 1269 1287 1298 1381 1385
1425 1460 1497 1591 1624 1631 1684 3099 3110 3115 3125 3129
3133 3134 3138

TS21

Atom	X	Y	Z
C	-2.8798	-1.6500	0.8100
C	-4.1034	-1.8097	0.1731
C	-4.5627	-0.8350	-0.7053
C	-3.8064	0.3031	-0.9525
C	-2.5902	0.4646	-0.3125
C	-2.1392	-0.5117	0.5638

H	-4.6920	-2.6958	0.3603
H	-5.5126	-0.9596	-1.2048
C	-0.0983	0.5476	0.7057
C	-0.5662	1.6081	-0.1102
C	1.3339	0.4310	1.0157
C	0.2568	2.6459	-0.4041
C	2.1155	1.6853	0.8348
C	1.6008	2.6948	0.1137
H	3.1117	1.7315	1.2488
H	2.1843	3.5839	-0.0786
H	-2.4855	-2.3882	1.4933
O	-1.8678	1.6097	-0.5415
H	-0.1277	3.4527	-1.0113
H	-4.1382	1.0743	-1.6327
O	1.3272	-0.4089	-0.1348
O	-0.9273	-0.3531	1.2257
Br	3.2710	-1.2543	-0.4540
H	1.5534	-0.1231	1.9267

Moment of Inertia (AMU): 2341.2308 7574.3170 9083.9105

Frequencies (cm**-1):

31 47 73 127 152 198 205 255 287 310 370 414
427 445 502 535 540 556 587 614 642 680 709 734
752 804 833 848 866 872 929 938 970 974 976 1019
1024 1090 1135 1141 1161 1173 1204 1231 1266 1270 1293 1295
1343 1395 1419 1462 1495 1545 1622 1635 1644 3025 3118 3118
3128 3134 3135 3141 3142

Imaginary Frequency (cm**-1): -527i

M20

Atom	X	Y	Z
C	2.4602	0.5911	1.1993
C	3.7372	0.4117	0.6863
C	3.9618	-0.5208	-0.3217
C	2.9125	-1.2850	-0.8110
C	1.6439	-1.1127	-0.2845
C	1.4133	-0.1734	0.7133
H	4.5543	1.0075	1.0669
H	4.9540	-0.6547	-0.7277
C	-0.8718	-0.3442	0.3251
C	-0.6228	-1.6764	-0.3065
C	-2.1824	-0.2605	1.0187
C	-1.6149	-2.5954	-0.4926
C	-3.1383	-1.1954	0.8145
C	-2.8887	-2.3542	0.0298

H	-4.1056	-1.0780	1.2828
H	-3.6733	-3.0798	-0.1187
H	2.2492	1.3173	1.9714
O	0.6301	-1.9177	-0.7525
H	-1.3806	-3.5130	-1.0131
H	3.0537	-2.0207	-1.5899
O	-0.7941	0.5226	-0.8251
O	0.1537	-0.0067	1.2355
Br	-0.9170	2.3350	-0.4346
H	-2.3336	0.6016	1.6514

Moment of Inertia (AMU): 3214.2766 4388.7873 6625.2102

Frequencies (cm**-1):

38 60 101 124 171 200 230 268 293 360 402 428
448 456 498 517 547 571 583 617 633 680 693 710
727 752 783 810 827 851 869 895 919 936 957 971
979 1023 1063 1094 1097 1133 1136 1178 1183 1248 1262 1288
1292 1305 1391 1400 1461 1494 1517 1583 1623 1635 3114 3115
3125 3126 3132 3138 3138 3145

TS22

Atom	X	Y	Z
C	3.0492	0.1775	1.3634
C	4.1616	0.5960	0.6446
C	4.1566	0.5422	-0.7441
C	3.0406	0.0650	-1.4187
C	1.9389	-0.3566	-0.6980
C	1.9411	-0.2971	0.6882
H	5.0276	0.9690	1.1719
H	5.0186	0.8724	-1.3053
C	-0.2962	-0.8949	0.7210
C	-0.2525	-1.1485	-0.6794
C	-1.4338	-1.3033	1.4540
C	-1.3685	-1.6218	-1.3353
C	-2.5403	-1.7632	0.7897
C	-2.5125	-1.9227	-0.6070
H	-3.4326	-2.0192	1.3419
H	-3.3887	-2.2879	-1.1223
H	3.0165	0.2164	2.4427
O	0.8566	-0.8510	-1.3936
H	-1.3242	-1.7477	-2.4072
H	3.0032	0.0106	-2.4973
O	-0.5980	1.0506	0.5589
O	0.8576	-0.7299	1.4208
Br	-2.1357	1.6277	-0.1688
H	-1.4049	-1.1752	2.5258

Moment of Inertia (AMU): 2388.8814 5920.8470 6586.2434

Frequencies (cm**-1):

35 48 89 104 147 181 223 246 269 318 382 397
432 447 505 517 542 558 591 635 654 692 698 720
741 750 826 832 841 849 879 931 934 968 969 1008
1025 1085 1102 1128 1135 1177 1199 1225 1260 1267 1286 1304
1317 1430 1458 1473 1499 1548 1584 1632 1641 3116 3122 3126
3132 3134 3139 3140 3146

Imaginary Frequency (cm**-1): -334i

DD

Atom	X	Y	Z
C	-1.1672	-0.6953	-0.0002
C	-1.1671	0.6953	-0.0002
C	-2.3645	-1.3885	0.0001
C	-2.3645	1.3885	0.0001
C	-3.5678	-0.6943	0.0004
C	-3.5678	0.6943	0.0004
H	-4.4998	-1.2408	0.0007
H	-4.4998	1.2408	0.0007
C	1.1671	-0.6953	-0.0002
C	1.1672	0.6953	-0.0002
C	2.3645	-1.3885	0.0001
C	2.3645	1.3885	0.0001
C	3.5678	-0.6943	0.0004
H	2.3295	-2.4687	0.0001
C	3.5678	0.6943	0.0004
H	4.4998	1.2408	0.0007
O	0.0000	-1.4221	-0.0006
O	0.0000	1.4221	-0.0006
H	2.3295	2.4687	0.0001
H	4.4998	-1.2408	0.0007
H	-2.3296	2.4687	0.0001
H	-2.3295	-2.4687	0.0001

Moment of Inertia (AMU): 836.9306 3743.3911 4580.3215

Frequencies (cm**-1):

118 221 233 259 287 383 428 436 449 489 522 537
552 599 607 659 671 722 743 744 833 835 836 838
874 928 929 958 959 1027 1027 1082 1098 1132 1133 1177
1185 1222 1259 1269 1281 1302 1306 1447 1466 1498 1506 1611

1611 1641 1652 3114 3114 3124 3124 3131 3131 3137 3137

M7

Atom	X	Y	Z
C	3.7860	-0.1113	-0.0330
C	2.6234	-0.2047	-0.8902
C	1.3591	-0.5270	-0.2260
C	1.2954	-0.7412	1.1356
C	2.4565	-0.6376	1.8993
C	3.6991	-0.3214	1.3127
O	0.3024	-0.6020	-1.0624
C	-0.9433	-0.8393	-0.5243
C	-1.7066	0.1995	-0.0037
C	-1.4542	-2.1274	-0.5653
C	-2.9809	-0.0522	0.4852
C	-2.7289	-2.3805	-0.0789
H	-0.8387	-2.9089	-0.9886
C	-3.4898	-1.3437	0.4476
H	-3.5653	0.7641	0.8840
H	-3.1271	-3.3845	-0.1150
H	-4.4842	-1.5343	0.8255
H	4.7183	0.1309	-0.5230
H	0.3531	-0.9802	1.6075
O	2.6824	-0.0278	-2.1116
H	2.3975	-0.8029	2.9654
H	4.5786	-0.2477	1.9367
Br	-1.0116	1.9578	0.0298

Moment of Inertia (AMU): 2528.1209 5168.5870 6202.5612

Frequencies (cm**-1):

25 34 73 119 133 184 217 260 267 318 429 432
462 477 490 494 538 553 605 650 697 699 739 759
785 807 834 865 874 928 950 963 983 1007 1020 1037
1099 1110 1127 1142 1167 1230 1249 1265 1275 1281 1383 1424
1439 1473 1483 1526 1569 1600 1608 3113 3115 3121 3125 3131
3133 3137 3139

