Elevated Reaction Order of 1,3,5-tri-*tert*-butylbenzene Bromination as Evidence of Clustered Polybromide Transition State: a Combined Kinetic and Computational Study

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Electronic Supplementary Information
(See also data repository, DOI: 10.14469/hpc/4748)

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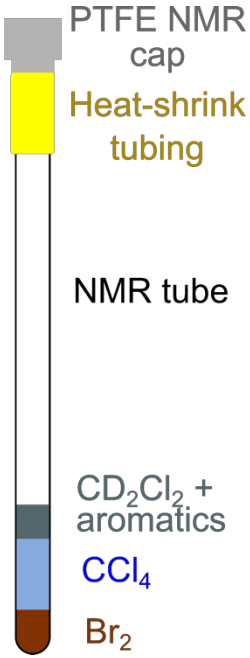
Experimental conditions of the bromination

Run	N	Aromatics	Temperature °C	Volume, mL				$[Br_2]_0$ mol/L	$[Aromatics]_0$ mol/L	Kinetics [c]
				Br_2	CCl_4	CD_2Cl_2	Aromatics			
1	1777	1,3,5-tri-t-Bu-benzene	23	0.10	0.28	0.1	20 mg	3.9	0.16	see p. S5
2	1782	1,3,5-tri-t-Bu-benzene	25	0.15	0.23	0.1	21 mg	5.8	0.17	see p. S6
3	1784	1,3,5-tri-t-Bu-benzene	27	0.20	0.18	0.1	21 mg	7.8	0.17	see p. S7
4	1790	1,3,5-tri-t-Bu-benzene	24	0.30	0.09	0.1	8.0 mg	11.6	0.065	see p. S8
5	1785	1,3,5-tri-t-Bu-benzene	0	0.15	0.23	0.1	21 mg	5.8	0.17	see p. S9
6	1780	1,3,5-tri-t-Bu-benzene	26	0.10	0.30	0.1	5.9 mg	3.9	0.048	see p. S10
7	1781	1,3,5-tri-t-Bu-benzene-d_3	26	0.10	0.30	0.1	6.4 mg	3.9	0.051	see p. S11
8	1912	1,3,5-tri-t-Bu-benzene [a]	20	0.10	0.30	0.1	7.4 mg	3.9	0.059	see p. S12
9	1913	1,3,5-tri-t-Bu-benzene [b]	21	0.10	0.30	0.1	8 mg	3.9	0.06	see p. S13
10										

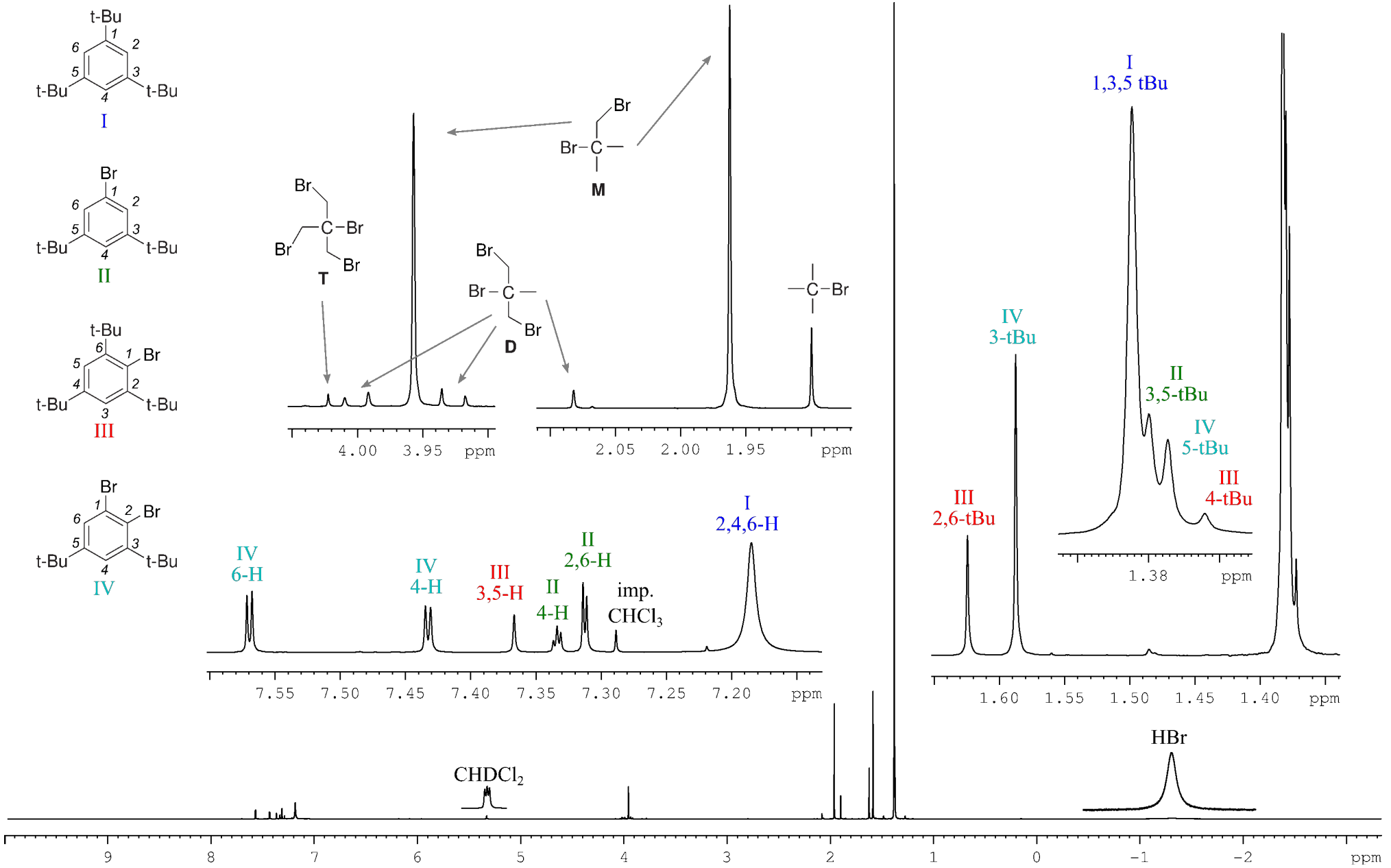
[a] CH_2Cl_2 instead of CCl_4; with $Bu_4N^+Br^-$ (9.0 mg, 0.056 mol/L)

[b] CH_2Cl_2 instead of CCl_4

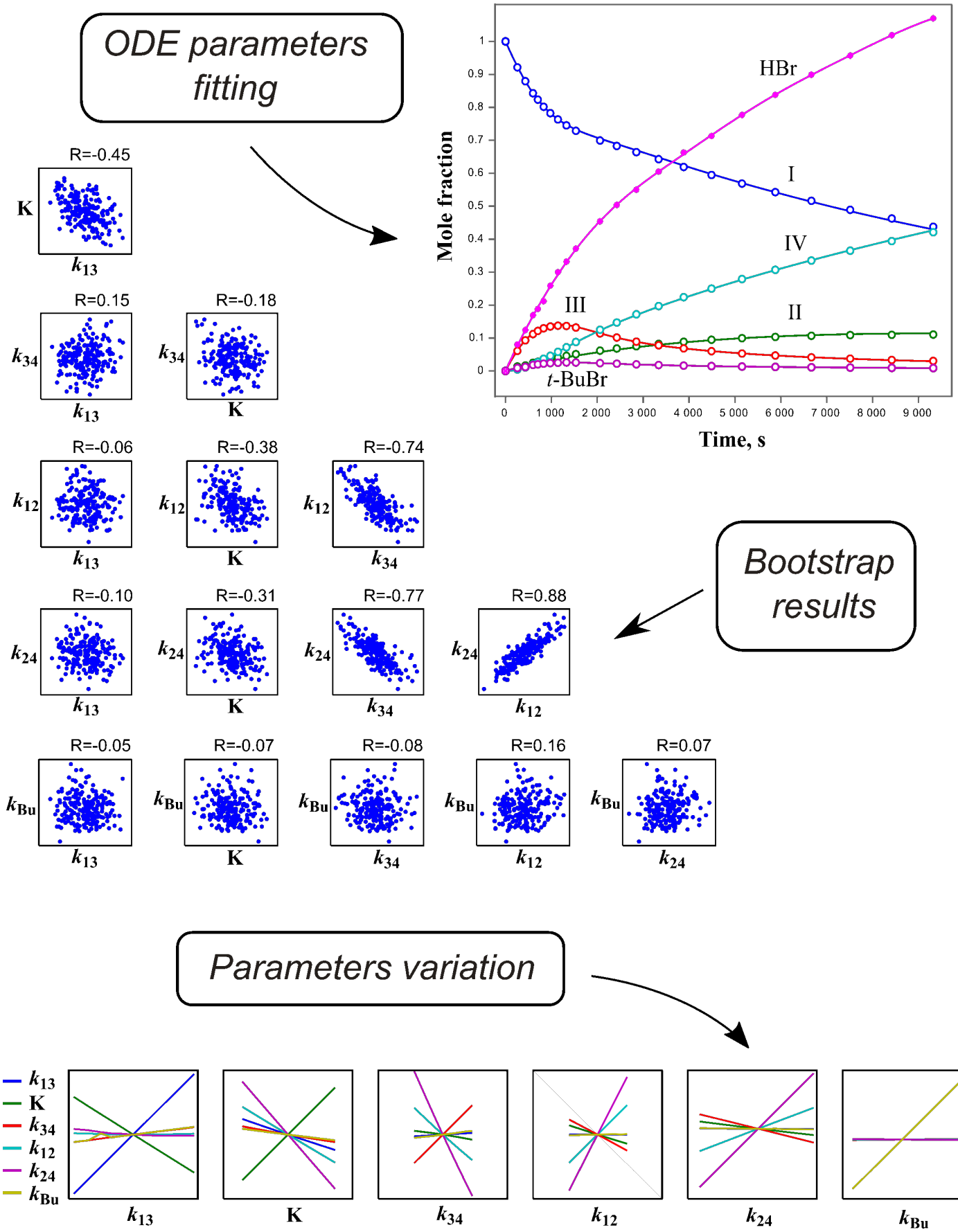
[c] True equilibrium constant of reaction I+Br_2=III+HBr is derived from the kinetic data by formula $K=K13*[Aromatics]_0/[Br_2]_0$



^{1}H NMR spectrum (600 MHz) of the reaction mixture (Br_2 (0.20 mL), CD_2Cl_2 (0.1 mL), CCl_4 (0.18 mL) and **I** (22 mg)) after 10 min at 27 °C.



Graphics from kinetics treatment program. *ODE parameters fitting*: circles are experimental concentrations, curves are ODE solution with optimized parameters. *Bootstrap results*: correlation of the parameters given by bootstrap Monte-Carlo method. *Parameters variation*: sensitivity of the parameters to variations of one of them (constant chi-square boundaries as confidence limits).



Data: 1777_data.txt
Experimental conditions see p. S2

HBr SSD: 3.080769e-03

time, s	I	II	III	IV	tBuBr	HBr
0	1	0	0	0	0	0
244	0.9857	0.0017	0.0125	0.0000	0.0010	0.0050
397	0.9777	0.0021	0.0195	0.0000	0.0016	0.0100
524	0.9707	0.0028	0.0260	0.0010	0.0016	0.0150
726	0.9603	0.0035	0.0355	0.0000	0.0021	0.0300
1189	0.9370	0.0050	0.0560	0.0020	0.0031	0.0320
1256	0.9350	0.0050	0.0585	0.0010	0.0032	0.0340
1383	0.9293	0.0054	0.0635	0.0020	0.0034	0.0470
2090	0.8987	0.0075	0.0895	0.0050	0.0049	0.1040
2756	0.8727	0.0093	0.1095	0.0080	0.0061	0.1540
3482	0.8510	0.0111	0.1255	0.0120	0.0071	0.1740
4268	0.8320	0.0132	0.1380	0.0170	0.0079	0.1920
5114	0.8160	0.0149	0.1465	0.0230	0.0086	0.2240
6020	0.8030	0.0173	0.1510	0.0290	0.0091	0.2420
6986	0.7930	0.0190	0.1520	0.0360	0.0096	0.2670
8011	0.7853	0.0211	0.1505	0.0430	0.0096	0.2690
9097	0.7793	0.0234	0.1470	0.0500	0.0094	0.2850
10243	0.7733	0.0255	0.1425	0.0590	0.0092	0.2960
11449	0.7693	0.0275	0.1370	0.0660	0.0091	0.3160
12715	0.7653	0.0292	0.1310	0.0740	0.0088	0.3240
14041	0.7600	0.0319	0.1250	0.0830	0.0084	0.3290
15427	0.7553	0.0339	0.1190	0.0910	0.0083	0.3490
16873	0.7507	0.0362	0.1140	0.0990	0.0080	0.3650
18379	0.7453	0.0383	0.1085	0.1080	0.0077	0.3790
19945	0.7393	0.0403	0.1035	0.1170	0.0073	0.3960
21571	0.7337	0.0427	0.0990	0.1250	0.0071	0.4090
23257	0.7280	0.0444	0.0945	0.1330	0.0069	0.4200
25003	0.7213	0.0464	0.0900	0.1420	0.0067	0.4420
26809	0.7147	0.0481	0.0860	0.1510	0.0064	0.4510
28675	0.7080	0.0501	0.0825	0.1600	0.0061	0.4680
30601	0.7003	0.0518	0.0795	0.1680	0.0061	0.4800
32587	0.6927	0.0539	0.0760	0.1770	0.0059	0.4930
34633	0.6860	0.0552	0.0730	0.1860	0.0057	0.5100
36740	0.6790	0.0566	0.0700	0.1940	0.0056	0.5310
38906	0.6710	0.0583	0.0670	0.2030	0.0053	0.5340
41132	0.6637	0.0593	0.0645	0.2120	0.0053	0.5540
43418	0.6557	0.0607	0.0620	0.2210	0.0051	0.5680
45764	0.6480	0.0618	0.0595	0.2300	0.0050	0.5890
48170	0.6390	0.0635	0.0580	0.2400	0.0047	0.5930
50637	0.6313	0.0642	0.0560	0.2480	0.0043	0.6090

k13	5.159558e-05	*
K13	5.754612e-02	*
k34	4.334222e-05	*
k12	3.011869e-06	*
k24	2.137391e-05	*
kBu	9.419645e-04	*

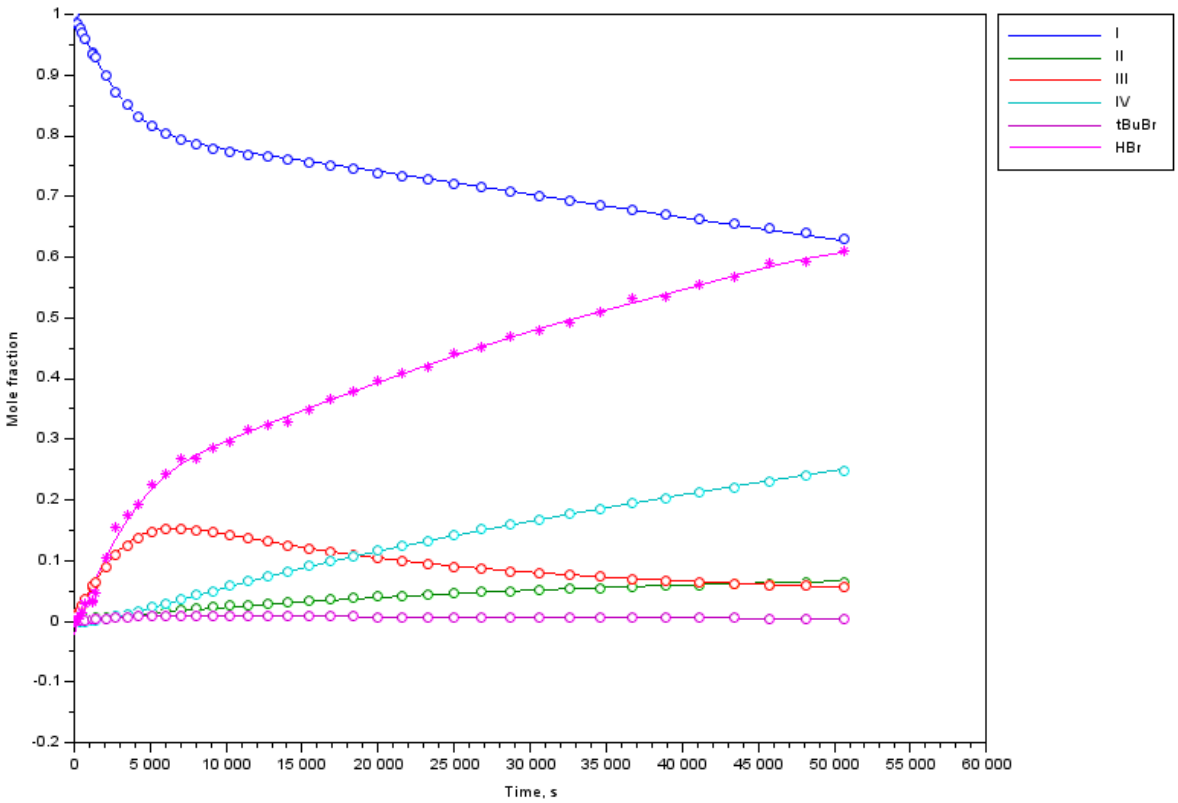
SSD (sum of squares): 3.571669e-04
Standard deviation: 1.356859e-03