TS13

Atom	X	Y	Z
C	-1.0219	-0.9346	-0.6027
C	-1.2319	0.2816	0.1096

C	-2.0118	-1.9045	-0.6363
C	-2.4582	0.4724	0.7901
C	-3.1960	-1.6965	0.0459
C	-3.4059	-0.5160	0.7835
H	-4.3330	-0.3749	1.3202
C	1.3137	-0.8694	-0.4696
C	1.2091	-0.4933	0.8799
C	2.5261	-0.9285	-1.1221
C	2.3892	-0.1648	1.5532
C	3.6918	-0.6363	-0.4215
H	2.5423	-1.2041	-2.1670
C	3.6182	-0.2617	0.9145
H	4.6468	-0.6922	-0.9234
O	0.1670	-1.1987	-1.1845
O	0.0278	-0.4293	1.4860
H	2.3096	0.1451	2.5854
H	4.5200	-0.0219	1.4604
H	-2.6178	1.4092	1.3024
H	-3.9607	-2.4598	0.0300
H	-1.8073	-2.8231	-1.1665
Br	-0.3255	1.8559	-0.4514

Moment of Inertia (AMU): 2224.4144 4321.9591 5228.6917

Frequencies (cm**-1):

48 92 120 142 182 226 270 306 339 356 413 435
466 501 519 540 579 599 634 682 703 735 743 755
826 835 843 860 926 941 962 972 1002 1016 1024 1083
1101 1132 1137 1161 1199 1228 1243 1251 1281 1308 1411 1427
1445 1463 1538 1577 1585 1610 3110 3118 3121 3129 3130 3136
3138 3143

Imaginary Frequency (cm**-1): -467i

M12

Atom	X	Y	Z
C	0.8267	-0.9507	0.7058
C	0.8267	-0.9509	-0.7057
C	2.0282	-1.0752	1.4055
C	2.0281	-1.0756	-1.4054
C	3.2136	-1.1991	0.7023
C	3.2135	-1.1994	-0.7021
H	4.1482	-1.2892	1.2419
H	4.1481	-1.2895	-1.2417
C	-1.4826	-0.6416	0.6986
C	-1.4826	-0.6417	-0.6985

C	-2.6501	-0.3726	1.4010
C	-2.6501	-0.3729	-1.4010
C	-3.8197	-0.1033	0.6988
H	-2.6190	-0.3716	2.4834
C	-3.8197	-0.1034	-0.6988
H	-4.7313	0.1127	-1.2422
O	-0.3391	-0.9334	1.4067
O	-0.3391	-0.9337	-1.4065
H	-2.6190	-0.3722	-2.4833
H	-4.7313	0.1131	1.2422
H	1.9988	-1.0699	-2.4874
Br	0.8697	2.0655	-0.0002
H	1.9988	-1.0691	2.4875

Moment of Inertia (AMU): 2502.0458 4772.9670 5588.4257

Frequencies (cm**-1):

31 45 71 90 112 214 246 257 314 383 425 427
438 479 516 528 559 593 616 644 663 709 731 734
815 818 823 834 872 915 920 946 949 1001 1005 1075
1095 1128 1131 1160 1181 1203 1238 1244 1258 1292 1309 1417
1425 1444 1461 1533 1549 1575 1589 3055 3057 3066 3069 3075
3079 3079 3083

TS14

Atom	X	Y	Z
C	-1.6271	0.0835	-1.5159
C	-2.9889	-0.1818	-1.6173
C	-3.7881	-0.1062	-0.4798
C	-3.2616	0.2187	0.7639
C	-1.8932	0.4800	0.8625
C	-1.0940	0.4055	-0.2828
C	0.3054	0.8152	0.0659
C	1.4384	-0.1399	-0.0526
C	0.6561	2.2060	-0.3737
C	2.7547	0.3021	-0.2092
C	1.9323	2.5809	-0.5735
C	2.9995	1.6317	-0.4562
H	3.5594	-0.4168	-0.1700
H	-3.8818	0.2723	1.6463
O	-1.3098	0.8282	2.0056
O	0.4311	0.6345	1.4640
H	-0.9847	0.0284	-2.3858
H	2.1674	3.6029	-0.8355
H	-3.4219	-0.4497	-2.5699
H	-4.8466	-0.3151	-0.5579
H	4.0193	1.9642	-0.5875

Br	1.0852	-1.9732	0.0398
H	-0.1655	2.9012	-0.4786

Moment of Inertia (AMU): 2621.1544 4229.6787 5403.4699

Frequencies (cm**-1):

50 58 81 142 156 206 244 265 321 354 376 428
466 479 502 546 561 589 607 643 710 730 734 742
812 822 847 933 936 956 970 971 978 982 991 1021
1097 1110 1136 1138 1173 1195 1232 1254 1287 1295 1359 1405
1434 1463 1474 1586 1608 1613 3100 3108 3112 3123 3129 3131
3136 3140

Imaginary Frequency (cm**-1): -805i

Zero-Point Energy (au): 0.1663006

Energies (au): -3186.5130645

Spin Multiplicity: 2

M13

Atom	X	Y	Z
C	0.4413	0.3398	0.2849
C	-0.2645	1.6467	0.4873
C	1.7874	0.2670	0.0483
C	0.5985	2.8354	0.2426
C	2.5608	1.4365	-0.0800
C	1.9319	2.7058	0.0017
H	3.6206	1.3575	-0.2771
H	2.5397	3.5925	-0.1395
C	-1.6930	-0.6207	0.2101
C	-2.2373	0.5973	-0.2147
C	-2.5007	-1.7364	0.3995
C	-3.6024	0.6795	-0.4793
C	-3.8647	-1.6440	0.1412
H	-2.0431	-2.6619	0.7273
C	-4.4120	-0.4398	-0.3067
H	-5.4731	-0.3684	-0.5135
O	-0.3273	-0.7715	0.3879
O	-1.4375	1.6956	-0.3847
H	-4.0071	1.6271	-0.8140
H	-0.6696	1.6689	1.5156
H	-4.4968	-2.5121	0.2832
Br	2.6302	-1.4373	-0.1575

H	0.1191	3.8050	0.2972

Moment of Inertia (AMU): 2193.2874 5715.8740 7748.5295

Frequencies (cm**-1):

52 70 108 153 183 233 271 289 303 373 433 441
472 489 508 540 554 599 615 653 698 701 730 742
766 799 829 856 874 911 928 942 968 1005 1007 1028
1081 1126 1133 1145 1178 1190 1225 1251 1265 1280 1296 1338
1374 1430 1454 1474 1527 1561 1580 2789 3046 3048 3059 3067
3068 3074 3089

TS16

Atom	X	Y	Z
C	4.0235	-0.3523	-1.0345
C	2.7681	0.1020	-1.3652
C	1.7808	0.0529	-0.2869
C	2.0792	0.5986	1.0313
C	2.8416	-0.6478	1.0224
C	4.0674	-0.8294	0.2707
H	4.8657	-0.3492	-1.7076
H	2.4572	0.4637	-2.3337
H	2.5603	-1.3370	1.8109
H	4.9194	-1.3178	0.7174
O	0.4956	-0.2882	-0.6306
C	-0.5203	0.6093	-0.3850
C	-0.3333	1.9810	-0.4863
C	-1.7816	0.1036	-0.0961
C	-1.4022	2.8398	-0.2852
H	0.6537	2.3662	-0.7032
C	-2.8540	0.9619	0.0958
C	-2.6634	2.3333	0.0037
H	-3.8260	0.5485	0.3217
H	-3.4985	3.0008	0.1603
O	1.5555	1.2963	1.8495
H	-1.2467	3.9068	-0.3548
Br	-2.0380	-1.7676	0.0409

Moment of Inertia (AMU): 2463.0274 5445.3187 6892.2405

Frequencies (cm**-1):

15 27 70 139 141 191 201 243 287 322 377 395
434 472 514 523 564 598 647 669 689 708 732 749
778 825 849 852 872 905 940 959 975 1019 1040 1043
1054 1081 1119 1143 1163 1182 1230 1249 1259 1281 1315 1375
1439 1465 1476 1604 1611 1815 3080 3113 3121 3131 3139 3139

3142 3161

Imaginary Frequency (cm**-1): -280i

M14

Atom	X	Y	Z
C	-3.5676	-0.6510	1.5185
C	-2.3525	0.0170	1.4390
C	-1.8003	-0.0694	0.0614
C	-2.6018	0.5809	-1.0154
C	-2.9233	-0.8563	-0.7326
C	-3.9388	-1.1891	0.2903
H	-4.1635	-0.7215	2.4193
H	-1.8570	0.5594	2.2315
H	-2.6712	-1.5409	-1.5384
H	-4.8419	-1.7412	0.0733
O	-0.4496	-0.3786	-0.1492
C	0.4977	0.6000	0.0265
C	0.1995	1.9566	0.1650
C	1.8380	0.1916	0.0468
C	1.2246	2.8858	0.3272
H	-0.8295	2.2892	0.1236
C	2.8582	1.1219	0.2061
C	2.5535	2.4744	0.3497
H	0.9752	3.9354	0.4289
H	3.8863	0.7832	0.2189
H	3.3526	3.1950	0.4746
O	-2.7243	1.4950	-1.7677
Br	2.2748	-1.6590	-0.1483

Moment of Inertia (AMU):   2511.6090 5784.1831 7283.7821

Frequencies (cm**-1):

22 37 72 102 129 155 179 223 259 290 310 375
426 449 503 524 547 580 605 646 659 684 701 728
738 748 795 826 832 892 896 912 918 947 971 1000
1023 1026 1043 1092 1101 1124 1139 1194 1203 1246 1263 1271
1340 1396 1411 1443 1547 1559 1822 3017 3049 3062 3073 3073
3078 3094 3102

M2

Atom	X	Y	Z
C	2.4698	-2.4312	-0.0312
C	1.2784	-2.1139	-0.6674

C	0.8042	-0.8107	-0.6418
C	1.5273	0.1770	0.0182
C	2.7179	-0.1364	0.6572
C	3.1874	-1.4430	0.6315
H	2.8365	-3.4475	-0.0542
H	0.6970	-2.8585	-1.1929
H	3.2682	0.6425	1.1642
H	4.1167	-1.6840	1.1280
O	-0.3572	-0.5063	-1.3165
C	-1.4929	-0.4718	-0.5482
C	-2.6846	-0.0585	-1.1378
C	-1.5319	-0.8356	0.7767
C	-3.8476	-0.0286	-0.3788
C	-2.6529	-0.8167	1.5625
C	-3.8442	-0.4019	0.9619
H	-2.6746	0.2362	-2.1783
H	-4.7694	0.2944	-0.8421
H	-4.7564	-0.3713	1.5412
H	-2.6229	-1.1096	2.6033
Br	0.8908	1.9593	0.0327

Moment of Inertia (AMU): 2294.2012 4346.3578 5673.8884

Frequencies (cm**-1):

21 38 65 129 160 231 249 266 348 404 433 457
485 509 556 590 613 649 655 710 730 748 796 824
858 865 921 947 951 965 981 1013 1020 1037 1091 1109
1129 1141 1204 1218 1241 1257 1275 1287 1424 1437 1441 1472
1561 1599 1606 1621 3103 3111 3113 3119 3123 3129 3132 3138

Zero-Point Energy (au): 0.1645387

TS3

Atom	X	Y	Z
C	3.7907	-1.4058	-0.1960
C	2.5320	-1.6323	0.3563
C	1.6461	-0.5701	0.3993
C	2.0081	0.6645	-0.0937
C	3.2504	0.9144	-0.6219
C	4.1514	-0.1542	-0.6846
H	4.4982	-2.2218	-0.2452
H	3.5273	1.8938	-0.9888
H	5.1329	-0.0037	-1.1131
O	0.3688	-0.7126	0.9199
C	-0.3479	0.4188	0.6428
C	0.3337	1.6555	0.7863

C	-1.5830	0.3594	0.0392
C	-0.2898	2.8205	0.2920
H	1.0564	1.7546	1.5866
C	-2.1894	1.5226	-0.4360
C	-1.5225	2.7412	-0.3306
H	-3.1601	1.4586	-0.9042
H	-1.9952	3.6356	-0.7112
H	2.2404	-2.5999	0.7403
H	0.1905	3.7778	0.4335
Br	-2.4320	-1.3143	-0.2022

Moment of Inertia (AMU): 2031.9111 4944.7696 6584.8441

Frequencies (cm**-1):

47 84 108 163 210 269 277 340 398 417 453 504
523 542 567 611 631 680 727 742 745 790 820 842
843 869 925 957 968 971 1008 1016 1039 1089 1105 1132
1141 1179 1209 1221 1237 1282 1295 1407 1429 1437 1464 1541
1568 1581 1615 3077 3100 3111 3115 3121 3129 3130 3140

Imaginary Frequency (cm**-1): -414i

TS2

Atom	X	Y	Z
C	3.7907	-1.4058	-0.1960
C	2.5320	-1.6323	0.3563
C	1.6461	-0.5701	0.3993
C	2.0081	0.6645	-0.0937
C	3.2504	0.9144	-0.6219
C	4.1514	-0.1542	-0.6846
H	4.4982	-2.2218	-0.2452
H	3.5273	1.8938	-0.9888
H	5.1329	-0.0037	-1.1131
O	0.3688	-0.7126	0.9199
C	-0.3479	0.4188	0.6428
C	0.3337	1.6555	0.7863
C	-1.5830	0.3594	0.0392
C	-0.2898	2.8205	0.2920
H	1.0564	1.7546	1.5866
C	-2.1894	1.5226	-0.4360
C	-1.5225	2.7412	-0.3306
H	-3.1601	1.4586	-0.9042
H	-1.9952	3.6356	-0.7112
H	2.2404	-2.5999	0.7403
H	0.1905	3.7778	0.4335
Br	-2.4320	-1.3143	-0.2022

Moment of Inertia (AMU): 2031.9111 4944.7696 6584.8441

Frequencies (cm**-1):

47 84 108 163 210 269 277 340 398 417 453 504
523 542 567 611 631 680 727 742 745 790 820 842
843 869 925 957 968 971 1008 1016 1039 1089 1105 1132
1141 1179 1209 1221 1237 1282 1295 1407 1429 1437 1464 1541
1568 1581 1615 3077 3100 3111 3115 3121 3129 3130 3140

Imaginary Frequency (cm**-1): -414i

M3

Atom	X	Y	Z
C	3.9081	-1.4390	-0.2894
C	2.5879	-1.8461	-0.1037
C	1.6629	-0.8514	0.1259
C	1.9918	0.4968	0.1862
C	3.3050	0.8874	0.0063
C	4.2645	-0.0946	-0.2406
H	4.6671	-2.1847	-0.4805
H	3.5859	1.9310	0.0544
H	5.2956	0.1904	-0.3938
O	0.3075	-1.0728	0.3052
C	-0.2838	0.1545	0.3407
C	0.7306	1.2405	0.5593
C	-1.5879	0.4178	0.1022
C	0.3209	2.5238	-0.0919
H	0.7872	1.4316	1.6487
C	-1.9870	1.7517	-0.1413
C	-0.9984	2.7535	-0.3268
H	-3.0303	1.9700	-0.3027
H	-1.3163	3.7196	-0.6947
H	2.2930	-2.8840	-0.1463
H	1.0667	3.2868	-0.2626
Br	-2.8371	-0.9956	-0.0750

Moment of Inertia (AMU): 1675.2357 5429.1092 6996.8179

Frequencies (cm**-1):

59 101 110 151 223 253 284 296 402 433 475 480
514 536 552 601 618 650 703 733 748 750 797 815
848 865 937 938 962 974 1012 1017 1034 1082 1124 1136
1138 1150 1187 1200 1219 1267 1276 1303 1329 1378 1459 1472
1505 1583 1619 1647 2786 3107 3108 3116 3126 3129 3140 3151

TS3

Atom	X	Y	Z
C	3.9729	-1.4097	-0.0978
C	2.6517	-1.8355	-0.0366
C	1.6905	-0.8465	0.0295
C	1.9919	0.5143	0.0421
C	3.3178	0.9236	-0.0137
C	4.3031	-0.0514	-0.0895
H	4.7618	-2.1464	-0.1555
H	3.5767	1.9731	0.0050
H	5.3422	0.2413	-0.1396
O	0.3333	-1.0700	0.0784
C	-0.2549	0.1536	0.0774
C	0.7006	1.1993	0.1672
C	-1.6052	0.4095	0.0110
C	0.2746	2.5255	-0.0605
H	0.7538	1.2426	1.8912
C	-2.0203	1.7339	-0.0657
C	-1.0813	2.7725	-0.1289
H	-3.0771	1.9500	-0.1171
H	-1.4375	3.7859	-0.2481
H	2.3797	-2.8804	-0.0438
H	0.9944	3.3291	-0.1157
Br	-2.8460	-1.0134	-0.0203