Use of constant chi-square boundaries as confidence limits
nsigma=3

k13	5.159558e-05 +/- 5.6e-07 (1.1%)
K13	5.754612e-02 +/- 4.5e-04 (0.8%)
k34	4.334222e-05 +/- 8.0e-07 (1.8%)
k12	3.011869e-06 +/- 1.1e-07 (3.6%)
k24	2.137391e-05 +/- 2.2e-06 (10.2%)
kBu	9.419645e-04 +/- 9.7e-05 (10.3%)

Confidence limits by Monte Carlo simulation (bootstrap method)
200 synthetic data sets, nsigma = 3

k13	5.158390e-05 +/- 5.7e-07 (1.1%)
K13	5.753813e-02 +/- 4.6e-04 (0.8%)
k34	4.338455e-05 +/- 7.5e-07 (1.7%)
k12	3.008495e-06 +/- 1.0e-07 (3.4%)
k24	2.130420e-05 +/- 2.0e-06 (9.6%)
kBu	9.630378e-04 +/- 1.0e-04 (10.9%)



Data: 1782_data.txt
Experimental conditions see p. S2

time, s	I	II	III	IV	tBuBr	HBr
0	1	0	0	0	0	0
258	0.9213	0.0131	0.0610	0.0050	0.0091	0.0800
431	0.8793	0.0166	0.0930	0.0110	0.0122	0.1240
598	0.8427	0.0248	0.1120	0.0200	0.0184	0.1690
704	0.8233	0.0279	0.1215	0.0270	0.0202	0.1880
830	0.8017	0.0320	0.1295	0.0370	0.0223	0.2120
976	0.7823	0.0361	0.1350	0.0460	0.0239	0.2590
1142	0.7633	0.0409	0.1375	0.0580	0.0250	0.3000
1327	0.7453	0.0459	0.1365	0.0720	0.0258	0.3320
1533	0.7287	0.0510	0.1320	0.0880	0.0256	0.3710
2059	0.6993	0.0618	0.1140	0.1250	0.0239	0.4540
2425	0.6827	0.0683	0.1015	0.1470	0.0222	0.5040
2851	0.6640	0.0750	0.0890	0.1720	0.0201	0.5500
3337	0.6427	0.0821	0.0780	0.1970	0.0181	0.6050
3883	0.6190	0.0886	0.0685	0.2240	0.0163	0.6630
4489	0.5947	0.0947	0.0600	0.2500	0.0149	0.7130
5154	0.5687	0.0995	0.0530	0.2790	0.0134	0.7770
5880	0.5427	0.1033	0.0470	0.3070	0.0123	0.8380
6666	0.5163	0.1068	0.0415	0.3350	0.0111	0.8990
7512	0.4890	0.1089	0.0375	0.3650	0.0103	0.9570
8418	0.4627	0.1097	0.0335	0.3940	0.0094	1.0190
9322	0.4377	0.1105	0.0305	0.4210	0.0088	1.0700

HBr SSD: 3.019890e-04

k13	2.722114e-04	*
K13	8.106878e-02	*
k34	4.869912e-04	*
k12	4.099485e-05	*
k24	1.537699e-04	*
kBu	3.789463e-03	*

SSD (sum of squares): 7.175647e-04
Standard deviation: 2.626721e-03

Use of Hessian matrix to obtain the standard deviations of the fitting parameters
nsigma=3

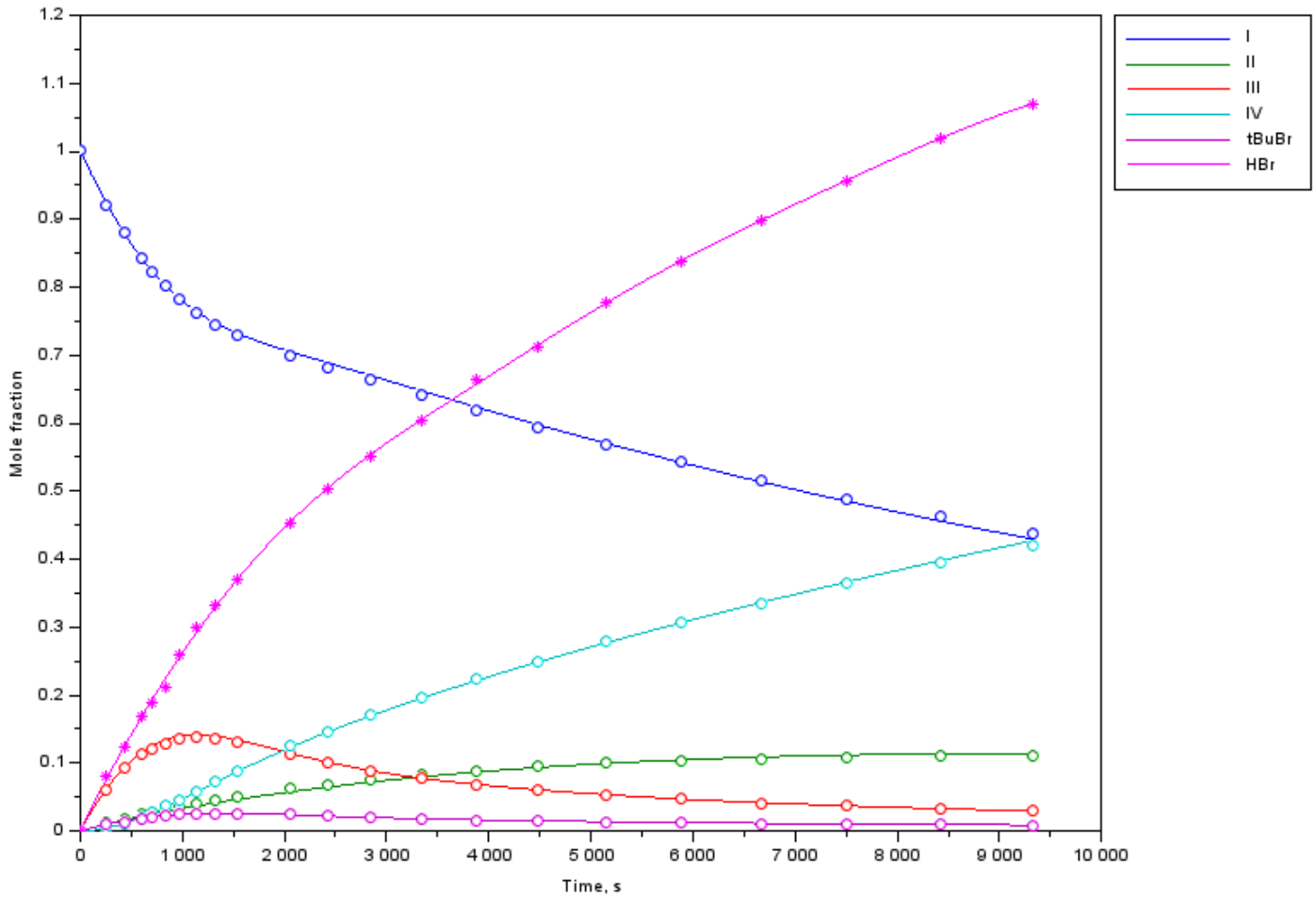
k13	2.722114e-04 +/- 5.9e-06 (2.2%)
K13	8.106880e-02 +/- 2.4e-03 (3.0%)
k34	4.869915e-04 +/- 1.5e-05 (3.1%)
k12	4.099479e-05 +/- 1.7e-06 (4.1%)
k24	1.537695e-04 +/- 1.4e-05 (9.3%)
kBu	3.789461e-03 +/- 3.9e-04 (10.2%)

Use of constant chi-square boundaries as confidence limits
nsigma=3

k13	2.722114e-04 +/- 5.9e-06 (2.2%)
K13	8.106878e-02 +/- 2.4e-03 (3.0%)
k34	4.869912e-04 +/- 1.5e-05 (3.1%)
k12	4.099485e-05 +/- 1.7e-06 (4.1%)
k24	1.537699e-04 +/- 1.4e-05 (9.3%)
kBu	3.789463e-03 +/- 3.9e-04 (10.3%)

Confidence limits by Monte Carlo simulation (bootstrap method)
200 synthetic data sets, nsigma = 3

k13	2.721434e-04 +/- 5.9e-06 (2.2%)
K13	8.129881e-02 +/- 2.3e-03 (2.8%)
k34	4.873166e-04 +/- 1.5e-05 (3.1%)
k12	4.098098e-05 +/- 1.7e-06 (4.0%)
k24	1.529057e-04 +/- 1.4e-05 (9.0%)
kBu	3.814127e-03 +/- 4.0e-04 (10.5%)



Data: 1784_data.txt
Experimental conditions see p. S2

time. s	I	II	III	IV	tBuBr	HBr
0	1.000	0.000	0.000	0.000	0.0000	0.000
176	0.792	0.058	0.107	0.044	0.0444	0.218
358	0.657	0.099	0.108	0.136	0.0550	0.482
458	0.609	0.116	0.093	0.182	0.0517	0.597
728	0.508	0.148	0.059	0.286	0.0383	0.853
899	0.456	0.159	0.046	0.339	0.0317	0.974
1146	0.391	0.168	0.035	0.407	0.0253	1.125
1422	0.330	0.169	0.027	0.473	0.0203	1.268
1728	0.277	0.164	0.021	0.538	0.0167	1.404
2064	0.229	0.155	0.017	0.600	0.0131	1.524
2431	0.188	0.142	0.013	0.657	0.0107	1.643
2827	0.153	0.127	0.011	0.710	0.0086	1.737
3253	0.122	0.111	0.009	0.758	0.0070	1.814
3710	0.097	0.095	0.007	0.802	0.0053	1.898
4196	0.077	0.080	0.006	0.838	0.0040	1.966
4712	0.060	0.066	0.005	0.869	0.0033	2.021
5258	0.046	0.054	0.004	0.897	0.0026	2.063
5835	0.035	0.044	0.003	0.918	0.0022	2.098
6441	0.026	0.036	0.003	0.936	0.0017	2.119

HBr SSD: 1.418445e-03

k13	1.105801e-03	*
K13	1.319586e-01	*
k34	3.811201e-03	*
k12	3.628205e-04	*
k24	6.948384e-04	*
kBu	1.216916e-02	*

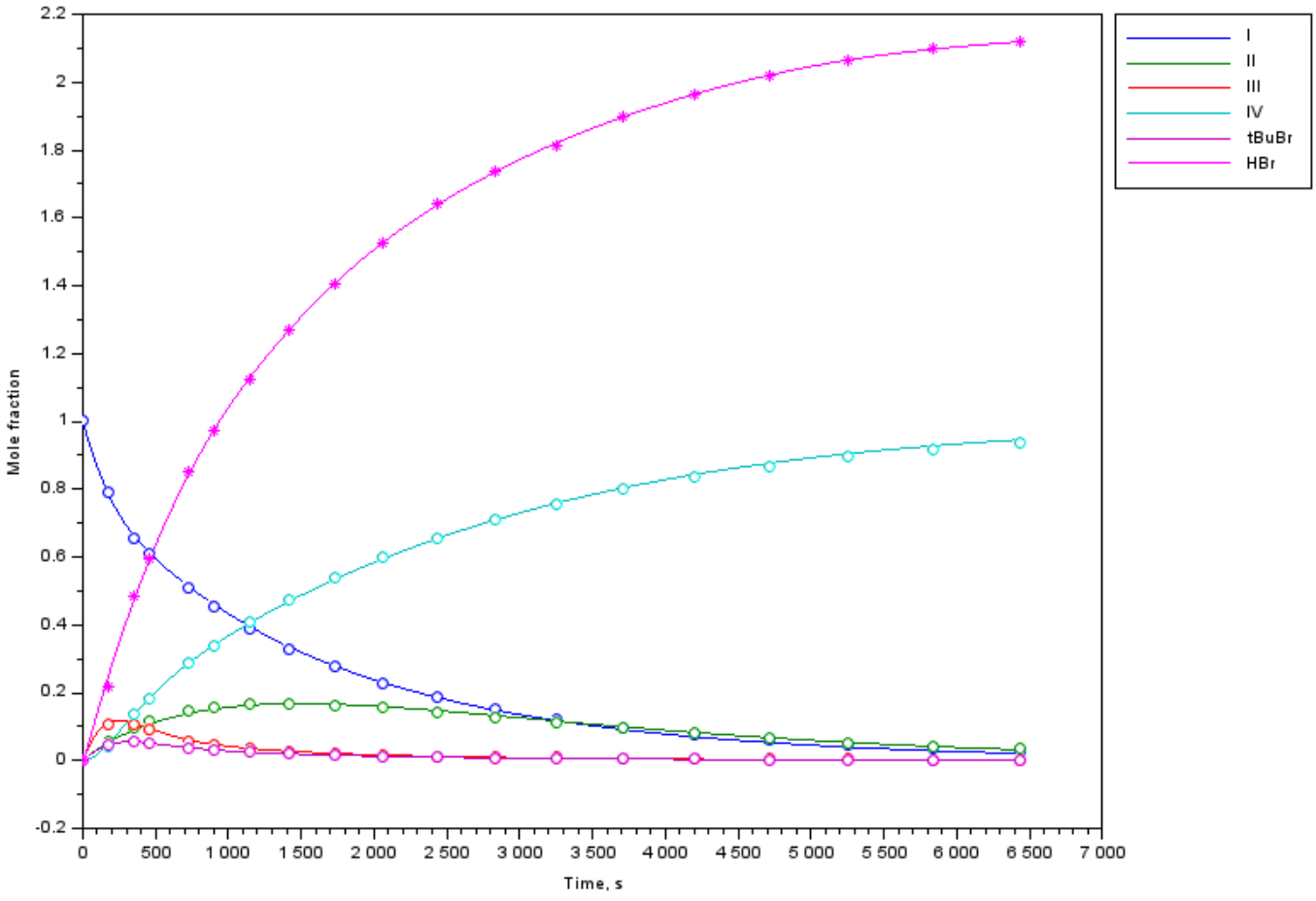
SSD (sum of squares): 1.426294e-03
Standard deviation: 4.003221e-03

Use of constant chi-square boundaries as confidence limits
nsigma=3

k13	1.105801e-03 +/- 5.6e-05 (5.1%)
K13	1.319586e-01 +/- 1.1e-02 (8.7%)
k34	3.811201e-03 +/- 2.1e-04 (5.4%)
k12	3.628205e-04 +/- 1.3e-05 (3.5%)
k24	6.948384e-04 +/- 3.3e-05 (4.8%)
kBu	1.216916e-02 +/- 1.4e-03 (11.5%)