Moment of Inertia (AMU): 1644.1275 5485.4600 7095.1183

Frequencies (cm**-1):

75 109 112 183 238 265 299 312 401 433 443 496
511 548 558 568 573 623 663 727 740 749 776 806
837 852 857 885 940 962 977 1006 1017 1050 1096 1128
1139 1164 1190 1227 1247 1288 1304 1329 1399 1446 1471 1482
1557 1601 1615 1648 3111 3117 3120 3131 3131 3139 3141

Imaginary Frequency (cm**-1): -963i

4-MBDF

Coordinates (Angstrom)

Atom	X	Y	Z
C	3.3970	-0.2536	0.0001
C	2.4180	-1.2462	0.0000
C	1.0995	-0.8202	-0.0001
C	0.7258	0.5347	-0.0003
C	1.7244	1.5131	-0.0001

C	3.0557	1.1074	0.0001
H	4.4421	-0.5408	0.0002
H	1.4696	2.5668	-0.0003
H	3.8430	1.8521	0.0003
O	-0.0000	-1.6473	-0.0001
C	-1.0995	-0.8202	-0.0000
C	-0.7258	0.5347	-0.0001
C	-2.4180	-1.2462	0.0000
C	-1.7244	1.5131	-0.0000
C	-3.3970	-0.2536	0.0001
C	-3.0557	1.1074	0.0001
H	-4.4422	-0.5408	0.0001
H	-3.8430	1.8521	0.0002
H	2.6678	-2.2997	-0.0001
H	-1.4696	2.5668	-0.0001
H	-2.6678	-2.2997	-0.0001

Moment of Inertia (AMU): 789.1869 3009.0975 3798.2844

Frequencies (cm**-1):

106 151 221 290 314 429 430 441 526 568 571 577
629 671 734 746 758 762 764 860 863 863 864 948
948 984 986 1019 1031 1041 1122 1132 1171 1178 1213 1217
1261 1307 1333 1356 1384 1469 1482 1501 1518 1618 1628 1636
1667 3168 3169 3177 3178 3190 3190 3201 3201

2,2-DBDE

Atom	X	Y	Z
C	2.0241	2.2444	-1.8413
C	0.9125	1.5913	-1.3321
C	1.0754	0.5078	-0.4761
C	2.3552	0.0807	-0.1419
C	3.4687	0.7293	-0.6578
C	3.3032	1.8147	-1.5061
H	1.8892	3.0838	-2.5086
H	-0.0897	1.9048	-1.5915
H	4.4543	0.3806	-0.3862
H	4.1717	2.3194	-1.9042
O	-0.0000	-0.1965	-0.0005
C	-1.0751	0.5079	0.4757
C	-0.9118	1.5913	1.3318
C	-2.3552	0.0811	0.1419
C	-2.0231	2.2444	1.8415
C	-3.4684	0.7297	0.6583
C	-3.3024	1.8150	1.5067
H	0.0905	1.9047	1.5908
H	-1.8879	3.0838	2.5088

H	-4.1707	2.3198	1.9051
Br	-2.5790	-1.3916	-1.0252
H	-4.4541	0.3812	0.3870
Br	2.5784	-1.3921	1.0252

Moment of Inertia (AMU): 3575.8140 8383.1874 9227.8236

Frequencies (cm**-1):

16 51 92 106 132 171 221 221 262 281 351 384
387 398 449 466 504 539 574 579 618 635 661 664
701 751 759 771 834 835 863 863 904 905 919 922
988 989 1010 1011 1070 1098 1114 1117 1128 1140 1269 1275
1305 1310 1414 1420 1421 1433 2755 2755 2762 2763 2771 2771
2778 2778

TS1

Atom	X	Y	Z
C	2.5681	0.9903	2.3264
C	2.9649	0.4073	1.1615
C	2.0381	0.2465	0.0617
C	0.6427	0.5476	0.3426
C	0.2674	1.1251	1.5275
C	1.2225	1.3595	2.5217
H	3.2872	1.1486	3.1174
H	3.9855	0.0970	0.9946
H	-0.7674	1.3896	1.6907
H	0.9175	1.8149	3.4515
Br	2.3307	-1.3636	-0.9766
O	2.4775	1.3647	-1.1169
O	2.3600	2.5495	-0.7029
O	-0.1883	0.2979	-0.6986
C	-1.5029	0.6997	-0.5906
C	-2.4636	-0.1588	-0.0725
C	-1.8599	1.9556	-1.0563
C	-3.7926	0.2388	-0.0203
C	-3.1876	2.3545	-1.0044
H	-1.0835	2.5947	-1.4547
C	-4.1513	1.4962	-0.4872
H	-4.5327	-0.4380	0.3808
H	-3.4687	3.3315	-1.3704
H	-5.1873	1.8014	-0.4481
Br	-1.9541	-1.8653	0.5630

Moment of Inertia (AMU): 4158.5683 8191.0029 9611.3132

Frequencies (cm**-1):

9 22 57 67 101 121 133 136 182 206 233 259
301 306 371 405 437 458 470 506 517 552 604 620
651 696 715 728 753 793 818 855 865 908 951 963
972 983 1011 1021 1037 1092 1111 1127 1142 1170 1221 1234
1248 1265 1278 1294 1395 1419 1438 1474 1517 1563 1603 1609
3114 3119 3122 3125 3131 3137 3138 3144

Imaginary Frequency (cm**-1): -526i

TS_U1

Atom	X	Y	Z
C	2.5436	-1.4036	1.1592
C	2.1833	-0.4965	0.1847
C	0.8325	-0.3153	-0.0916
C	-0.1793	-1.1907	0.4486
C	0.2451	-2.0684	1.5119
C	1.5631	-2.1526	1.8530
H	3.5864	-1.4967	1.4261
H	-0.4878	-2.7228	1.9631
H	1.8844	-2.8336	2.6283
O	0.3854	0.8188	-0.6202
C	-0.8450	1.1547	-0.0946
C	-1.5882	0.0731	0.4146
C	-1.1520	2.4772	0.1624
C	-2.5583	0.3688	1.3957
C	-2.1730	2.7439	1.0582
C	-2.8246	1.6843	1.7084
H	-2.4277	3.7658	1.2968
H	-3.5798	1.8998	2.4518
H	-3.1320	-0.4344	1.8342
Br	-2.7223	-0.9553	-1.2142
H	-0.5484	3.2584	-0.2779
H	-0.7124	-1.7439	-0.3175
Br	3.4666	0.6270	-0.6231

Moment of Inertia (AMU): 3088.3249 8499.3095 9187.3585

Frequencies (cm**-1):

28 74 86 100 140 168 175 226 276 289 333 406
416 484 498 523 559 568 602 631 683 723 741 764
766 805 832 848 888 921 960 964 974 1006 1011 1052
1084 1116 1138 1145 1166 1202 1233 1256 1308 1338 1383 1409
1415 1433 1517 1554 1586 1594 2987 3110 3114 3123 3128 3130
3138 3139

Imaginary Frequency (cm**-1): -527i

TS_U2

Atom	X	Y	Z
C	2.9867	2.2063	0.0667
C	2.1660	1.9571	-1.0143
C	1.1222	1.0612	-0.8450
C	0.9827	0.2108	0.3109
C	1.7738	0.6191	1.4443
C	2.7255	1.5882	1.3143
H	3.7808	2.9335	-0.0179
H	1.6633	0.0645	2.3657
H	3.3287	1.8536	2.1713
O	-0.0002	1.2126	-1.5802
C	-1.1225	1.0613	-0.8447
C	-0.9827	0.2106	0.3110
C	-2.1662	1.9573	-1.0137
C	-1.7737	0.6185	1.4446
C	-2.9868	2.2062	0.0676
C	-2.7254	1.5877	1.3150
H	-3.7808	2.9334	-0.0167
H	-3.3286	1.8528	2.1721
H	-1.6632	0.0636	2.3658
Br	-1.5795	-1.6593	-0.1128
H	-2.2377	2.5214	-1.9329
Br	1.5796	-1.6593	-0.1121
H	2.2373	2.5210	-1.9337

Moment of Inertia (AMU): 3576.8452 4643.6506 6750.1888

Frequencies (cm**-1):

19 82 97 144 149 179 181 237 249 256 355 394
426 467 508 546 568 581 585 600 705 712 736 737
793 800 800 844 894 902 924 924 960 964 998 999
1081 1084 1134 1138 1162 1175 1236 1244 1306 1329 1397 1398
1405 1427 1517 1524 1583 1590 3109 3110 3121 3121 3126 3126
3138 3138