Confidence limits by Monte Carlo simulation (bootstrap method)
200 synthetic data sets, nsigma = 3

k13	1.107748e-03 +/- 5.2e-05 (4.7%)
K13	1.326303e-01 +/- 1.1e-02 (8.1%)
k34	3.829810e-03 +/- 2.1e-04 (5.6%)
k12	3.616882e-04 +/- 1.2e-05 (3.3%)
k24	6.941455e-04 +/- 3.4e-05 (4.8%)
kBu	1.223432e-02 +/- 1.3e-03 (10.4%)



Data: 1790_data.txt
Experimental conditions see p. S2

time, s	I	II	III	IV	tBuBr	HBr
0	1	0	0	0	0	0
293	0.0369	0.1585	0.0033	0.8013	0.0113	2.0820
483	0.0044	0.0754	0.0006	0.9196	0.0031	2.2401
553	0.0022	0.0528	0.0006	0.9445	0.0018	2.2643
689	0.0003	0.0273	0.0006	0.9719	0.0005	2.2957
769	-0.0001	0.0183	0.0001	0.9816	0.0000	2.2953
895	0.0002	0.0108	0.0000	0.9887	0.0000	2.3168
1051	-0.0005	0.0058	0.0000	0.9943	0.0000	2.3201
1237	-0.0003	0.0037	0.0000	0.9964	0.0000	2.3224

HBr SSD: 4.982481e-05

k13	2.335738e-02	*
K13	4.300000e-01	
k34	2.850024e-02	*
k12	6.497140e-03	*
k24	4.961653e-03	*
kBu	4.518262e-02	*

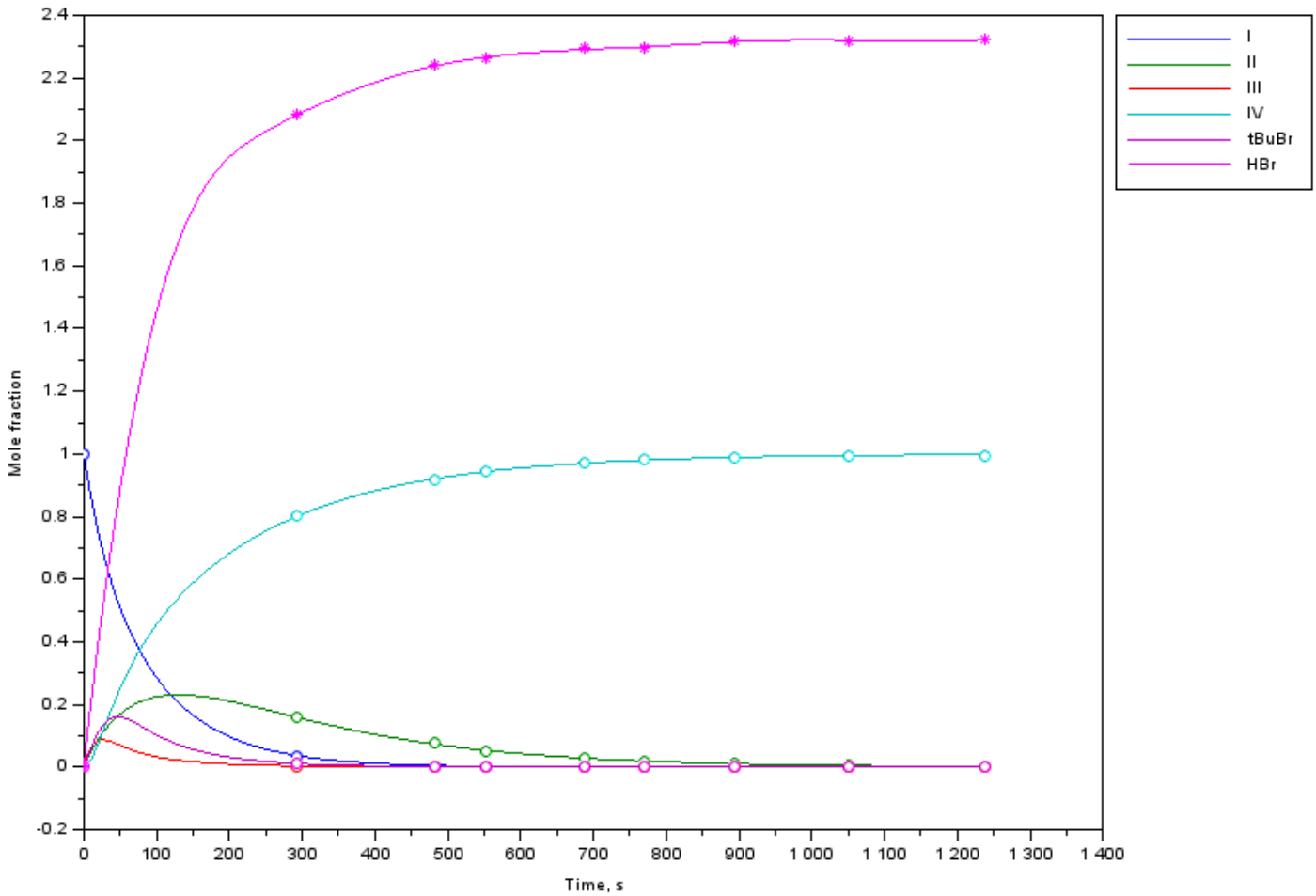
SSD (sum of squares): 4.870542e-05
Standard deviation: 1.103465e-03

Use of constant chi-square boundaries as confidence limits
nsigma=3

k13	2.335738e-02 +/- >100%
k34	2.850024e-02 +/- >100%
k12	6.497140e-03 +/- 1.1e-03 (16.6%)
k24	4.961653e-03 +/- 1.9e-04 (3.9%)
kBu	4.518262e-02 +/- 1.0e-02 (23.1%)

Confidence limits by Monte Carlo simulation (bootstrap method)
200 synthetic data sets, nsigma = 3

k13	2.437594e-02 +/- 1.2e-02 (51.2%)
k34	3.979518e-02 +/- 3.2e-02 (79.7%)
k12	6.296914e-03 +/- 6.4e-04 (10.2%)
k24	4.942876e-03 +/- 1.2e-04 (2.5%)
kBu	4.628966e-02 +/- 8.8e-03 (19.1%)



Data: 1785_data.txt
Experimental conditions see p. S2

time, s	I	II	III	IV	tBuBr	HBr
0	1	0	0	0	0	0
350	0.9553	0.0070	0.0350	0.0020	0.0078	0.0000
606	0.9270	0.0120	0.0545	0.0060	0.0138	0.0000
897	0.9003	0.0170	0.0720	0.0100	0.0212	0.0000
1202	0.8737	0.0220	0.0870	0.0180	0.0288	0.0100
1567	0.8463	0.0260	0.0995	0.0280	0.0377	0.0310
1993	0.8187	0.0320	0.1085	0.0410	0.0471	0.0820
2478	0.7933	0.0380	0.1120	0.0560	0.0560	0.1060
3023	0.7693	0.0440	0.1115	0.0750	0.0640	0.1440
3628	0.7467	0.0510	0.1065	0.0950	0.0699	0.1660
4293	0.7297	0.0560	0.0985	0.1160	0.0733	0.2070
5019	0.7100	0.0630	0.0890	0.1380	0.0750	0.2510
5804	0.6930	0.0690	0.0795	0.1590	0.0744	0.2870
6649	0.6760	0.0740	0.0705	0.1800	0.0718	0.3220
7554	0.6587	0.0790	0.0620	0.2000	0.0679	0.3720
8520	0.6407	0.0850	0.0550	0.2200	0.0633	0.4300
9545	0.6223	0.0890	0.0490	0.2400	0.0590	0.4670
10630	0.6033	0.0920	0.0445	0.2600	0.0546	0.5080
11776	0.5847	0.0960	0.0400	0.2800	0.0506	0.5480
12981	0.5643	0.0990	0.0365	0.3000	0.0466	0.5890
14246	0.5440	0.1020	0.0335	0.3200	0.0431	0.6340
15571	0.5253	0.1030	0.0310	0.3410	0.0402	0.6700
16957	0.5060	0.1040	0.0285	0.3610	0.0372	0.7040
18402	0.4880	0.1050	0.0260	0.3810	0.0349	0.7500
19907	0.4697	0.1050	0.0240	0.4010	0.0324	0.7770
21473	0.4510	0.1060	0.0225	0.4200	0.0304	0.8180
23098	0.4337	0.1050	0.0205	0.4410	0.0284	0.8540
24783	0.4160	0.1030	0.0195	0.4610	0.0268	0.8910
26529	0.3993	0.1030	0.0180	0.4800	0.0252	0.9250
28334	0.3837	0.1000	0.0165	0.5000	0.0239	0.9520
30200	0.3667	0.0980	0.0155	0.5200	0.0221	0.9910
32125	0.3503	0.0970	0.0145	0.5380	0.0212	1.0230
34110	0.3357	0.0940	0.0135	0.5570	0.0196	1.0480
36156	0.3210	0.0910	0.0125	0.5750	0.0187	1.0840
38261	0.3067	0.0880	0.0115	0.5930	0.0176	1.1080
40426	0.2927	0.0870	0.0110	0.6100	0.0166	1.1370
42652	0.2790	0.0840	0.0105	0.6270	0.0157	1.1600
44937	0.2660	0.0800	0.0095	0.6440	0.0148	1.1910
47283	0.2537	0.0770	0.0090	0.6600	0.0140	1.2160
49688	0.2417	0.0750	0.0080	0.6750	0.0131	1.2410
52154	0.2297	0.0720	0.0080	0.6900	0.0122	1.2620
54679	0.2183	0.0700	0.0075	0.7040	0.0121	1.2850
57265	0.2073	0.0660	0.0070	0.7200	0.0110	1.3070
59910	0.1973	0.0630	0.0065	0.7330	0.0107	1.3320
62616	0.1867	0.0610	0.0060	0.7460	0.0100	1.3400
65381	0.1773	0.0580	0.0055	0.7600	0.0092	1.3670

HBr SSD: 4.126753e-03

k13	9.045607e-05	*
K13	3.888798e-02	*
k34	2.792278e-04	*
k12	1.544423e-05	*
k24	6.412574e-05	*
kBu	4.717469e-04	*

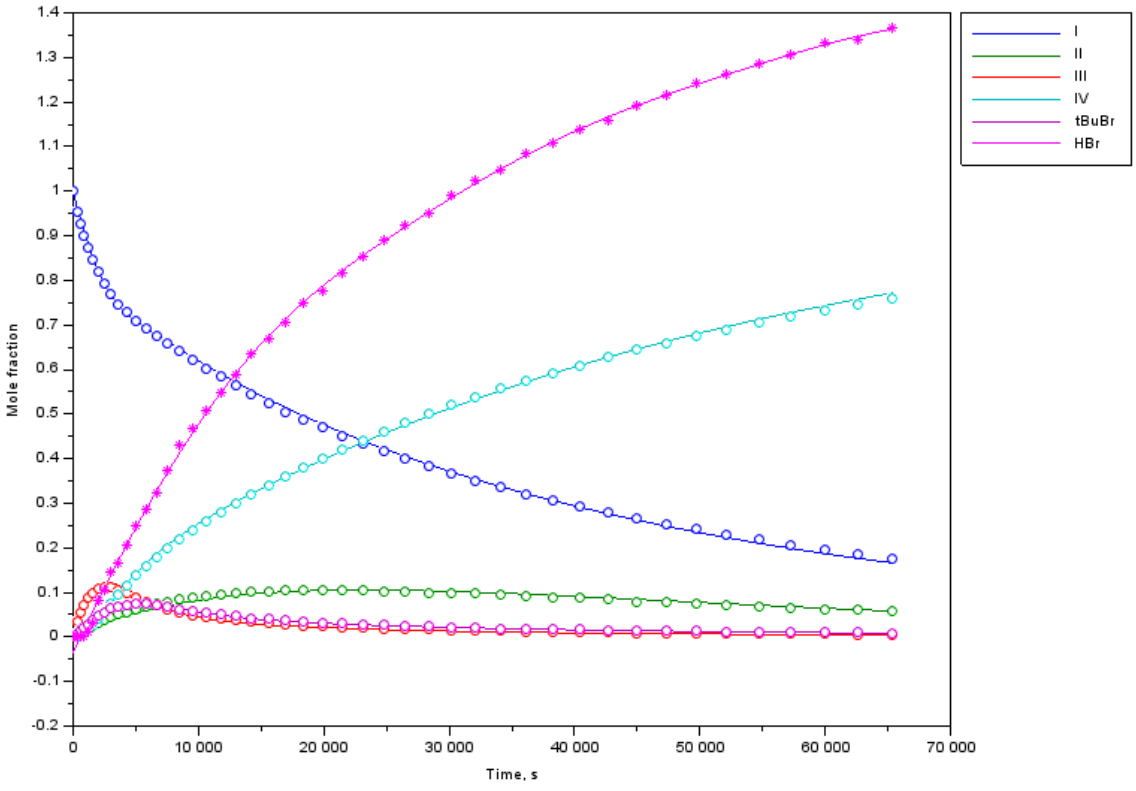
SSD (sum of squares): 4.929760e-03
Standard deviation: 4.691253e-03

Use of constant chi-square boundaries as confidence limits
nsigma=3

k13	9.045607e-05 +/- 3.1e-06 (3.4%)
K13	3.888798e-02 +/- 2.3e-03 (5.9%)
k34	2.792278e-04 +/- 1.1e-05 (4.1%)
k12	1.544423e-05 +/- 5.1e-07 (3.3%)
k24	6.412574e-05 +/- 3.0e-06 (4.7%)
kBu	4.717469e-04 +/- 2.8e-05 (5.9%)

Confidence limits by Monte Carlo simulation (bootstrap method)
200 synthetic data sets, nsigma = 3

k13	9.051925e-05 +/- 3.1e-06 (3.5%)
K13	3.899622e-02 +/- 2.5e-03 (6.3%)
k34	2.796895e-04 +/- 1.1e-05 (4.1%)
k12	1.540805e-05 +/- 5.2e-07 (3.4%)
k24	6.391375e-05 +/- 2.8e-06 (4.4%)
kBu	4.752015e-04 +/- 2.7e-05 (5.7%)



Data: 1780_data_HBr_teor_Me.txt
Experimental conditions see p. S2

time, s	I	II	III	IV	tBuBr	HBr_teor
0	1.00000	0.00000	0.00000	0.00000	0.00000	0.00000
590	0.96621	0.00227	0.03098	0.00054	0.00156	0.03600
811	0.95360	0.00347	0.04192	0.00101	0.00211	0.04300
1185	0.92992	0.00861	0.05968	0.00179	0.00400	0.06400
1431	0.92092	0.00481	0.07136	0.00291	0.00367	0.07750
1736	0.90642	0.00570	0.08397	0.00391	0.00389	0.09250
2102	0.88813	0.00751	0.09910	0.00527	0.00467	0.11200
2528	0.86918	0.00839	0.11482	0.00761	0.00522	0.13400
3014	0.84844	0.00942	0.13149	0.01065	0.00589	0.15650
3560	0.82648	0.01140	0.14803	0.01408	0.00667	0.18250
4166	0.80437	0.01268	0.16417	0.01878	0.00744	0.20800
4832	0.78241	0.01476	0.17902	0.02382	0.00800	0.23950
5227	0.77050	0.01582	0.18639	0.02728	0.00833	0.25500

HBr SSD: 1.045144e-05

k13	5.378125e-05	*
K13	1.486477e-01	*
k34	4.162369e-05	*
k12	4.182856e-06	*
k24	8.242562e-05	*
kBu	1.290152e-03	*

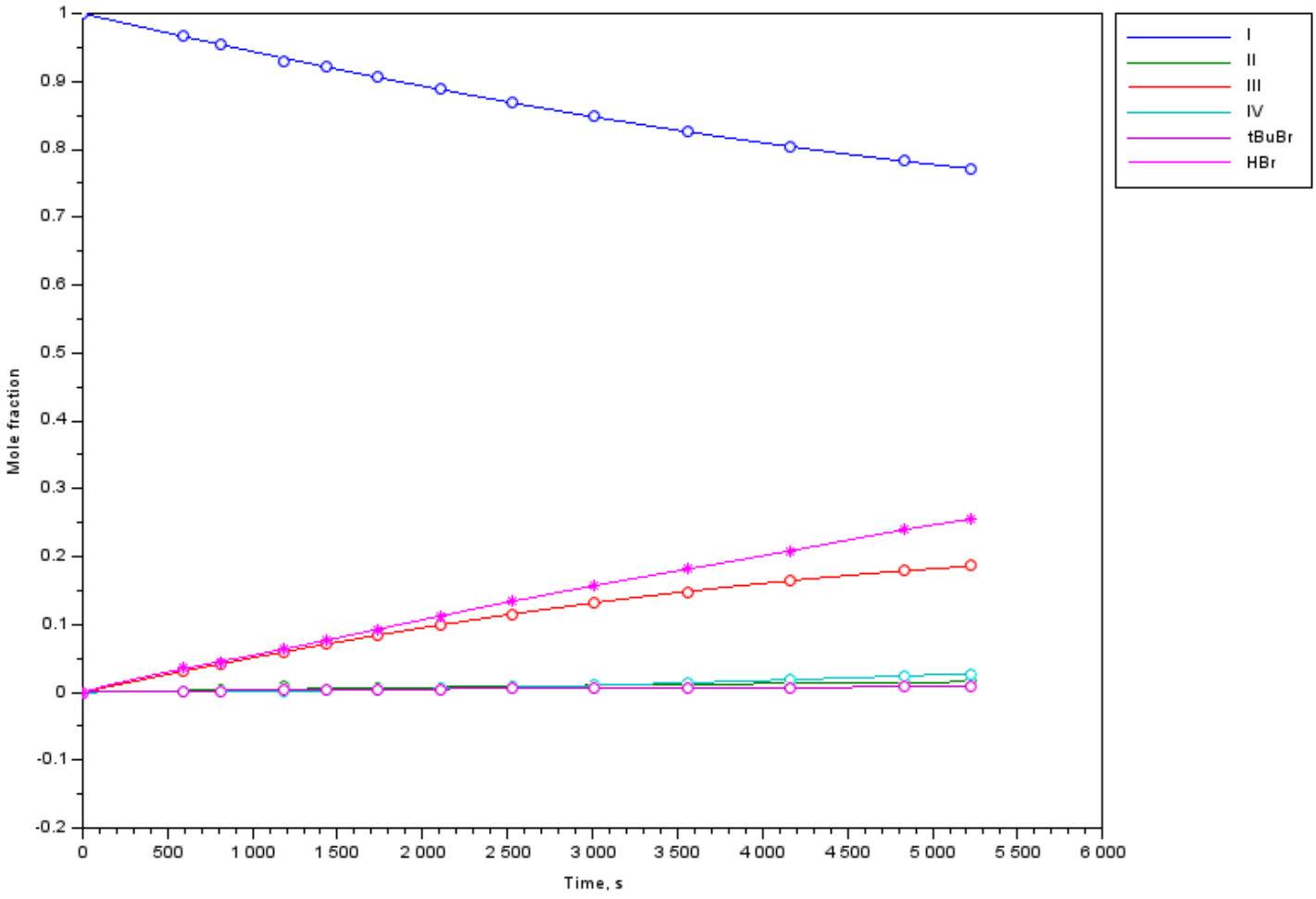
SSD (sum of squares): 4.422388e-05
Standard deviation: 8.657697e-04

Use of constant chi-square boundaries as confidence limits
nsigma=3

k13	5.378125e-05 +/- 7.8e-07 (1.4%)
K13	1.486477e-01 +/- 1.5e-02 (9.9%)
k34	4.162369e-05 +/- 8.3e-06 (20.0%)
k12	4.182856e-06 +/- 8.4e-07 (20.1%)
k24	8.242562e-05 +/- >100%
kBu	1.290152e-03 +/- 2.3e-04 (17.5%)

Confidence limits by Monte Carlo simulation (bootstrap method)
200 synthetic data sets, nsigma = 3

k13	5.377062e-05 +/- 8.1e-07 (1.5%)
K13	1.503349e-01 +/- 1.5e-02 (9.7%)
k34	4.210131e-05 +/- 9.0e-06 (21.5%)
k12	4.143184e-06 +/- 9.0e-07 (21.8%)
k24	7.398219e-05 +/- 1.1e-04 (154.6%)
kBu	1.373550e-03 +/- 2.7e-04 (19.5%)



Data: 1781_data_HBr_teor.txt
Experimental conditions see p. S2

time	I	II	III	IV	tBuBr	HBr_teor
0	1	0	0	0	0	0
386	0.9929	0.0009	0.0063	0.0000	0.0007	0.0064
465	0.9910	0.0014	0.0075	0.0000	0.0009	0.0082
638	0.9875	0.0019	0.0104	0.0002	0.0013	0.0116
841	0.9838	0.0021	0.0136	0.0005	0.0014	0.0155
997	0.9810	0.0027	0.0160	0.0004	0.0016	0.0178
1183	0.9776	0.0031	0.0190	0.0003	0.0018	0.0210
1398	0.9731	0.0039	0.0223	0.0006	0.0020	0.0260
1644	0.9685	0.0047	0.0260	0.0008	0.0022	0.0306
1920	0.9638	0.0048	0.0302	0.0012	0.0025	0.0354
2226	0.9579	0.0060	0.0346	0.0015	0.0027	0.0418
2562	0.9523	0.0062	0.0393	0.0021	0.0028	0.0479
2928	0.9456	0.0075	0.0444	0.0025	0.0031	0.0550
3323	0.9385	0.0084	0.0497	0.0034	0.0035	0.0630
3749	0.9312	0.0095	0.0551	0.0042	0.0036	0.0712
4205	0.9240	0.0102	0.0605	0.0053	0.0037	0.0797
4691	0.9158	0.0115	0.0662	0.0065	0.0041	0.0892
5207	0.9074	0.0127	0.0719	0.0079	0.0042	0.0992
5753	0.8993	0.0139	0.0776	0.0093	0.0044	0.1089
6329	0.8909	0.0151	0.0829	0.0111	0.0047	0.1194
6934	0.8821	0.0162	0.0884	0.0133	0.0049	0.1307
7570	0.8736	0.0172	0.0936	0.0156	0.0050	0.1418
8236	0.8643	0.0193	0.0985	0.0179	0.0053	0.1541
8930	0.8555	0.0204	0.1032	0.0209	0.0054	0.1664

HBr SSD: 1.351053e-06

k13	1.664691e-05	*
K13	6.461039e-02	*
k34	3.620841e-05	*
k12	2.660959e-06	*
k24	1.625905e-05	*
kBu	1.106073e-03	*

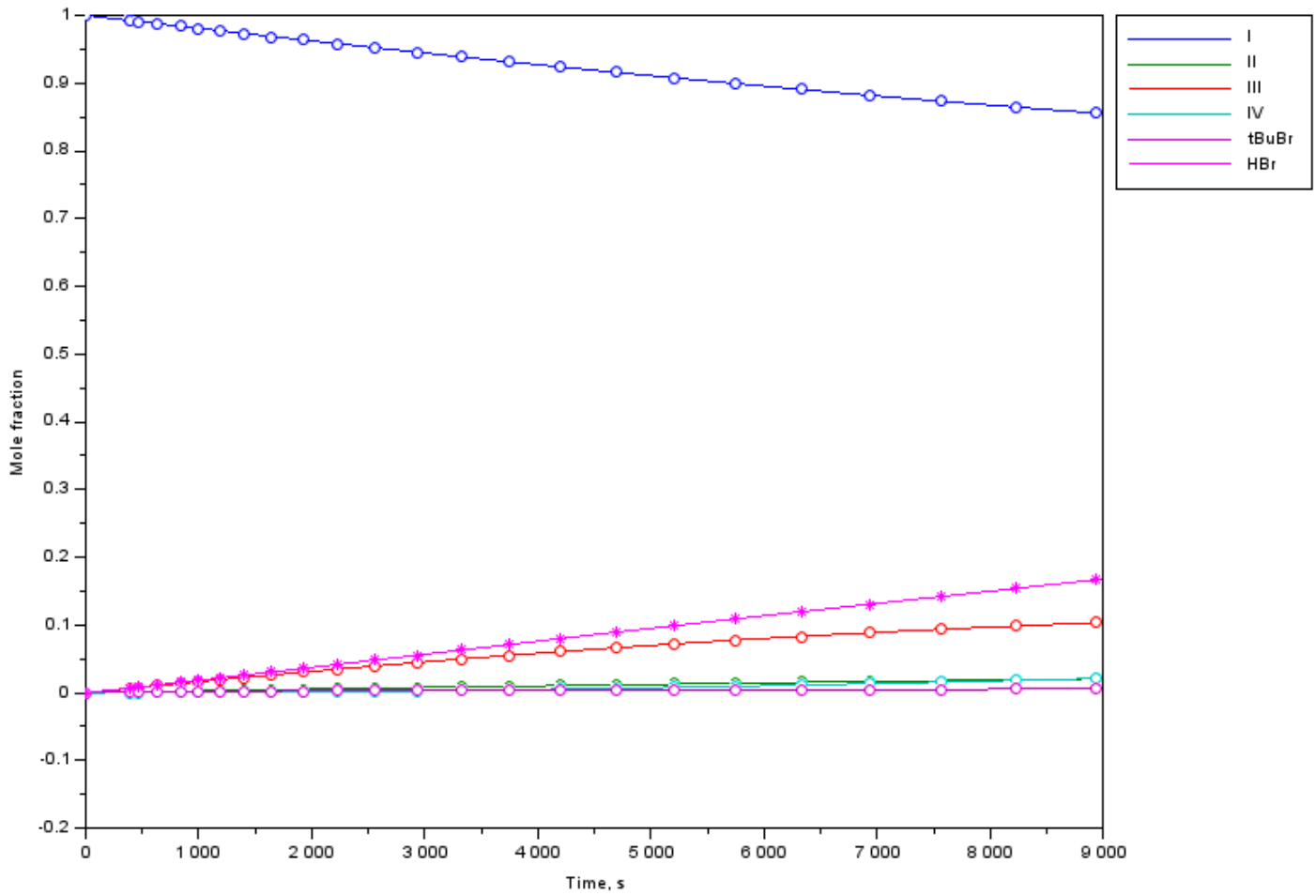
SSD (sum of squares): 3.178641e-06
Standard deviation: 1.669815e-04

Use of constant chi-square boundaries as confidence limits
nsigma=3

k13	1.664691e-05 +/- 6.2e-08 (0.4%)
K13	6.461039e-02 +/- 2.5e-03 (3.8%)
k34	3.620841e-05 +/- 1.4e-06 (3.8%)
k12	2.660959e-06 +/- 6.9e-08 (2.6%)
k24	1.625905e-05 +/- 7.7e-06 (47.6%)
kBu	1.106073e-03 +/- 4.0e-05 (3.6%)

Confidence limits by Monte Carlo simulation (bootstrap method)
200 synthetic data sets, nsigma = 3

k13	1.664273e-05 +/- 6.5e-08 (0.4%)
K13	6.471300e-02 +/- 2.3e-03 (3.6%)
k34	3.613187e-05 +/- 1.3e-06 (3.7%)
k12	2.664834e-06 +/- 6.8e-08 (2.5%)
k24	1.663560e-05 +/- 7.6e-06 (45.7%)
kBu	1.105484e-03 +/- 4.0e-05 (3.7%)



Data: 1912-data.txt
Experimental conditions see p. S2

time	I	II	III	IV	HBr
0	1.000	0.000	0.000	0.000	0.000
262	0.835	0.124	0.023	0.019	0.28
783	0.573	0.295	0.025	0.107	0.7315
1024	0.499	0.335	0.022	0.143	0.896
1977	0.296	0.417	0.012	0.276	1.3272
2986	0.183	0.426	0.006	0.384	1.5451

HBr SSD: 3.696766e-06

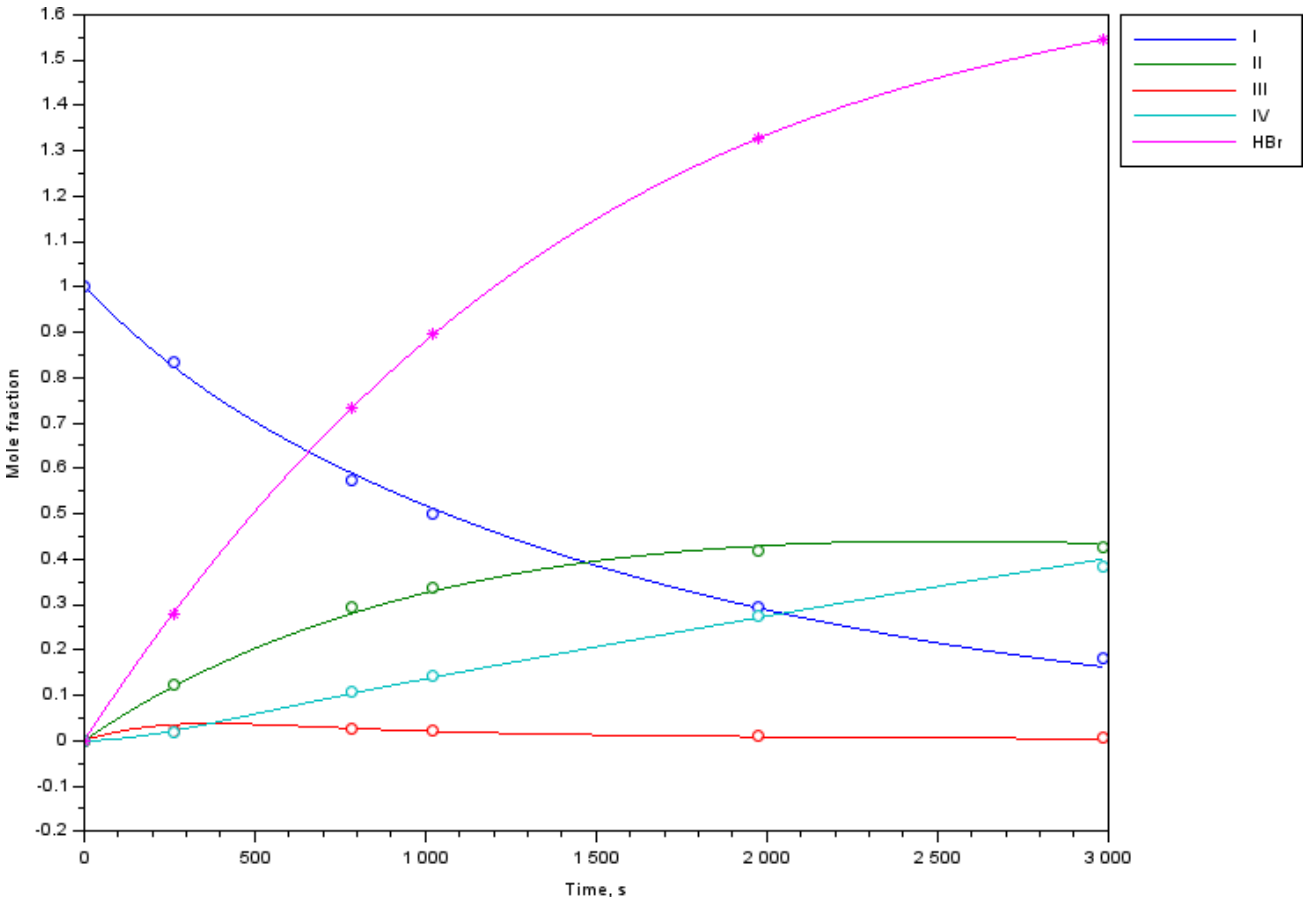
k13 2.418009e-04 *
K13 5.247835e-02 *
k34 3.092900e-03 *
k12 5.165345e-04 *
k24 2.503739e-04 *
SSD (sum of squares): 1.948359e-03
Standard deviation: 1.012646e-02