Imaginary Frequency (cm**-1): -420i

TS_H2

Atom	X	Y	Z
C	-2.8726	1.1344	-0.7560
C	-2.4819	2.2272	-1.4973
C	-1.1533	2.6272	-1.3874
C	-0.2725	1.9428	-0.5584

C	-0.7064	0.8404	0.1705
C	-2.0370	0.4290	0.0689
H	-4.2398	0.7110	-0.8615
H	-3.1786	2.7498	-2.1376
H	-0.7966	3.4796	-1.9490
H	0.7578	2.2586	-0.4782
Br	-2.6487	-1.0760	1.0413
H	-5.0635	0.4704	-0.9366
O	0.1039	0.1381	1.0218
C	1.4637	0.3009	0.9038
C	2.1351	1.0380	1.8677
C	2.1750	-0.3094	-0.1247
C	3.5148	1.1735	1.8008
H	1.5547	1.4896	2.6601
C	3.5534	-0.1706	-0.1972
C	4.2221	0.5733	0.7665
H	4.0347	1.7461	2.5555
H	4.0920	-0.6524	-1.0000
H	5.2964	0.6753	0.7089
Br	1.2622	-1.3489	-1.4150

Moment of Inertia (AMU): 3407.5350 7633.8439 7906.9874

Frequencies (cm**-1):

15 28 64 109 120 137 178 188 228 248 261 295
315 397 439 451 460 503 524 564 603 638 649 677
714 747 750 786 848 854 863 882 947 961 963 981
1006 1021 1037 1070 1106 1111 1142 1153 1224 1240 1256 1274
1277 1394 1437 1446 1473 1558 1599 1600 1613 1909 3109 3114
3122 3124 3130 3132 3138

Imaginary Frequency (cm**-1): -1415i

TS_H1

Atom	X	Y	Z
C	1.4552	0.5819	-0.8181
C	2.1840	1.5149	-1.5433
C	3.5670	1.5602	-1.4201
C	4.2253	0.6797	-0.5706
C	3.5008	-0.2620	0.1548
C	2.1272	-0.2934	0.0202
H	1.6470	2.1873	-2.1980
H	4.1297	2.2858	-1.9903
H	5.3014	0.7145	-0.4751
H	3.9963	-0.9656	0.8087
Br	1.0807	-1.7024	1.0315
H	0.0961	-3.0738	1.5818

O	0.0939	0.5161	-0.9938
C	-0.7092	0.9317	0.0366
C	-0.2710	1.7904	1.0371
C	-2.0290	0.4896	0.0418
C	-1.1481	2.1946	2.0345
H	0.7544	2.1323	1.0333
C	-2.9042	0.8977	1.0349
C	-2.4636	1.7526	2.0372
H	-0.7960	2.8597	2.8103
H	-3.9225	0.5379	1.0184
H	-3.1469	2.0659	2.8133
Br	-2.6240	-0.6947	-1.3092

Moment of Inertia (AMU): 3509.9641 7416.6145 7707.0425

Frequencies (cm**-1):

16 26 62 64 115 120 132 164 208 245 256 313
316 405 430 432 467 500 528 569 605 650 675 691
709 747 751 791 846 859 869 937 944 973 980 1001
1019 1027 1043 1101 1119 1138 1144 1206 1231 1253 1259 1276
1285 1432 1438 1460 1477 1584 1600 1606 1617 3111 3112 3120
3122 3127 3129 3134 3137

Imaginary Frequency (cm**-1): -549i

TS_H4

Atom	X	Y	Z
C	-1.0310	2.5101	1.6166
C	-0.2075	1.8441	0.7171
C	-0.7264	0.8227	-0.0700
C	-2.0722	0.4820	0.0516
C	-2.8909	1.1506	0.9457
C	-2.3702	2.1696	1.7337
H	-0.6151	3.3001	2.2259
H	0.8352	2.1139	0.6316
H	-3.9300	0.8650	1.0208
H	-3.0103	2.6874	2.4334
O	0.0064	0.1254	-0.9962
C	1.3792	0.2606	-0.9608
C	1.9813	1.2521	-1.7544
C	2.1327	-0.3419	0.0658
C	3.3351	1.5013	-1.6397
C	3.4875	-0.0891	0.1729
C	4.0924	0.8232	-0.6864
H	1.3604	1.7650	-2.4751
H	3.8025	2.2326	-2.2836
H	5.1517	1.0155	-0.5958

Br	1.2990	-1.5875	1.2098
H	4.0628	-0.6015	0.9300
Br	-2.7829	-0.9151	-1.0083
H	1.5690	-1.1029	-2.1262

Moment of Inertia (AMU): 3429.8192 7444.8002 7969.9713

Frequencies (cm**-1):

12 32 68 117 121 137 186 244 260 292 310 382
393 430 452 482 488 526 532 589 602 645 654 691
724 746 759 789 845 858 874 936 946 973 979 1016
1019 1029 1044 1108 1120 1138 1146 1201 1233 1245 1259 1263
1283 1429 1437 1448 1475 1563 1587 1598 1612 3113 3115 3124
3125 3131 3133 3138 3138

Imaginary Frequency (cm**-1): -880i

TS_H3

Atom	X	Y	Z
C	3.4923	-0.1920	-0.2609
C	2.1119	-0.3201	-0.1660
C	1.4213	0.2845	0.8740
C	2.1248	0.9649	1.8761
C	3.5090	1.1456	1.7418
C	4.1845	0.5540	0.6893
H	4.0123	-0.6703	-1.0776
H	4.0435	1.7209	2.4837
H	5.2552	0.6680	0.5967
O	0.0653	0.1481	1.0138
C	-0.7484	0.8584	0.1674
C	-0.3134	1.9711	-0.5415
C	-2.0737	0.4479	0.0568
C	-1.2001	2.6604	-1.3579
C	-2.9577	1.1399	-0.7547
C	-2.5211	2.2499	-1.4667
H	0.7169	2.2874	-0.4561
H	-0.8509	3.5225	-1.9084
H	-3.2121	2.7848	-2.1021
Br	-2.6651	-1.0747	1.0111
H	-3.9806	0.8003	-0.8266
H	2.0987	-0.3897	3.1846
H	1.5518	1.5142	2.6098
Br	1.1699	-1.3255	-1.4614

Moment of Inertia (AMU): 3428.8316 7521.4101 7766.8585

Frequencies (cm**-1):

16 27 63 117 123 135 185 232 255 288 291 328
354 398 432 462 486 505 528 570 601 649 651 695
733 745 757 793 846 867 882 937 965 973 996 1012
1020 1035 1042 1101 1119 1141 1144 1204 1233 1251 1258 1269
1284 1422 1438 1470 1476 1573 1584 1602 1613 3112 3116 3121
3122 3129 3133 3137 3139

Imaginary Frequency (cm**-1): -753i

TS_H5

Atom	X	Y	Z
C	-1.1922	-0.8538	2.8083
C	-0.3181	-0.2387	1.9173
C	-0.7767	0.1836	0.6813
C	-2.1098	-0.0800	0.3087
C	-3.0028	-0.6020	1.2531
C	-2.5335	-1.0248	2.4837
H	-0.8208	-1.1802	3.7692
H	0.7168	-0.0818	2.1857
H	-4.0416	-0.7110	0.9796
H	-3.2152	-1.4717	3.1928
O	0.0016	0.8081	-0.2488
C	1.3440	0.9535	0.0148
C	1.8064	2.1743	0.4824
C	2.2392	-0.0801	-0.2388
C	3.1637	2.3622	0.7018
C	3.5967	0.1045	-0.0177
C	4.0569	1.3271	0.4536
H	1.0852	2.9598	0.6600
H	3.5217	3.3158	1.0629
H	5.1153	1.4681	0.6208
Br	1.6012	-1.7363	-0.8896
H	4.2810	-0.7059	-0.2220
Br	-2.8188	0.7707	-1.2466
H	-1.6836	-1.6145	-0.5809

Moment of Inertia (AMU): 3457.7384 8016.7805 8161.0261

Frequencies (cm**-1):

26 32 66 109 122 137 188 245 261 289 310 370
423 439 461 473 488 506 545 567 609 643 650 714
723 743 752 793 848 864 869 934 948 974 982 1009
1020 1036 1041 1109 1116 1141 1143 1200 1237 1255 1258 1274
1277 1427 1437 1459 1473 1578 1585 1600 1610 3115 3115 3124
3125 3133 3133 3139 3141