Use of constant chi-square boundaries as confidence limits
nsigma=1

k13 2.418009e-04 +/- 3.1e-05 (12.9%)
K13 5.247835e-02 +/- 1.7e-02 (32.0%)
k34 3.092900e-03 +/- 6.8e-04 (21.9%)
k12 5.165345e-04 +/- 1.2e-05 (2.4%)
k24 2.503739e-04 +/- 1.9e-05 (7.4%)

Confidence limits by Monte Carlo simulation (bootstrap method)
200 synthetic data sets, nsigma = 1

k13 2.455044e-04 +/- 2.7e-05 (11.1%)
K13 5.308848e-02 +/- 1.5e-02 (27.7%)
k34 3.265734e-03 +/- 8.0e-04 (24.5%)
k12 5.165577e-04 +/- 1.1e-05 (2.1%)
k24 2.500796e-04 +/- 1.6e-05 (6.3%)



Data: 1913-data.txt

time, s	I	II	III	IV	HBr
0	1.000	0.000	0.000	0.000	0.000
233	0.832	0.135	0.022	0.012	0.200
367	0.764	0.182	0.028	0.026	0.294
529	0.686	0.235	0.032	0.047	0.412
640	0.638	0.267	0.034	0.061	0.477
833	0.575	0.316	0.034	0.075	0.619
1183	0.467	0.381	0.030	0.122	0.788
1598	0.367	0.436	0.025	0.171	0.982
2081	0.281	0.470	0.019	0.230	1.147
2632	0.211	0.484	0.014	0.290	1.308
3251	0.153	0.480	0.011	0.355	1.463
3938	0.107	0.464	0.012	0.418	1.600
4693	0.073	0.439	0.008	0.480	1.698
5516	0.050	0.396	0.007	0.547	1.785
6407	0.032	0.357	0.009	0.602	1.898
7367	0.024	0.312	0.007	0.657	1.946

HBr SSD: 9.893464e-04

k13	2.060058e-04	*
K13	6.268796e-02	*
k34	1.899235e-03	*
k12	5.214668e-04	*
k24	1.825199e-04	*

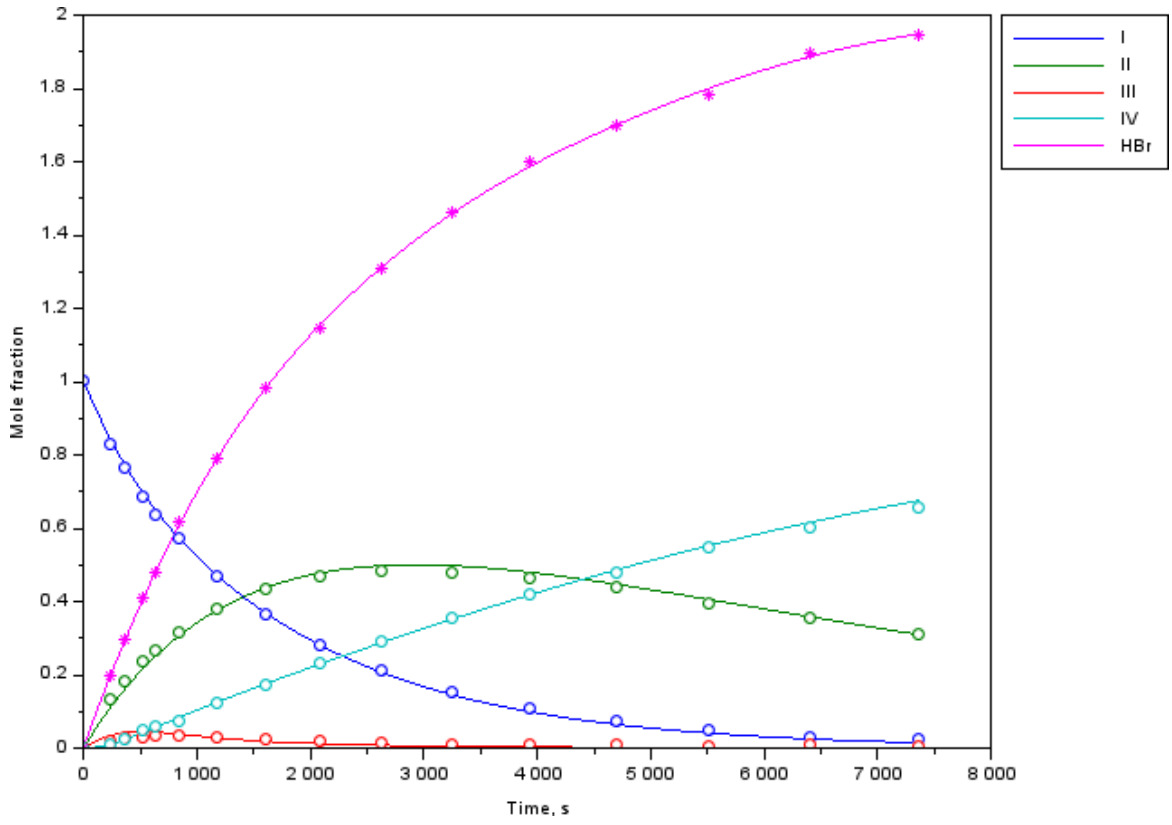
SSD (sum of squares): 5.254032e-03
Standard deviation: 9.436704e-03

Use of constant chi-square boundaries as confidence limits
nsigma=1

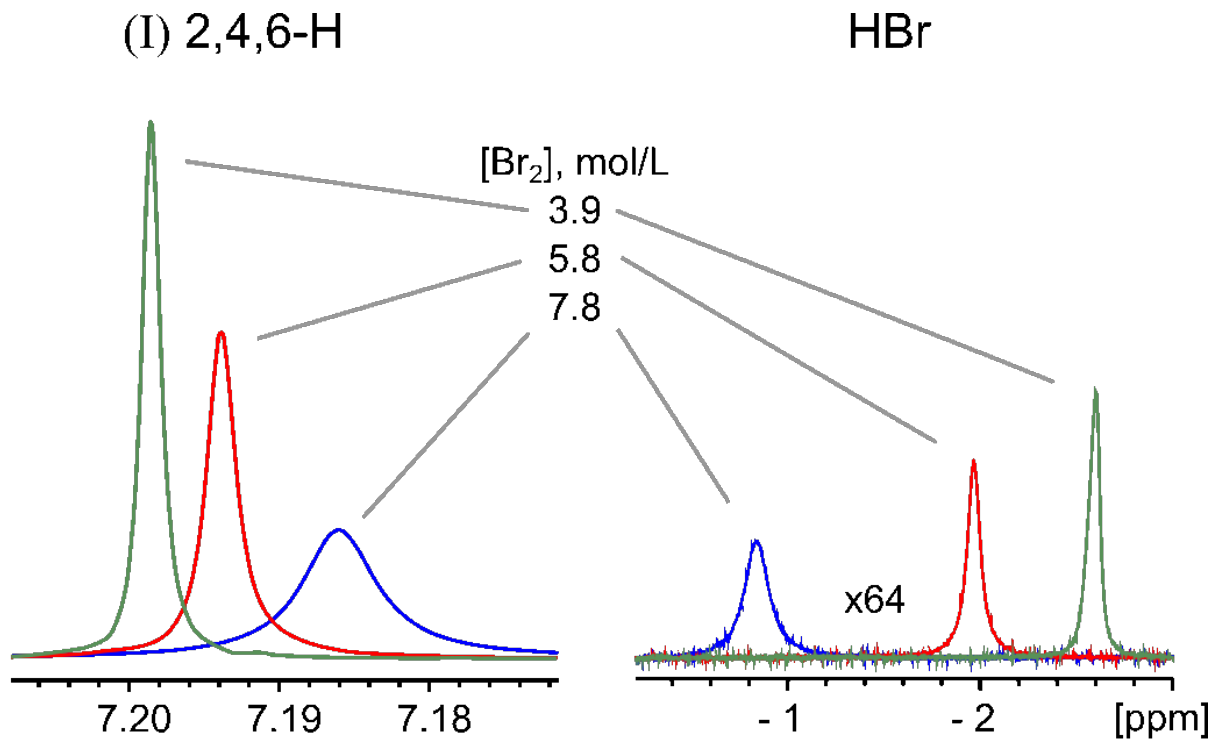
k13	2.060058e-04 +/- 1.7e-05 (8.2%)
K13	6.268796e-02 +/- 1.3e-02 (20.5%)
k34	1.899235e-03 +/- 2.1e-04 (11.1%)
k12	5.214668e-04 +/- 5.5e-06 (1.1%)
k24	1.825199e-04 +/- 3.9e-06 (2.2%)

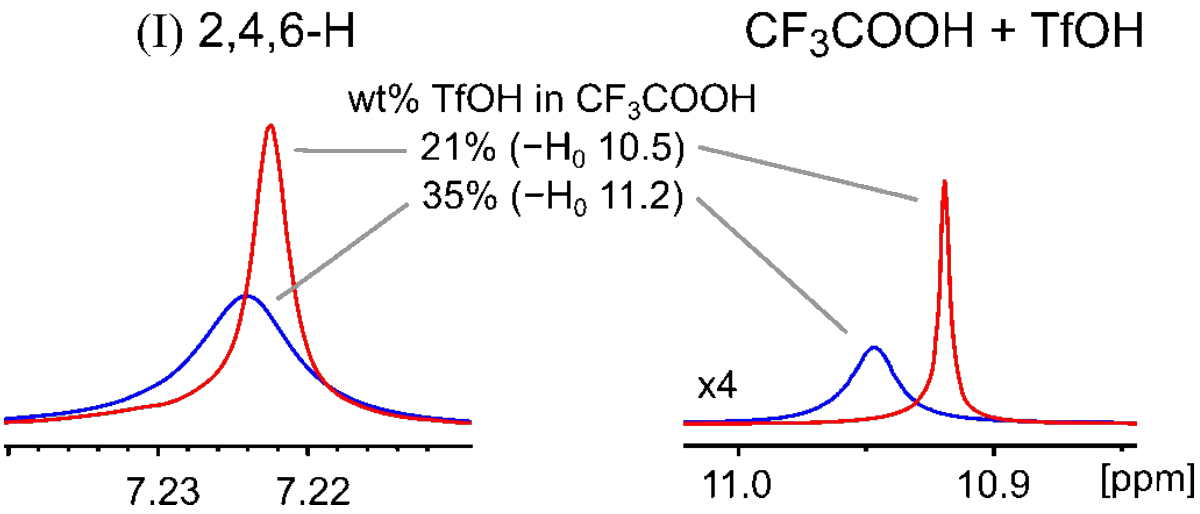
Confidence limits by Monte Carlo simulation (bootstrap method)
200 synthetic data sets, nsigma = 1

k13	2.078995e-04 +/- 1.8e-05 (8.5%)
K13	6.557147e-02 +/- 1.5e-02 (23.5%)
k34	1.907406e-03 +/- 2.5e-04 (13.0%)
k12	5.206950e-04 +/- 5.4e-06 (1.0%)
k24	1.821183e-04 +/- 3.7e-06 (2.0%)



^{1}H NMR signals of compound I (2,4,6-H) and acid protons. [I] = [HBr] = [CF_3COOH+TfOH] = 0.1 mol/L, CD_2Cl_2: 0.1 mL. Br_2+ CCl_4 (mL): 0.1+0.28 (a), 0.15+0.23 (b), 0.2+0.18 (c), 0+0.38 (d,e); wt% TfOH in CF_3COOH: 35 (d), 21 (e).





For measurement of broadening of aromatic signals of compound I the width of $CHCl_3$ signal present as a small impurity in CCl_4 was taken as a reference width.

Transition states of the bromination reactions (DFT/PBE/Λ01), see also Fig. 7 of the main text.
DFT energy and ZPE are in a.u., free energy G and Grimme's E_{disp} are in kcal/mol
Br_2 and 1,3,5-tri-*tert*-butylbenzene (zero level for Fig. 8 of the main text) see on p. S24

I→III (n=1)

Energy -5850.770394628 Dipole 11.026145 ZPE 0.425003 G(298.15) 231.72 Edisp -43.59

C	-0.66176950	-0.41602230	-1.23443578
C	-0.66848074	-0.39837925	1.19011529
C	-1.28000208	-0.78482533	-0.02514831
C	0.53971728	0.26442274	1.24980195
C	0.54866799	0.25540076	-1.28517858
C	1.25532502	0.51158652	-0.01677966
H	-1.16371796	-0.65254086	-2.17263093
H	-1.18476186	-0.62418131	2.12528016
H	1.96233754	1.35897745	-0.01784778
Br	2.75892120	-1.03664783	-0.02916038
Br	4.90928334	2.29336572	-0.02159124
C	1.09604440	0.72262775	2.60399448
C	1.10336729	0.71803933	-2.63638130
C	2.33561477	1.62084854	2.48076239
H	3.18208094	1.13378089	1.97392515
H	2.11630426	2.55170112	1.93381760
H	2.67201197	1.90585311	3.49038768
C	2.36954510	1.57843315	-2.52110097
H	2.19198813	2.50796854	-1.95783694
H	3.20806244	1.05745512	-2.03524564
H	2.69802384	1.86690679	-3.53233538
C	-0.00252521	1.53694924	3.33958192
H	-0.90312132	0.93937792	3.54877962
H	0.40036256	1.88624636	4.30391900
H	-0.29970262	2.42004426	2.75212851
C	1.45111508	-0.52244017	3.45664116
H	2.24146767	-1.11267389	2.96989383
H	1.81615563	-0.19426315	4.44356726
H	0.57530346	-1.17220824	3.61309640
C	0.01440375	1.57671722	-3.33847841
H	0.40929519	1.92622720	-4.30604763
H	-0.90799147	1.00880134	-3.53386934
H	-0.24201038	2.46060635	-2.73330742
C	1.40893434	-0.52097080	-3.51671828
H	1.77141257	-0.18411513	-4.50161818
H	2.18802847	-1.14227119	-3.05061538
H	0.51364742	-1.14257966	-3.67570689
C	-2.59865980	-1.55848930	0.01420901
C	-3.66825447	-0.70328687	0.73924395
H	-4.61792355	-1.26176039	0.77993562
H	-3.37448955	-0.46154387	1.77187821
H	-3.84588450	0.24191688	0.20210388
C	-3.12744077	-1.91024009	-1.38786835
H	-2.41454520	-2.53604836	-1.94844697
H	-4.06475638	-2.48030712	-1.28834786
H	-3.34983122	-1.00878963	-1.98146823
C	-2.37622166	-2.87772286	0.79635317
H	-2.04481781	-2.69366846	1.82953934
H	-3.32171823	-3.44313534	0.83865853
H	-1.61879537	-3.50514291	0.30055172

I→III (n=2)

Energy -10998.42107182 Dipole 13.940750 ZPE 0.424528 G(298.15) 225.67 Edisp -48.12

C	-0.75535949	-0.59366691	-1.22596764
C	-0.82292091	-0.49226242	1.19039721
C	-1.42371066	-0.87864491	-0.02625357
C	0.43310989	0.07490236	1.27533543
C	0.50161008	-0.00805297	-1.27583482
C	1.13471066	0.35821215	0.00410495
H	-1.24244068	-0.84930206	-2.16608782
H	-1.36956192	-0.67948121	2.11453211
H	1.24630499	1.56992600	-0.04884002

Br	3.02237747	-0.32972984	0.06087488
Br	3.89328310	4.11183199	-0.09475825
Br	6.33666513	4.49830007	0.02092296
Br	1.13909485	3.59598061	-0.22126422
C	0.98862855	0.41883700	2.67475179
C	1.04745304	0.35044605	-2.67454445
C	2.04975369	1.54005077	2.68318478
H	2.94541073	1.29599433	2.09932715
H	1.63815126	2.48428369	2.29810184
H	2.36596012	1.70355767	3.72582569
C	2.41548168	1.05952352	-2.74047181
H	2.48320262	1.92126845	-2.06166781
H	3.24967006	0.37815877	-2.53411608
H	2.54245560	1.44035026	-3.76691582
C	-0.16091065	0.90353904	3.59665486
H	-0.88730448	0.11262811	3.83981170
H	0.27796309	1.23702117	4.55005270
H	-0.69607541	1.75677012	3.15140872
C	1.58587751	-0.87580852	3.28900947
H	2.43722202	-1.24381287	2.69938523
H	1.93857912	-0.65487864	4.30990303
H	0.82891534	-1.67450242	3.34929578
C	0.01093726	1.32173555	-3.31542240
H	0.34867520	1.57109649	-4.33421523
H	-0.99460051	0.88110564	-3.38806555
H	-0.05000285	2.25528125	-2.73407874
C	1.14259242	-0.94252450	-3.52375363
H	1.51098911	-0.68018483	-4.52861431
H	1.85319159	-1.65238754	-3.07165768
H	0.17177315	-1.44796592	-3.64252831
C	-2.78800037	-1.56903526	0.00119608
C	-3.81994933	-0.60046173	0.63333511
H	-4.80738544	-1.08938974	0.66337461
H	-3.54764618	-0.32126892	1.66239957
H	-3.90924105	0.32272324	0.03927288
C	-3.28580834	-1.96602874	-1.40004730
H	-2.59399824	-2.66396034	-1.89866906
H	-4.25927534	-2.47269656	-1.30647755
H	-3.43258895	-1.08759602	-2.04887901
C	-2.68504727	-2.85165297	0.86428566
H	-2.38489160	-2.63276796	1.90007081
H	-3.66815616	-3.34871288	0.89629730
H	-1.95516351	-3.55674760	0.43601878

I→III (n=3)

Energy -16146.05511219 ZPE 0.425409 G(298.15) 222.30 HoF -26.87 kcal Edisp -53.00

C	0.80146658	0.96259085	-1.11621718
C	1.40655465	-0.54919710	0.66397152
C	1.78878341	0.24097635	-0.43349633
C	0.10284450	-0.65684955	1.12034525
C	-0.54328492	0.95029828	-0.76308154
C	-0.93454455	0.02395470	0.31628008
H	1.10558871	1.57849596	-1.95796125
H	2.18377309	-1.09781491	1.19229193
H	-1.25587100	-0.95345963	-0.41363476
Br	-2.63735631	0.44042612	1.25713577
Br	-6.24683664	-0.84120374	1.38524069
Br	-6.58916674	-3.01100227	-0.36478912
Br	-4.12814894	-2.84847937	-1.05812650
Br	-1.54468658	-2.50323684	-1.63592447
Br	-5.60028703	1.07820114	2.81692385
C	-0.17232823	-1.55237330	2.34971573
C	-1.52099868	1.81518202	-1.58923008
C	-1.35336275	-2.52833815	2.12132851
H	-2.30457477	-2.02559134	1.91240127
H	-1.13564458	-3.21389363	1.28837091
H	-1.48483351	-3.12737418	3.03665182
C	-2.78167180	1.03096959	-2.03179070
H	-2.50543963	0.18542371	-2.67980085

H	-3.37476755	0.64338320	-1.19571097
H	-3.42391116	1.71432374	-2.61010921
C	1.04908341	-2.43916171	2.69081784
H	1.92158531	-1.85524764	3.02620436
H	0.76665237	-3.09854886	3.52588109
H	1.34318824	-3.08036763	1.84420474
C	-0.42241796	-0.65073316	3.58925874
H	-1.31464040	-0.02281445	3.48000350
H	-0.56301819	-1.29926055	4.46955007
H	0.44752243	-0.00061275	3.77736653
C	-0.86427599	2.33021962	-2.89234976
H	-1.62947100	2.87794465	-3.46365877
H	-0.03837153	3.03564541	-2.70606916
H	-0.50185361	1.50482991	-3.52592372
C	-1.90530833	3.07245018	-0.76160792
H	-2.55974519	3.70890091	-1.37958645
H	-2.44237691	2.82122932	0.16077589
H	-1.00653618	3.65484062	-0.50135492
C	3.26147355	0.28355795	-0.84881329
C	3.70314268	-1.14889917	-1.24163027
H	4.76296408	-1.13460167	-1.54403238
H	3.59820889	-1.85603416	-0.40481774
H	3.10728333	-1.52732575	-2.08723349
C	3.51771177	1.21764424	-2.04490973
H	3.24200987	2.26051086	-1.81927627
H	4.59174637	1.20413614	-2.28869151
H	2.97034518	0.89341274	-2.94457514
C	4.11051501	0.77794696	0.34851764
H	4.01783818	0.11818433	1.22442659
H	5.17299138	0.80206018	0.05675824
H	3.81245766	1.79468185	0.64998091

I→III (n=4)

Energy -21293.67708776 Dipole 14.569397 ZPE 0.425776 G(298.15) 214.66 Edisp -56.34

C	0.94530272	0.88491457	-0.98684635
C	1.69319996	-0.53925093	0.80475572
C	1.98044851	0.17540953	-0.37017197
C	0.42942731	-0.62274677	1.37031541
C	-0.37031335	0.89162844	-0.52710459
C	-0.66693099	-0.02398963	0.58556455
H	1.18115803	1.47845588	-1.86528634
H	2.51508363	-1.04483857	1.30702848
H	-0.86773591	-1.07398016	-0.16139522
Br	-2.42189304	0.15361395	1.46690038
Br	-6.15405799	-0.95864102	1.03991876
Br	-6.22658035	-2.60508843	-1.37733723
Br	-3.65255574	-2.73732808	-1.35032397
Br	-1.01309824	-2.64732584	-1.24802031
Br	-5.78536545	0.42588369	3.00730899
C	0.26429832	-1.41490439	2.68828255
C	-1.40092594	1.76027904	-1.28177806
C	-0.78519805	-2.54868701	2.56309156
H	-1.79109961	-2.18779357	2.32113014
H	-0.48296168	-3.27247876	1.79059107
H	-0.83850340	-3.07646149	3.52896130
C	-2.60600452	0.92657020	-1.78642577
H	-2.26934260	0.14033576	-2.47948104
H	-3.18188480	0.45384483	-0.98381766
H	-3.28726140	1.59464135	-2.33692162
C	1.58250833	-2.10663554	3.10797076
H	2.39036210	-1.38767687	3.32016298
H	1.39130247	-2.66129762	4.03942540
H	1.92910684	-2.83370011	2.35595313
C	-0.09233836	-0.43229873	3.83551607
H	-1.04300668	0.08802349	3.67048587
H	-0.17285570	-1.00374083	4.77469201
H	0.70428301	0.31906064	3.95968614
C	-0.78592143	2.41646565	-2.54029696
H	-1.57656956	3.00200931	-3.03360942

H	0.03324681	3.11374939	-2.30030589
H	-0.42882864	1.66915549	-3.26696571
C	-1.85824804	2.92716128	-0.36518025
H	-2.56733099	3.55395154	-0.92986337
H	-2.36111523	2.58368256	0.54617252
H	-0.99781029	3.55428582	-0.08021720
C	3.40784181	0.16731946	-0.92443376
C	3.79171405	-1.29463548	-1.26471642
H	4.81645301	-1.31963276	-1.66973634
H	3.76182866	-1.94486480	-0.37702667
H	3.11046525	-1.71528249	-2.02134863
C	3.55597418	1.01898080	-2.19779050
H	3.32448049	2.08037270	-2.01247519
H	4.59856372	0.96413011	-2.54863804
H	2.91206286	0.65314127	-3.01363683
C	4.37503065	0.72108581	0.15056796
H	4.36233630	0.11855680	1.07154612
H	5.40413366	0.70954382	-0.24354943
H	4.11870071	1.75947330	0.41432817
Br	-6.40290774	-0.35142190	-3.31064964
Br	-6.49066769	1.49897533	-4.86500567

I→III (n=5)

Energy -26441.29533457 Dipole 17.446627 ZPE 0.425830 G(298.15) 205.63 Edisp -57.62

C	1.31586149	1.19429238	-1.07110526
C	1.93989562	-0.32122069	0.68961171
C	2.29014019	0.39392954	-0.46598934
C	0.67074342	-0.31020810	1.25409666
C	0.00480799	1.30075463	-0.60889041
C	-0.36099164	0.40825270	0.49410253
H	1.59915751	1.77900264	-1.94147526
H	2.71309359	-0.90885258	1.17977927
H	-0.65254053	-0.63373730	-0.30936917
Br	-2.09390286	0.71011455	1.37478565
Br	-5.85374039	-0.42893215	1.58583677
Br	-6.01833591	-2.65998312	-0.37941882
Br	-3.51419239	-2.42012172	-0.94227568
Br	-0.93968673	-2.07317746	-1.43915400
Br	-5.44358603	1.40259476	3.10778455
C	0.43489400	-1.12349995	2.54934355
C	-0.95703684	2.25525171	-1.35507808
C	-0.70524576	-2.16096392	2.38623226
H	-1.67633502	-1.71270964	2.14784294
H	-0.45644991	-2.88797888	1.59771954
H	-0.81221417	-2.70896094	3.33607375
C	-2.22350756	1.52205302	-1.86699787
H	-1.94920012	0.72957700	-2.58041113
H	-2.82561281	1.07421161	-1.06855497
H	-2.85604037	2.25362634	-2.39480323
C	1.68848914	-1.93712547	2.94811065
H	2.55325393	-1.29597939	3.18409654
H	1.44739404	-2.50302854	3.86097623
H	1.97537161	-2.66693443	2.17399497
C	0.15950928	-0.15190806	3.72754259
H	-0.74594405	0.44903428	3.58424438
H	0.03421962	-0.74424083	4.64862662
H	1.01476444	0.52791291	3.87260982
C	-0.29324493	2.87128111	-2.60904627
H	-1.03507350	3.52093491	-3.09829418
H	0.57674282	3.50142388	-2.36332649
H	0.00702965	2.10459181	-3.34120678
C	-1.32152761	3.44736648	-0.43050181
H	-1.97233331	4.13817824	-0.99092479
H	-1.85469054	3.13854567	0.47603167
H	-0.41312516	3.99730493	-0.13565698
C	3.71595816	0.28536802	-1.01559802
C	3.98718219	-1.19325051	-1.38925434
H	5.01011321	-1.28955889	-1.78807615
H	3.89881310	-1.86036019	-0.51815592

H	3.28183961	-1.54117869	-2.16066360
C	3.93746591	1.15300108	-2.26739329
H	3.78695683	2.22436788	-2.05741268
H	4.97503724	1.02658452	-2.61454986
H	3.27316503	0.85728404	-3.09535969
C	4.71732925	0.73660542	0.07573946
H	4.65170021	0.11569068	0.98213990
H	5.74485434	0.65362900	-0.31387304
H	4.54137426	1.78541403	0.36311163
Br	-7.46085896	-1.85921188	-2.93305770
Br	-8.65146770	-1.22180893	-4.91329700
Br	-6.29035279	-5.40029710	0.91112197
Br	-6.56992007	-7.54295042	1.94761620

I→II (n=1)

Energy -5850.75695777 Dipole 12.797972 ZPE 0.421149 G(298.15) 227.69 Edisp -42.84

C	-0.26302819	-1.39846315	-0.78626588
C	-1.03585904	0.16238127	0.86863440
C	-1.32367838	-0.69264274	-0.21920502
C	0.24929766	0.31364002	1.40804444
C	1.04293701	-1.25142624	-0.28361284
C	1.29009643	-0.41318331	0.80954284
H	-0.42813042	-2.09061892	-1.61479584
H	-1.85995400	0.71965684	1.31831541
H	2.30980891	-0.34928881	1.20110411
Br	4.21897180	-4.76661434	-1.22624219
C	0.54282697	1.21108061	2.62409638
C	2.06440601	0.20424450	-2.10901980
C	1.59873913	2.27343220	2.24073863
H	2.53868523	1.81105612	1.90053502
H	1.22377174	2.93003782	1.43803653
H	1.83391113	2.90443602	3.11395982
C	1.20250494	1.40257172	-1.93278381
H	0.13155706	1.15556099	-1.98996772
H	1.41289190	1.93653583	-0.99629532
H	1.41736477	2.09791986	-2.77214906
C	-0.71282696	1.94276683	3.13139825
H	-1.49013041	1.23643224	3.46523015
H	-0.44365843	2.57205011	3.99495156
H	-1.14378275	2.60183204	2.35976768
C	1.09239154	0.33338785	3.77280673
H	2.01675535	-0.18884099	3.48137861
H	1.31874423	0.95990874	4.65167516
H	0.35371416	-0.42753870	4.07095125
C	1.78042189	-0.73677168	-3.21901728
H	2.45501329	-0.50632117	-4.06810528
H	2.03703566	-1.77231569	-2.91456007
H	0.74034535	-0.68687192	-3.56908800
C	3.44679542	0.20582341	-1.58001642
H	4.15548431	0.40675328	-2.40835835
H	3.60358100	0.94970316	-0.78708798
H	3.71227434	-0.81047184	-1.21725980
C	-2.77475461	-0.83054604	-0.71257596
C	-3.65234623	-1.36877836	0.44184492
H	-3.29590035	-2.35636214	0.77514733
H	-3.64486040	-0.69246430	1.31090010
H	-4.69687858	-1.47337836	0.10403977
C	-3.30350969	0.55272531	-1.15776337
H	-3.27183252	1.28834376	-0.33887431
H	-2.70991040	0.95034528	-1.99755670
H	-4.35086579	0.46579619	-1.49163954
C	-2.89543283	-1.80016123	-1.90166669
H	-3.94984950	-1.86483959	-2.21490988
H	-2.31023675	-1.45790445	-2.77108762
H	-2.56293302	-2.81627342	-1.63550244
Br	2.33003200	-2.83634463	-0.56769192

I→II (n=2)

Energy -10998.40548862 Dipole 15.090025 ZPE 0.424053 G(298.15) 225.29 Edisp -49.40

C	-0.50174383	-1.32037399	-0.99458454
C	-1.22074108	0.18116244	0.72877045
C	-1.53901790	-0.62569559	-0.39199834
C	0.06913877	0.29820303	1.27632708
C	0.83588836	-1.18288166	-0.51928578
C	1.09067238	-0.42363354	0.65618625
H	-0.68120218	-1.98616242	-1.83969678
H	-2.03491643	0.72483565	1.21251708
H	2.11095757	-0.41723501	1.05616937
Br	5.01011599	-1.88515589	1.04758017
Br	4.73576219	-4.27776030	-0.04255922
Br	4.99456833	0.52907309	2.01270038
C	0.37009949	1.14478761	2.52487057
C	1.74954111	0.09992989	-1.97274964
C	1.33865994	2.28591700	2.13531625
H	2.30121966	1.89219404	1.76906654
H	0.89454191	2.94025575	1.36616146
H	1.55565581	2.90476572	3.02154108
C	0.94818908	1.36912678	-1.90003733
H	-0.12314076	1.20798348	-2.08641221
H	1.08792953	1.89962070	-0.94919882
H	1.32727659	2.02819278	-2.70516009
C	-0.90591146	1.76028004	3.12668831
H	-1.62826378	0.98755843	3.43859238
H	-0.63507962	2.34039300	4.02275407
H	-1.40466908	2.45131897	2.42638804
C	1.04071921	0.25272355	3.59663561
H	2.01728171	-0.13018944	3.26232721
H	1.21838943	0.84760263	4.50743395
H	0.39588731	-0.60042916	3.86205200
C	1.55420823	-0.70925516	-3.22667475
H	2.15743299	-0.22886513	-4.02022788
H	1.93497131	-1.73609320	-3.11165473
H	0.50707988	-0.72791618	-3.55997130
C	3.16311091	0.18682938	-1.49145622
H	3.78678785	0.50759121	-2.34784610
H	3.30274425	0.90098663	-0.66825752
H	3.57165541	-0.79098705	-1.17615185
C	-2.99919032	-0.72736104	-0.86232385
C	-3.86227429	-1.29067614	0.29106237
H	-3.51742599	-2.29474932	0.58482040
H	-3.83171818	-0.64455788	1.18233643
H	-4.91358259	-1.36666287	-0.03174930
C	-3.51064446	0.67909505	-1.25172780
H	-3.45541820	1.38631901	-0.40930175
H	-2.92553653	1.09612313	-2.08774066
H	-4.56435995	0.61880730	-1.56973274
C	-3.15058510	-1.65579721	-2.07998986
H	-4.20996706	-1.69474213	-2.37911334
H	-2.57445987	-1.29301601	-2.94726873
H	-2.83158310	-2.68563421	-1.85173495
Br	1.95094656	-2.82584577	-0.63369138