Imaginary Frequency (cm**-1): -870i

TS_H4

Atom	X	Y	Z
C	0.6151	2.9738	0.0281
C	-0.0353	1.8709	-0.4953
C	0.6223	0.6354	-0.6437
C	1.9735	0.5728	-0.2476
C	2.6294	1.6741	0.2760
C	1.9459	2.8753	0.4239
H	0.0895	3.9139	0.1218
H	-1.0622	1.9287	-0.8296
H	3.6698	1.5915	0.5546
H	2.4603	3.7339	0.8321
O	-0.0040	-0.4003	-1.1785
C	-1.0020	-1.3977	-0.0273
C	-0.0350	-1.8711	0.9218
C	-1.9714	-0.4689	0.4693
C	0.1575	-1.2021	2.1033
C	-1.7851	0.1974	1.6498
C	-0.6912	-0.1448	2.4608
H	0.5981	-2.6972	0.6380
H	0.9548	-1.4987	2.7700
H	-0.5293	0.3931	3.3834
Br	-3.4335	-0.0378	-0.6484
H	-2.4789	0.9656	1.9585
Br	2.9504	-1.0297	-0.5142
H	-1.3045	-2.0588	-0.8243

Moment of Inertia (AMU): 2840.4580 7927.1100 8738.5965

Frequencies (cm**-1):

28 56 66 76 126 152 188 215 260 284 304 315
400 448 465 487 517 555 584 638 641 664 713 724
762 814 840 859 928 945 963 969 978 992 1013 1016
1034 1049 1069 1110 1123 1139 1149 1232 1251 1267 1284 1285
1396 1424 1442 1443 1515 1560 1564 1588 3109 3117 3120 3128
3128 3135 3137 3138 3150

Imaginary Frequency (cm**-1): -559i

TS2_Br

Atom	X	Y	Z
C	0.4922	-0.1493	2.4179
C	0.0233	-1.0478	1.4971
C	-0.9096	-0.6321	0.4888
C	-1.5808	0.6205	0.7020
C	-1.1009	1.5075	1.6311
C	-0.0459	1.1425	2.4781
H	1.2652	-0.4486	3.1113
H	0.4035	-2.0549	1.4412
H	-1.5509	2.4862	1.7106
H	0.3279	1.8568	3.1965
O	0.1761	-0.2476	-0.9296
C	1.0844	0.6947	-0.7349
C	0.7619	2.0508	-0.9303
C	2.4138	0.3895	-0.3769
C	1.7083	3.0452	-0.7612
C	3.3640	1.3819	-0.2071
C	3.0079	2.7134	-0.3894
H	-0.2481	2.2805	-1.2411
H	1.4386	4.0789	-0.9267
H	3.7527	3.4857	-0.2580
Br	2.9406	-1.4215	-0.2060
H	4.3765	1.1108	0.0537
Br	-2.9713	1.1631	-0.4462
Br	-1.8689	-2.0592	-0.3347

Moment of Inertia (AMU): 4644.1293 8684.239511129.2585

Frequencies (cm**-1):

25 53 59 70 117 129 138 155 192 222 248 289
310 356 366 409 448 468 488 529 561 605 638 646
687 711 725 764 830 838 858 929 946 968 977 992
1004 1014 1033 1037 1105 1106 1129 1139 1220 1231 1234 1265
1274 1387 1400 1424 1439 1507 1550 1564 1586 3109 3120 3121
3128 3129 3136 3141 3159

Imaginary Frequency (cm**-1): -584i

Table S1: Zero-point corrections (M052X/6-311+G(d,p)) and single-point energies (M052X/GTLarge). All values are in Hartress.

Structure	Zero-point correction	Single Point energies	Structure	Zero-point correction	Single Point energies
O_2	0.004035	-150.3524698	**TS10**	0.166334	-3261.863624
H	0.000	-0.4992931	**TS12**	0.169604	-3261.8274
H2	0.010332	-1.1698001	**TS14**	0.166301	-3186.59376
Br2	0.000773	-5148.211687	**TS13**	0.168083	-3186.697265
OH	0.008663	-75.7488401	**M11**	0.172794	-3261.882947
HBr	0.006111	-2574.711367	**M13**	0.170433	-3186.728362
OBr	0.00161	-2649.230192	**M12**	0.170625	-3186.756127
O	0.000	-75.0805261	**TS16**	0.165369	-3186.649973
Br	0.000	-2574.065971	**M7**	0.168975	-3186.74183
M1	0.17337	-3261.881659	**1-MBDD**	0.159925	-3186.183607
TS5	0.17227	-3261.853714	**DD**	0.169971	-612.6730522
TS6	0.171073	-3261.838647	**M2**	0.164539	-3111.455228
TS7	0.171127	-3261.806873	**2,2-DBDE**	0.16741	-5685.656838
M4	0.173471	-3261.873373	**TS1**	0.170997	-5835.942784
M8	0.172039	-3261.853182	**M14**	0.166337	-3186.656259
M8	0.172625	-3261.92029	**TS2**	0.163673	-3111.437561
M9	0.174719	-3261.938695	**TS3**	0.163654	-3111.431003
M10	0.174623	-3261.98323	**4-MBDF**	0.156577	-3110.963411
M3	0.165261	-3111.487554	**TS22**	0.172811	-3261.904153
TS9	0.171647	-3261.885466	**TS21**	0.17333	-3261.891548
TS11	0.169946	-3261.887826	**TS8**	0.170046	-3261.847271
TS19	0.170089	-3261.84551	**M18**	0.174648	-3261.948027
M18	0.174648	-3261.948027	**M20**	0.174124	-3261.924419
DF	0.166793	-537.4522146	**M19**	0.174932	-687.851143
TS20	0.171599	-3261.879996	**TS_H2**	0.164309	-5686.125725
TS2_Br	0.164852	-8259.693083	**TS_H3**	0.16938	-5686.142764
TS1_Br	0.157039	-8259.68462	**TS_H1**	0.167866	-5686.142447
M21	0.15443	-5684.966848	**TS_H4**	0.169001	-5686.146212
M22	0.177287	-5686.199592	**TS_U1**	0.164443	-5685.524547
TS_H6	0.175851	-5686.1877	**M23**	0.176268	-5686.201951
TS_H5	0.169547	-5686.143698	**TS_U2**	0.163896	-5685.4959