I→II (n=3)

Energy -16146.04800999 Dipole 16.419325 ZPE 0.425775 G(298.15) 220.07 Edisp -51.19

C	-1.26641914	-0.02392505	0.01959590
C	-0.65712901	-1.27202313	-0.30213891
C	0.56675641	-1.63861693	0.24357239
C	1.14493285	-0.75163006	1.17625062
C	0.54701499	0.45373886	1.60111229
C	-0.67610413	0.78696843	1.03276243
C	-1.03634360	1.08545653	-1.68824644
C	1.27881552	-2.95645416	-0.10237734
C	1.23832766	1.31580939	2.66989478
C	2.62680664	1.75463248	2.14955078
C	0.42258616	2.57562910	3.00937682
C	1.40769410	0.48011215	3.96023275
C	0.45304145	1.22054536	-1.87420219
C	-1.71576356	0.26318502	-2.74552644

C	-1.73632551	2.37686052	-1.37551010
C	2.66954076	-2.64141676	-0.70058542
C	1.44584886	-3.79342397	1.18742369
C	0.48430858	-3.78897171	-1.12391487
H	-1.17562107	-1.92476186	-1.00583409
H	2.10846320	-1.02712343	1.61489227
H	-1.20782288	1.69008210	1.33568545
H	3.13739454	2.36071104	2.91547509
H	3.27358791	0.89300746	1.91985313
H	2.53355376	2.36553498	1.23707861
H	0.95559062	3.15768104	3.77755774
H	-0.57136257	2.32429768	3.41356985
H	0.29070651	3.22940086	2.13165513
H	1.90595253	1.08632629	4.73417930
H	2.02274181	-0.41830974	3.79297932
H	0.42959301	0.15769844	4.35115583
H	0.57657151	1.82003307	-2.79806706
H	0.93895356	1.76477833	-1.05272141
H	0.95383603	0.25516321	-2.03031700
H	-1.72212436	0.89940409	-3.65450274
H	-2.76636884	0.04520198	-2.50398396
H	-1.17078064	-0.66118990	-2.98296066
H	-1.74076079	2.94714322	-2.32729758
H	-1.20675333	2.97805655	-0.62320050
H	-2.78793450	2.23116192	-1.08831099
H	3.19477408	-3.58088254	-0.93765332
H	3.30196533	-2.07303787	-0.00025256
H	2.57826151	-2.05732312	-1.63063790
H	1.95890841	-4.74041083	0.95346008
H	0.46615848	-4.03218511	1.63087988
H	2.04629737	-3.26732763	1.94644637
H	1.03223880	-4.71981901	-1.33906231
H	-0.50969615	-4.07008520	-0.73993944
H	0.35452032	-3.25342981	-2.07868002
Br	-3.27901266	-0.14855524	0.18284728
Br	-6.29303207	-0.09785106	0.05751111
Br	-6.20919842	1.30145505	-2.10651826
Br	-6.14871433	2.74311149	-4.33647078
Br	-3.48791508	3.06170091	-4.77732891
Br	-0.98056064	3.31386656	-5.11875772

I→II (n=4)

Energy -21293.680336774 Dipole 13.443430 ZPE 0.427254 G(298.15) 215.72 Edisp -55.02

C	-1.14271961	0.63025082	0.38624533
C	-0.88127456	-0.66223225	-0.18091283
C	0.24534857	-1.39270118	0.17004844
C	1.10569199	-0.81441559	1.12854467
C	0.87623043	0.42146657	1.77455776
C	-0.27322463	1.10984506	1.42085529
C	-0.92829648	1.92233919	-1.11459923
C	0.55474729	-2.79004349	-0.38778670
C	1.86525262	0.92105573	2.83899457
C	3.25800406	1.09607051	2.19009531
C	1.43045132	2.26960417	3.43901914
C	1.94940037	-0.11886448	3.98066118
C	0.52624912	1.82752572	-1.51470454
C	-1.89396183	1.43841200	-2.16725963
C	-1.31382461	3.25557161	-0.51292838
C	1.94967738	-2.78284895	-1.05456049
C	0.54359085	-3.79621896	0.78820781
C	-0.48802828	-3.23637837	-1.42694468
H	-1.59660684	-1.05291635	-0.90659725
H	2.00195988	-1.37630691	1.40726335
H	-0.53926186	2.04673864	1.91237065
H	3.98064203	1.44152214	2.94707363
H	3.64022124	0.15252188	1.76953199
H	3.22701052	1.84223047	1.37983748
H	2.16854781	2.58613152	4.19261871
H	0.45233725	2.19914080	3.94214602

H	1.37851058	3.06207567	2.67429176
H	2.66087626	0.22764056	4.74768879
H	2.29898903	-1.09984312	3.62192125
H	0.96714126	-0.25916344	4.45919898
H	0.67727142	2.53432742	-2.35132160
H	1.20639440	2.12454216	-0.70353238
H	0.80712499	0.83587422	-1.89481281
H	-1.95110829	2.22632860	-2.94099250
H	-2.91666826	1.30855253	-1.77926401
H	-1.55515503	0.52075030	-2.66744110
H	-1.36656094	3.98042850	-1.34539526
H	-0.56985152	3.62651446	0.20679151
H	-2.30971213	3.22742204	-0.04561281
H	2.17604212	-3.79106449	-1.43760210
H	2.74776595	-2.51435642	-0.34293066
H	1.98879939	-2.08025519	-1.90246467
H	0.77074246	-4.80585304	0.40959746
H	-0.44414692	-3.82517332	1.27566348
H	1.29809221	-3.54960001	1.55293946
H	-0.22784945	-4.24406597	-1.78720564
H	-1.50096667	-3.29304705	-0.99537496
H	-0.50736437	-2.57033398	-2.30469034
Br	-3.06628278	0.79580520	0.90980512
Br	-6.09148971	1.19555712	1.18016335
Br	-6.18795450	1.32278239	-1.35635200
Br	-6.22831594	1.47413718	-4.04246361
Br	-4.36618353	-0.24771103	-4.77132785
Br	-2.59670678	-1.97345089	-5.54233355
Br	-0.06809825	-1.03207856	-4.89513087
Br	2.25850098	-0.31424214	-4.33359004

I→II (n=5)

Energy -26441.306053914 Dipole 14.668281 ZPE 0.428668 G(298.15) 211.29 Edisp -59.67

C	-1.07977004	0.35118845	0.54632129
C	-0.77203014	-0.93220016	-0.01302579
C	0.39615684	-1.60243466	0.32229246
C	1.23857832	-0.97934737	1.26868180
C	0.95515938	0.24434307	1.91549802
C	-0.23456263	0.87142761	1.57835695
C	-0.83512047	1.62238424	-0.96768409
C	0.76005684	-2.98945651	-0.22915081
C	1.92783501	0.79489657	2.97002765
C	3.30378022	1.03966820	2.30790144
C	1.43043003	2.12024036	3.57289364
C	2.07580354	-0.23875246	4.11095907
C	0.62391105	1.53551089	-1.35107429
C	-1.77850607	1.10987810	-2.02377788
C	-1.23750395	2.95828768	-0.38990804
C	2.15719596	-2.93921189	-0.88845140
C	0.77682264	-3.98874698	0.95283735
C	-0.25932483	-3.47731403	-1.27328523
H	-1.47970503	-1.36098873	-0.72408424
H	2.16410805	-1.49597015	1.53932521
H	-0.54586302	1.79150179	2.07439779
H	4.01516761	1.42007242	3.05866110
H	3.72871177	0.11656491	1.88281989
H	3.22876381	1.78475844	1.49950618
H	2.15988445	2.47746084	4.31654532
H	0.46370890	2.00011177	4.08846970
H	1.32712899	2.90667647	2.80721455
H	2.77567130	0.14466576	4.87098887
H	2.47227552	-1.20077969	3.74955649
H	1.10669141	-0.42878588	4.59901849
H	0.76719682	2.25349293	-2.17959111
H	1.29721946	1.83497552	-0.53557357
H	0.91170543	0.54849587	-1.73835306
H	-1.85137153	1.90138366	-2.79367144
H	-2.80280097	0.96651838	-1.64689157
H	-1.41605406	0.19781168	-2.51713854

H	-1.27722787	3.67145712	-1.23667126
H	-0.50841939	3.34258473	0.33778625
H	-2.24386999	2.93823720	0.05345991
H	2.42688620	-3.94558867	-1.24751124
H	2.94037508	-2.62134846	-0.18098778
H	2.16595574	-2.25795679	-1.75430925
H	1.03984630	-4.99250941	0.58192382
H	-0.21154563	-4.04757219	1.43629208
H	1.51872121	-3.71098597	1.71916532
H	0.04618846	-4.47088452	-1.63702617
H	-1.26976578	-3.58138261	-0.84460354
H	-0.30815296	-2.80910621	-2.14848040
Br	-3.01869742	0.49952400	1.01554672
Br	-6.17569575	0.95173240	1.13871722
Br	-6.03800472	1.57284880	-1.25810297
Br	-5.77567751	2.26011880	-3.95610083
Br	-3.60045702	4.14076072	-3.67136791
Br	-1.70373997	5.65412632	-3.35996618
Br	-4.36251898	0.12053568	-4.81936984
Br	-3.03994886	-1.89254711	-5.61390267
Br	-0.37229818	-1.31870884	-4.94086519
Br	1.99669642	-0.86166208	-4.37423826

Br_2 and 1,3,5-tri-*tert*-butylbenzene (zero level)

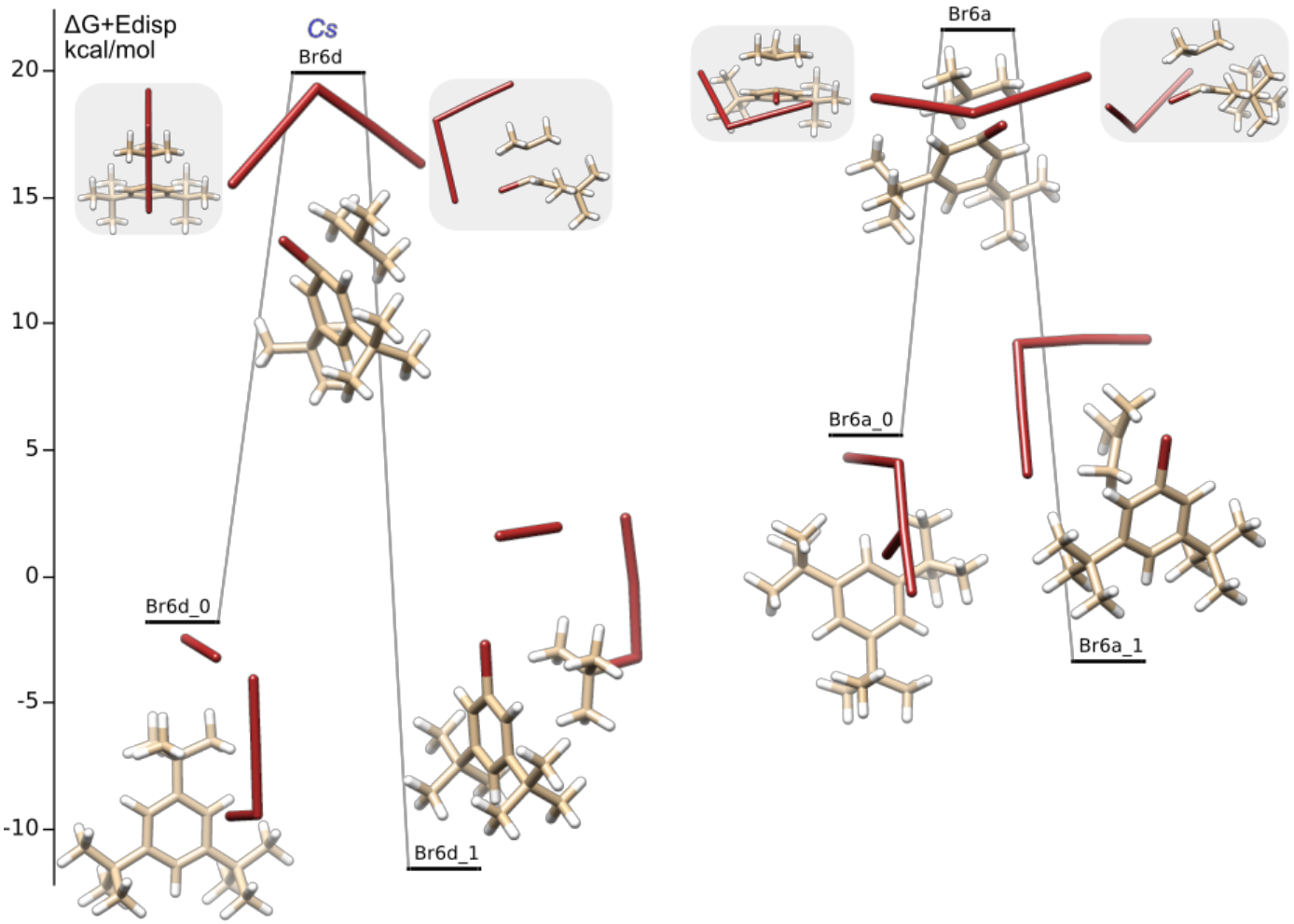
Br_2

```
Energy -5147.612945443  ZPE 0.000688  G(298) -14.75  Edisp -0.80
 Br  -0.97011655  -0.63390917  -0.18653487
 Br   0.97011655   0.63390917   0.18653487
```

1,3,5-tri-*tert*-butylbenzene

```
Energy -703.2159711986  ZPE 0.424741  G(298.15) 236.63 Edisp -36.80
 C    0.20798034   1.17889394  -0.70087958
 C    0.82297750  -0.32623274   1.06823566
 C    1.04976414   0.87539455   0.36982023
 C   -0.20576900  -1.20207964   0.71942795
 C   -0.84267643   0.32581048  -1.09007607
 C   -1.02971556  -0.85349032  -0.36807738
 H    0.36514442   2.10501279  -1.25695564
 H    1.47421425  -0.57612961   1.90791990
 H   -1.83833415  -1.52980418  -0.65154348
 C   -0.46695943  -2.51858727   1.47401973
 C   -1.73455717   0.71992025  -2.28173604
 C    0.52748158  -2.74398629   2.62733900
 H    1.56642620  -2.80163767   2.26379198
 H    0.46465487  -1.94294848   3.38183700
 H    0.29517953  -3.69681757   3.13052449
 C   -2.82904672  -0.32385164  -2.56900104
 H   -2.39844828  -1.30644552  -2.82193603
 H   -3.50750527  -0.44975690  -1.70951138
 H   -3.43491203   0.00749202  -3.42818459
 C   -1.89431941  -2.49431782   2.06869253
 H   -2.65905234  -2.37683692   1.28525963
 H   -2.09957986  -3.43669674   2.60458005
 H   -2.00605925  -1.66012351   2.78004099
 C   -0.34096515  -3.70716458   0.49277859
 H    0.67253619  -3.75160171   0.06238338
 H   -0.53599074  -4.65724257   1.01878832
 H   -1.05904812  -3.62677898  -0.33803014
 C   -0.86235866   0.86229592  -3.55079234
 H   -1.48761997   1.15464061  -4.41158770
 H   -0.08164503   1.62828800  -3.42382403
 H   -0.36598977  -0.09163312  -3.79168771
 C   -2.42597148   2.07016572  -1.98127131
 H   -3.06120123   2.37011842  -2.83207848
 H   -3.06227722   1.99134190  -1.08500888
 H   -1.69245943   2.87264549  -1.80704409
 C    2.20182180   1.79845175   0.80750515
 C    3.54133290   1.03268607   0.70387560
 H    4.37549752   1.67987141   1.02435351
 H    3.54636421   0.13412189   1.34021678
 H    3.72922189   0.71454139  -0.33433602
 C    2.30629987   3.06366093  -0.06324144
 H    1.38980253   3.67341119  -0.00739950
 H    3.14422139   3.68520681   0.29260811
 H    2.49818898   2.81610308  -1.12001537
 C    1.97675328   2.24104611   2.27207790
 H    1.93403716   1.37872144   2.95540714
 H    2.80116002   2.89547705   2.60289839
 H    1.03140116   2.79884458   2.36983624
```