Polynomial NASA coefficients

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THERMO
M3              H   8C  12O   1Br  1g    300.00   5000.00 1000.00     1
 2.69832922E+01 3.62122535E-02-1.45005877E-05 2.64003053E-09-1.79844397E-13    2
-2.13082871E+04-1.16083730E+02-8.62865165E+00 1.40900443E-01-1.26629755E-04    3
 5.14897938E-08-6.07011277E-12-1.17294692E+04 6.64431694E+01                  4
END
C1              H   8C  12O   3Br  1g    300.00   5000.00 1000.00     1
 3.15407690E+01 3.75727034E-02-1.50341200E-05 2.73597560E-09-1.86330482E-13    2
-1.38096018E+04-1.33318130E+02-6.29269861E+00 1.49308448E-01-1.35443791E-04    3
 5.57347295E-08-6.77439468E-12-3.67173215E+03 6.04372423E+01                  4
END
M1              H   8C  12O   3Br  1g    300.00   5000.00 1000.00     1
 3.20031169E+01 3.71140045E-02-1.48489439E-05 2.70209609E-09-1.84015368E-13    2
-2.43566072E+04-1.38184302E+02-7.93903789E+00 1.60374644E-01-1.58278196E-04    3
 7.57988825E-08-1.32671806E-11-1.39243016E+04 6.50472582E+01                  4
END
M5              H   8C  12O   3Br  1g    300.00   5000.00 1000.00     1
 3.20031169E+01 3.71140045E-02-1.48489439E-05 2.70209609E-09-1.84015368E-13    2
-2.43566072E+04-1.38184302E+02-7.93903789E+00 1.60374644E-01-1.58278196E-04    3
 7.57988825E-08-1.32671806E-11-1.39243016E+04 6.50472582E+01                  4
END
M17             H   8C  12O   3Br  1g    300.00   5000.00 1000.00     1
 3.20031170E+01 3.71140044E-02-1.48489439E-05 2.70209608E-09-1.84015368E-13    2
-2.41553155E+04-1.38324111E+02-7.93903748E+00 1.60374642E-01-1.58278192E-04    3
 7.57988786E-08-1.32671793E-11-1.37230098E+04 6.49074471E+01                  4
END
M12             H   8C  12O   2Br  1g    300.00   5000.00 1000.00     1
 2.90202900E+01 3.71898847E-02-1.49022577E-05 2.71449222E-09-1.84983253E-13    2
-5.36685215E+03-1.26274979E+02-8.51420064E+00 1.48531351E-01-1.36212772E-04    3
 5.75639604E-08-7.62791817E-12 4.67788290E+03 6.58567919E+01                  4
END
M7              H   8C  12O   2Br  1g    300.00   5000.00 1000.00     1
 2.93176027E+01 3.67518494E-02-1.46886395E-05 2.67093985E-09-1.81795640E-13    2
-2.49713921E+04-1.23310589E+02-6.70942183E+00 1.42668116E-01-1.27985265E-04    3
 5.18071088E-08-6.00442231E-12-1.52876487E+04 6.13266937E+01                  4
END
M2              H   8C  12O   1Br  1g    300.00   5000.00 1000.00     1
 2.71710822E+01 3.58461692E-02-1.43066218E-05 2.59893769E-09-1.76771319E-13    2
-1.21973304E+04-1.12940412E+02-7.15243564E+00 1.36378843E-01-1.21000375E-04    3
 4.79840254E-08-5.16752367E-12-2.95372946E+03 6.30553841E+01                  4
END
M4              H   8C  12O   3Br  1g    300.00   5000.00 1000.00     1
 3.21150537E+01 3.70118886E-02-1.48105935E-05 2.69548258E-09-1.83584512E-13    2
-9.69083206E+03-1.40200577E+02-9.92882363E+00 1.70164258E-01-1.76060847E-04    3
 9.02425781E-08-1.76868000E-11 1.10913962E+03 7.28562150E+01                  4
END
M11             H   8C  12O   3Br  1g    300.00   5000.00 1000.00     1
```

3.24851769E+01 3.63414639E-02-1.44666150E-05 2.62404610E-09-1.78314892E-13 2
-1.55408028E+04-1.39459882E+02-7.86199522E+00 1.64190220E-01-1.69423791E-04 3
8.68906336E-08-1.70832935E-11-5.18152085E+03 6.49792197E+01 4
END
M9 H 8C 12O 3Br 1g 300.00 5000.00 1000.00 1
3.15243557E+01 3.77519254E-02-1.51488494E-05 2.76216074E-09-1.88367353E-13 2
-2.62291774E+04-1.39572306E+02-9.87099088E+00 1.64587161E-01-1.60940185E-04 3
7.54847921E-08-1.26597600E-11-1.53736993E+04 7.12742367E+01 4
END
M20 H 8C 12O 3Br 1g 300.00 5000.00 1000.00 1
3.08310710E+01 3.81044691E-02-1.52077861E-05 2.76307106E-09-1.87971725E-13 2
-3.86967210E+04-1.34950652E+02-9.23142735E+00 1.59833169E-01-1.53014511E-04 3
6.95656682E-08-1.09480116E-11-2.81438897E+04 6.93495353E+01 4
END
1-MBDD H 7C 12O 2Br 1g 300.00 5000.00 1000.00 1
2.83856576E+01 3.49689332E-02-1.40388860E-05 2.56063723E-09-1.74666289E-13 2
-1.92275011E+04-1.21424613E+02-7.63421164E+00 1.41415913E-01-1.29425073E-04 3
5.43684939E-08-7.11633351E-12-9.56338400E+03 6.30670580E+01 4
END
DF H 8C 12O 1 0g 300.00 5000.00 1000.00 1
2.33365586E+01 3.67162488E-02-1.46689038E-05 2.66657999E-09-1.81458673E-13 2
-5.45456797E+03-1.01846997E+02-1.05711959E+01 1.33291202E-01-1.11872765E-04 3
3.91154096E-08-2.18613596E-12 3.82471557E+03 7.27206591E+01 4
END
4-MBDF H 7C 12O 1Br 1g 300.00 5000.00 1000.00 1
2.52995437E+01 3.48121721E-02-1.39146566E-05 2.53062237E-09-1.72274668E-13 2
-1.81756852E+04-1.07613755E+02-7.45631708E+00 1.27083610E-01-1.04725524E-04 3
3.46337633E-08-1.06874450E-12-9.16155386E+03 6.12768660E+01 4
END
M10 H 8C 12O 3Br 1g 300.00 5000.00 1000.00 1
3.20047810E+01 3.68695022E-02-1.46936330E-05 2.66732462E-09-1.81357122E-13 2
-4.10102884E+04-1.40805398E+02-8.76227121E+00 1.64031583E-01-1.64786947E-04 3
8.07679055E-08-1.46787090E-11-3.04498936E+04 6.62413575E+01 4
END
M18 H 8C 12O 3Br 1g 300.00 5000.00 1000.00 1
3.07513134E+01 3.82080316E-02-1.52564852E-05 2.77287481E-09-1.88686043E-13 2
-3.25750423E+04-1.36011311E+02-9.41055716E+00 1.58832183E-01-1.48760080E-04 3
6.45722745E-08-9.04449266E-12-2.19352912E+04 6.91196161E+01 4
END
M13 H 8C 12O 2Br 1g 300.00 5000.00 1000.00 1
2.87620566E+01 3.72992705E-02-1.49090903E-05 2.71124664E-09-1.84550158E-13 2
-5.23158146E+03-1.21880313E+02-7.21189119E+00 1.42039000E-01-1.25081369E-04 3
4.88490547E-08-5.01118611E-12 4.49579643E+03 6.27545470E+01 4
END
M8 H 8C 12O 3Br 1g 300.00 5000.00 1000.00 1
3.21476758E+01 3.69561570E-02-1.47815958E-05 2.68934120E-09-1.83123552E-13 2
-4.25202797E+03-1.37008423E+02-7.63141524E+00 1.59632201E-01-1.57283529E-04 3
7.50431466E-08-1.30283997E-11 6.13874830E+03 6.54060694E+01 4
END
M6 H 8C 12O 3Br 1g 300.00 5000.00 1000.00 1
3.23747223E+01 3.67269488E-02-1.46883442E-05 2.67222007E-09-1.81951781E-13 2

5.63097835E+03-1.40417834E+02-8.91842766E+00 1.66949877E-01-1.71264851E-04 3
8.66729170E-08-1.66323684E-11 1.62634226E+04 6.89650529E+01 4
END
TS2 H 8C 12O 1Br 1g 300.00 5000.00 1000.00 1
2.64631281E+01 3.55728907E-02-1.42004131E-05 2.57999458E-09-1.75499584E-13 2
-7.09793911E+03-1.12612496E+02-8.58803594E+00 1.39974324E-01-1.28407396E-04 3
5.43538873E-08-7.18272612E-12 2.24963549E+03 6.66723119E+01 4
END
TS_U2 H 8C 12O 1Br 2g 300.00 5000.00 1000.00 1
2.90693154E+01 3.57219079E-02-1.42016272E-05 2.57334830E-09-1.74731033E-13 2
3.69637176E+04-1.22231534E+02-6.36034738E+00 1.42120036E-01-1.31954255E-04 3
5.70227698E-08-7.92856949E-12 4.63542797E+04 5.87394102E+01 4
END
TS_U1 H 8C 12O 1Br 2g 300.00 5000.00 1000.00 1
2.87137650E+01 3.61433027E-02-1.43888206E-05 2.60961920E-09-1.77303361E-13 2
2.81821926E+04-1.19798482E+02-5.66278397E+00 1.36317939E-01-1.19420195E-04 3
4.59380511E-08-4.36205058E-12 3.74567787E+04 5.65746630E+01 4
END
TS16 H 8C 12O 2Br 1g 300.00 5000.00 1000.00 1
2.94713398E+01 3.55093350E-02-1.41609855E-05 2.57115242E-09-1.74819933E-13 2
2.75845260E+03-1.23670441E+02-7.53719273E+00 1.50286473E-01-1.48694976E-04 3
7.18539469E-08-1.27829691E-11 1.23944785E+04 6.44874686E+01 4
END
TS_H4 H 9C 12O 1Br 2g 300.00 5000.00 1000.00 1
3.07410042E+01 3.71076895E-02-1.47795139E-05 2.68141155E-09-1.82229325E-13 2
1.73623209E+04-1.29573218E+02-5.89416220E+00 1.46273057E-01-1.34387292E-04 3
5.72026215E-08-7.71951898E-12 2.71303519E+04 5.78054526E+01 4
END
TS_H5 H 9C 12O 1Br 2g 300.00 5000.00 1000.00 1
3.08071361E+01 3.70382078E-02-1.47501229E-05 2.67583901E-09-1.81838101E-13 2
1.64167053E+04-1.28736617E+02-4.88830810E+00 1.41884363E-01-1.26621251E-04 3
5.08931387E-08-5.77160909E-12 2.60122932E+04 5.42161010E+01 4
END
TS9 H 8C 12O 3Br 1g 300.00 5000.00 1000.00 1
3.13483513E+01 3.67841365E-02-1.47196626E-05 2.67897421E-09-1.82462682E-13 2
-1.48783890E+04-1.38198761E+02-1.02113030E+01 1.67251608E-01-1.70282596E-04 3
8.49208503E-08-1.58657256E-11-4.15352280E+03 7.26679569E+01 4
END
TS20 H 8C 12O 3Br 1g 300.00 5000.00 1000.00 1
3.05427477E+01 3.73968993E-02-1.49218077E-05 2.71071285E-09-1.84392333E-13 2
-1.19409435E+04-1.34846534E+02-9.51272836E+00 1.59223253E-01-1.52488129E-04 3
6.87188473E-08-1.04923081E-11-1.41534546E+03 6.93397613E+01 4
END
TS11 H 8C 12O 3Br 1g 300.00 5000.00 1000.00 1
3.27982921E+01 3.55372525E-02-1.42666882E-05 2.60231098E-09-1.77520915E-13 2
-1.18234831E+04-1.41082156E+02-5.82980331E+00 1.52391477E-01-1.46057096E-04 3
6.64042948E-08-1.05104862E-11-1.60757190E+03 5.60703993E+01 4
END
TS22 H 8C 12O 3Br 1g 300.00 5000.00 1000.00 1
2.98366593E+01 3.80498093E-02-1.51721199E-05 2.75480178E-09-1.87320722E-13 2
-3.23062340E+04-1.27964435E+02-7.01002579E+00 1.45657796E-01-1.28859526E-04 3

5.07740471E-08-5.37671488E-12-2.23666321E+04 6.10515837E+01 4
END
TS12 H 8C 12O 3Br 1g 300.00 5000.00 1000.00 1
3.12998467E+01 3.70771522E-02-1.48995146E-05 2.71922355E-09-1.85555500E-13 2
-2.99775758E+03-1.36807515E+02-8.09823721E+00 1.56526841E-01-1.50494122E-04 3
6.93015773E-08-1.13246096E-11 7.42331926E+03 6.42437558E+01 4
END
TS10 H 8C 12O 3Br 1g 300.00 5000.00 1000.00 1
3.25526252E+01 3.59399825E-02-1.44702316E-05 2.64453809E-09-1.80642945E-13 2
-9.59042894E+03-1.43364742E+02-9.08923752E+00 1.64657998E-01-1.64763145E-04 3
7.98410133E-08-1.42587678E-11 1.27430124E+03 6.84639217E+01 4
END
TS5 H 8C 12O 3Br 1g 300.00 5000.00 1000.00 1
3.10445744E+01 3.70662517E-02-1.48280118E-05 2.69806967E-09-1.83731071E-13 2
-5.84441788E+03-1.35300400E+02-8.55352120E+00 1.58575713E-01-1.54824888E-04 3
7.27859558E-08-1.22827387E-11 4.53072882E+03 6.63464573E+01 4
END
TS14 H 8C 12O 2Br 1g 300.00 5000.00 1000.00 1
2.84348906E+01 3.66417649E-02-1.46460128E-05 2.66338000E-09-1.81291048E-13 2
-1.34956442E+04-1.22309357E+02-8.09219257E+00 1.44697611E-01-1.31386481E-04 3
5.42701093E-08-6.66987406E-12-3.71808820E+03 6.47075723E+01 4
END
TS13 H 8C 12O 2Br 1g 300.00 5000.00 1000.00 1
2.87756168E+01 3.62733491E-02-1.44894255E-05 2.63377138E-09-1.79222168E-13 2
-1.17497579E+04-1.24424734E+02-8.36188204E+00 1.48498270E-01-1.40425429E-04 3
6.26847568E-08-9.47458415E-12-1.93036864E+03 6.51250086E+01 4
END
TS7 H 8C 12O 3Br 1g 300.00 5000.00 1000.00 1
3.13401343E+01 3.67378794E-02-1.46862784E-05 2.67101106E-09-1.81828195E-13 2
8.36018744E+03-1.34806157E+02-7.89343158E+00 1.57499485E-01-1.54484526E-04 3
7.32054628E-08-1.25414847E-11 1.86194515E+04 6.48879983E+01 4
END
TS21 H 8C 12O 3Br 1g 300.00 5000.00 1000.00 1
2.95578074E+01 3.83963292E-02-1.53295451E-05 2.78569597E-09-1.89529455E-13 2
-2.81360617E+04-1.26270242E+02-6.68696800E+00 1.41751233E-01-1.19536780E-04 3
4.20635253E-08-2.46732149E-12-1.82294302E+04 6.02861470E+01 4
END
TS8 H 8C 12O 3Br 1g 300.00 5000.00 1000.00 1
3.15849693E+01 3.65038440E-02-1.45941759E-05 2.65445810E-09-1.80711511E-13 2
-2.23427057E+03-1.37429581E+02-8.68954994E+00 1.62554218E-01-1.64414689E-04 3
8.15997124E-08-1.51767418E-11 8.18707716E+03 6.70332954E+01 4
END
TS19 H 8C 12O 3Br 1g 300.00 5000.00 1000.00 1
3.08891728E+01 3.69952064E-02-1.47443929E-05 2.67636751E-09-1.81954894E-13 2
-2.55121823E+03-1.33787078E+02-8.34066271E+00 1.56624524E-01-1.50518057E-04 3
6.84840554E-08-1.07092081E-11 7.74431240E+03 6.61190105E+01 4
END
TS6 H 8C 12O 3Br 1g 300.00 5000.00 1000.00 1
3.10894782E+01 3.69978241E-02-1.47939147E-05 2.69101323E-09-1.83208976E-13 2
-1.27657706E+03-1.31804717E+02-6.63452359E+00 1.49652998E-01-1.38572066E-04 3
5.93335109E-08-8.07377695E-12 8.76516368E+03 6.10711414E+01 4

END
TS1_Br H 8C 12O 1Br 3g 300.00 5000.00 1000.00 1
3.28090042E+01 3.51629847E-02-1.40186451E-05 2.54483984E-09-1.73010397E-13 2
9.34470990E+03-1.35026190E+02-3.58660349E+00 1.46938488E-01-1.42758961E-04 3
6.67816710E-08-1.11387119E-11 1.88706714E+04 5.02742868E+01 4
END
TS2_Br H 8C 12O 1Br 3g 300.00 5000.00 1000.00 1
3.41145268E+01 3.42948294E-02-1.37789876E-05 2.51453954E-09-1.71583787E-13 2
1.09855395E+04-1.38967388E+02-3.48396859E+00 1.48947475E-01-1.44773253E-04 3
6.73450679E-08-1.11540648E-11 2.08810923E+04 5.26972684E+01 4
END
TS_H3 H 9C 12O 1Br 2g 300.00 5000.00 1000.00 1
3.07861812E+01 3.70653293E-02-1.47630372E-05 2.67847207E-09-1.82031985E-13 2
1.76015407E+04-1.29177010E+02-5.91032156E+00 1.46517470E-01-1.34854407E-04 3
5.75535881E-08-7.81495742E-12 2.73793951E+04 5.84863506E+01 4
END
TS_H1 H 9C 12O 1Br 2g 300.00 5000.00 1000.00 1
3.17362656E+01 3.64788256E-02-1.46178805E-05 2.66304094E-09-1.81503679E-13 2
2.10671835E+04-1.33075577E+02-4.15633056E+00 1.40236552E-01-1.22659788E-04 3
4.71798137E-08-4.61707455E-12 3.08210985E+04 5.13566613E+01 4
END
TS_H2 H 9C 12O 1Br 2g 300.00 5000.00 1000.00 1
3.09586184E+01 3.68731405E-02-1.46791595E-05 2.66228097E-09-1.80882617E-13 2
1.72762319E+04-1.27367787E+02-3.65998421E+00 1.37163211E-01-1.18881804E-04 3
4.48938714E-08-3.97300901E-12 2.66539875E+04 5.04143276E+01 4
END