PES I→II, n=3 (DFT/PBE/L1+ΔG+D3)



Br6d (point 20.0 on Fig.8 of the paper)

Energy -16146.04800999 Dipole 16.419325 ZPE 0.425775 G(298.15) 220.07 Edisp -51.19

C	-1.26641914	-0.02392505	0.01959590
C	-0.65712901	-1.27202313	-0.30213891
C	0.56675641	-1.63861693	0.24357239
C	1.14493285	-0.75163006	1.17625062
C	0.54701499	0.45373886	1.60111229
C	-0.67610413	0.78696843	1.03276243
C	-1.03634360	1.08545653	-1.68824644
C	1.27881552	-2.95645416	-0.10237734
C	1.23832766	1.31580939	2.66989478
C	2.62680664	1.75463248	2.14955078
C	0.42258616	2.57562910	3.00937682
C	1.40769410	0.48011215	3.96023275
C	0.45304145	1.22054536	-1.87420219
C	-1.71576356	0.26318502	-2.74552644
C	-1.73632551	2.37686052	-1.37551010
C	2.66954076	-2.64141676	-0.70058542
C	1.44584886	-3.79342397	1.18742369
C	0.48430858	-3.78897171	-1.12391487
H	-1.17562107	-1.92476186	-1.00583409
H	2.10846320	-1.02712343	1.61489227
H	-1.20782288	1.69008210	1.33568545
H	3.13739454	2.36071104	2.91547509
H	3.27358791	0.89300746	1.91985313
H	2.53355376	2.36553498	1.23707861
H	0.95559062	3.15768104	3.77755774
H	-0.57136257	2.32429768	3.41356985
H	0.29070651	3.22940086	2.13165513
H	1.90595253	1.08632629	4.73417930
H	2.02274181	-0.41830974	3.79297932
H	0.42959301	0.15769844	4.35115583

```
 H    0.57657151   1.82003307  -2.79806706
 H    0.93895356   1.76477833  -1.05272141
 H    0.95383603   0.25516321  -2.03031700
 H   -1.72212436   0.89940409  -3.65450274
 H   -2.76636884   0.04520198  -2.50398396
 H   -1.17078064  -0.66118990  -2.98296066
 H   -1.74076079   2.94714322  -2.32729758
 H   -1.20675333   2.97805655  -0.62320050
 H   -2.78793450   2.23116192  -1.08831099
 H    3.19477408  -3.58088254  -0.93765332
 H    3.30196533  -2.07303787  -0.00025256
 H    2.57826151  -2.05732312  -1.63063790
 H    1.95890841  -4.74041083   0.95346008
 H    0.46615848  -4.03218511   1.63087988
 H    2.04629737  -3.26732763   1.94644637
 H    1.03223880  -4.71981901  -1.33906231
 H   -0.50969615  -4.07008520  -0.73993944
 H    0.35452032  -3.25342981  -2.07868002
 Br  -3.27901266  -0.14855524   0.18284728
 Br  -6.29303207  -0.09785106   0.05751111
 Br  -6.20919842   1.30145505  -2.10651826
 Br  -6.14871433   2.74311149  -4.33647078
 Br  -3.48791508   3.06170091  -4.77732891
 Br  -0.98056064   3.31386656  -5.11875772
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Br6d_0

```
 Energy -16146.08739154  Dipole 10.033835  ZPE 0.428820  G(298.15) 221.22  Edisp -49.35
 C    0.14929295   0.49836649  -0.86348064
 C    0.59954887  -0.82173458  -0.93724356
 C    0.86441554  -1.58589971   0.20813959
 C    0.68362046  -0.99069285   1.47306238
 C    0.23481046   0.31605105   1.62299151
 C   -0.08035099   1.04790657   0.43505358
 C   -0.03350701   1.32419939  -2.14375398
 C    1.34624633  -3.04108236   0.12664963
 C    0.13082818   0.94604048   3.02108340
 C    1.54592430   0.96545304   3.65113567
 C   -0.39920141   2.39153593   2.98649216
 C   -0.81210078   0.09898252   3.90784083
 C    1.34890261   1.44913571  -2.83561031
 C   -1.01400995   0.60509613  -3.10130215
 C   -0.56212298   2.74524368  -1.87454651
 C    2.71486621  -3.16668251   0.83822117
 C    0.31019966  -3.94857090   0.83371411
 C    1.50898652  -3.53186622  -1.32309314
 H    0.76047644  -1.26442281  -1.92037853
 H    0.91350238  -1.57567050   2.36648076
 H   -0.28149333   2.11634162   0.51535249
 H    1.49634095   1.41499541   4.65671351
 H    1.96187325  -0.04889756   3.75198545
 H    2.24220452   1.56247454   3.04056632
 H   -0.46263113   2.77604339   4.01686603
 H   -1.40636762   2.44848734   2.54460958
 H    0.27339544   3.06248374   2.42738872
 H   -0.87088966   0.54249739   4.91534977
 H   -0.45217559  -0.93585076   4.01660613
 H   -1.82616497   0.06797171   3.48036410
 H    1.23589758   2.03999497  -3.75923833
 H    2.07516592   1.96003009  -2.18274379
 H    1.76106720   0.46468935  -3.10663143
 H   -1.12015452   1.19483302  -4.02554930
 H   -2.00887644   0.50388295  -2.64174614
 H   -0.65451609  -0.39856563  -3.37750706
 H   -0.67909212   3.27095377  -2.83505611
 H    0.13869018   3.33368266  -1.25870738
 H   -1.54715905   2.73062556  -1.38268191
 H    3.06176939  -4.21213985   0.79198182
 H    2.65695340  -2.87836253   1.89902362
 H    3.47086903  -2.53045403   0.35085753
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 H    0.64270765  -4.99870074   0.78563599
 H   -0.67431317  -3.87437210   0.34516720
 H    0.18590258  -3.68059766   1.89421953
 H    1.85159333  -4.57890512  -1.31468013
 H    0.55661211  -3.49790183  -1.87619874
 H    2.25854474  -2.94123580  -1.87432502
 Br  -2.56052307   0.57321255   0.44439473
 Br  -5.09109887   0.30951187   0.41466680
 Br  -5.64160524   1.63290699  -1.97208184
 Br  -6.11006391   2.81662381  -4.10489879
 Br  -3.45962757   3.39566447  -5.09127044
 Br  -1.23316270   3.89668786  -5.95988885
```

Br6d_1

```
Energy -16146.09810614  Dipole 8.556305  ZPE 0.426798  G(298.15) 215.92  Edisp -47.03
 C   -1.45016015  -0.66313198   0.99601833
 C   -0.77198240  -1.72964918   0.40939329
 C    0.61937067  -1.82697774   0.56149837
 C    1.27178823  -0.83219926   1.30600477
 C    0.59488738   0.24154620   1.90465115
 C   -0.79622432   0.31774791   1.73880163
 C   -1.17832627   1.70660048  -2.64981819
 C    1.43023825  -2.98131239  -0.05524886
 C    1.37969892   1.28776578   2.71700456
 C    2.43016471   1.96171884   1.80408237
 C    0.46778973   2.38535028   3.29413217
 C    2.09483095   0.58484589   3.89422608
 C    0.28344678   1.49465670  -2.29206946
 C   -1.90080657   0.42791449  -3.02655997
 C   -1.93019116   2.55732305  -1.64488399
 C    2.48133500  -2.40395186  -1.03146948
 C    2.14702133  -3.75853889   1.07324225
 C    0.54297332  -3.97037363  -0.83234332
 H   -1.33380000  -2.47462056  -0.15413660
 H    2.35582701  -0.90014153   1.43039288
 H   -1.37642063   1.12617374   2.18381421
 H    3.00706625   2.70612332   2.37791355
 H    3.14108497   1.23016426   1.38946984
 H    1.94266485   2.47935447   0.96190822
 H    1.07777302   3.10431875   3.86437558
 H   -0.28696359   1.96951418   3.98105476
 H   -0.05228307   2.94535520   2.49984796
 H    2.66582464   1.32196298   4.48326554
 H    2.79859888  -0.18571457   3.54305924
 H    1.36443550   0.10003226   4.56151194
 H    0.79917043   2.44749048  -2.10150912
 H    0.31493851   0.89379251  -1.36459284
 H    0.81982825   0.94202399  -3.07760464
 H   -2.92165743   0.62781882  -3.38234943
 H   -1.97824444  -0.18938422  -2.11346189
 H   -1.35017567  -0.13940350  -3.79083251
 H   -2.95110823   2.78162155  -1.98562739
 H   -1.39998057   3.49656109  -1.43074176
 H   -2.00893166   1.97305894  -0.71040671
 H    3.07670887  -3.22116296  -1.47184080
 H    3.17552121  -1.71570347  -0.52460653
 H    1.99303268  -1.85348078  -1.85207860
 H    2.73660265  -4.58666847   0.64553317
 H    1.41639405  -4.18326410   1.78005372
 H    2.83410759  -3.11246429   1.64145705
 H    1.17102575  -4.77337562  -1.25056405
 H   -0.21075772  -4.44137422  -0.18082001
 H    0.02329625  -3.48153300  -1.67254113
 Br  -3.35971304  -0.52293963   0.74519217
 Br  -7.10018838   0.22890497  -0.48833043
 Br  -6.78509737   1.53808673  -2.50322813
 Br  -6.34132178   3.13187837  -4.95478984
 Br  -3.87635494   3.07735443  -4.81923233
 Br  -1.09675724   2.86030517  -4.42621681
```

Br6a

Energy -16146.04300925 Dipole 16.392028 ZPE 0.425728 G(298.15) 220.24 Edisp -52.76

C	-0.61881075	-1.09639550	-0.95947728
C	-1.32265706	0.37962611	0.78449741
C	-1.65067812	-0.40539800	-0.34932028
C	-0.03282679	0.48253138	1.33505468
C	0.72696122	-0.96624129	-0.49316088
C	0.98977099	-0.22282884	0.69518360
H	-0.80288116	-1.75908919	-1.80583146
H	-2.13358735	0.91788115	1.27971454
H	2.01278518	-0.21460156	1.08651313
Br	4.81394919	-1.59660151	1.63032933
Br	4.86424337	-4.27421593	1.49383535
Br	3.82827412	-5.01777748	-0.95420739
Br	2.90763364	-5.75183182	-3.17011312
Br	4.72553359	0.96234992	1.79447034
C	0.25413000	1.30528174	2.60320124
C	1.58319423	0.30830270	-1.94464531
C	1.09841239	2.54156672	2.21411402
H	2.06782862	2.24374230	1.78355076
H	0.55963469	3.18043570	1.49429796
H	1.30737791	3.14401278	3.11338474
C	0.89195494	1.63076074	-1.75495012
H	-0.20446613	1.54259953	-1.76211677
H	1.21876685	2.14711639	-0.84313226
H	1.17076371	2.26223322	-2.62002765
C	-1.04143387	1.78526830	3.28333298
H	-1.69467523	0.94237242	3.56449149
H	-0.77997507	2.32491919	4.20692859
H	-1.61343811	2.48351669	2.64953793
C	1.04352684	0.43944714	3.61272668
H	2.03380384	0.15080017	3.22907505
H	1.20945342	1.01787137	4.53596398
H	0.48426041	-0.47311659	3.87413800
C	1.23905430	-0.42090459	-3.21778169
H	1.85015014	0.03185075	-4.02114243
H	1.52079956	-1.48491524	-3.16983925
H	0.18065127	-0.31926454	-3.49490254
C	3.04132210	0.28580370	-1.59867801
H	3.55830495	0.83129181	-2.41290110
H	3.28776077	0.79062866	-0.65298500
H	3.45455569	-0.73375420	-1.58787181
C	-3.11233882	-0.49379723	-0.81541423
C	-3.97415726	-1.06609674	0.33458245
H	-3.63442778	-2.07561334	0.61510960
H	-3.93866512	-0.43058189	1.23339462
H	-5.02644671	-1.13237117	0.01356260
C	-3.61535132	0.92092142	-1.18558142
H	-3.55418328	1.61751650	-0.33454127
H	-3.03065827	1.34440615	-2.01862648
H	-4.67018108	0.87081946	-1.50100566
C	-3.27080653	-1.40686428	-2.04360681
H	-4.33078656	-1.43593794	-2.34125211
H	-2.69450463	-1.03728473	-2.90790400
H	-2.95802533	-2.44143496	-1.82874919
Br	1.78110439	-2.62895551	-0.67122561

Br6a_0

Energy -16146.07335091 Dipole 11.197152 ZPE 0.428925 G(298.15) 222.33 Edisp -51.85

C	-0.55336720	0.31762394	-1.48956315
C	-1.44883596	-0.17524627	0.71352487
C	-1.63601251	-0.05869757	-0.69047568
C	-0.22250885	0.00512973	1.31787265
C	0.72243395	0.52907155	-0.95877783
C	0.92017610	0.25456678	0.45164723
H	-0.70571413	0.46582468	-2.55810578
H	-2.31596320	-0.40087401	1.33383836
H	1.83825130	0.62556848	0.91694495

```
 Br    4.88103149  -0.78400639   1.88012829
 Br    5.20213131  -3.37177786   0.94335747
 Br    2.89161511  -4.33391719  -0.14929490
 Br    0.90898937  -5.51623925  -1.19199503
 Br    4.58317554   1.56082976   2.68684651
 C    -0.04260410   0.03546383   2.83715601
 C     1.83378549   1.10660854  -1.83951850
 C     0.38252827   1.47716973   3.22770804
 H     1.37211481   1.73950152   2.82224434
 H    -0.35673307   2.21846982   2.88327845
 H     0.45145520   1.54304913   4.32589448
 C     1.37139704   2.53280061  -2.25259233
 H     0.43403720   2.51109327  -2.82922817
 H     1.22327589   3.17407355  -1.36919536
 H     2.15300916   2.98995021  -2.88101276
 C    -1.35016205  -0.30179162   3.57656936
 H    -1.70685286  -1.31563485   3.33191170
 H    -1.16447735  -0.26716970   4.66138756
 H    -2.15155718   0.42217894   3.35541400
 C     1.04927322  -0.95399065   3.30422730
 H     2.03259970  -0.74530102   2.85842127
 H     1.15682799  -0.86992820   4.39777470
 H     0.77391591  -1.99171429   3.06110067
 C     2.01993073   0.24544125  -3.11124957
 H     2.79643313   0.70228309  -3.74538253
 H     2.34063713  -0.77317153  -2.84609071
 H     1.09794267   0.17619862  -3.70880501
 C     3.18759752   1.23226305  -1.12065772
 H     3.92401011   1.65202875  -1.82378032
 H     3.14502886   1.91085410  -0.25378596
 H     3.57035236   0.25948038  -0.77756032
 C    -3.02131528  -0.33906825  -1.27638314
 C    -3.39325916  -1.80899283  -0.95303964
 H    -2.66343977  -2.50632238  -1.39365566
 H    -3.43114190  -1.99445514   0.13113349
 H    -4.38770070  -2.03445660  -1.37188894
 C    -4.05751223   0.61279195  -0.62936209
 H    -4.11520406   0.48553128   0.46217902
 H    -3.81197188   1.66561589  -0.84150581
 H    -5.05605970   0.40105209  -1.04502665
 C    -3.07324003  -0.14843733  -2.80246732
 H    -4.08963633  -0.37669887  -3.16020609
 H    -2.84425417   0.88921290  -3.09517527
 H    -2.37814562  -0.82616657  -3.32362359
 Br    1.71371269  -1.84766904   0.00884509
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Br6a_1

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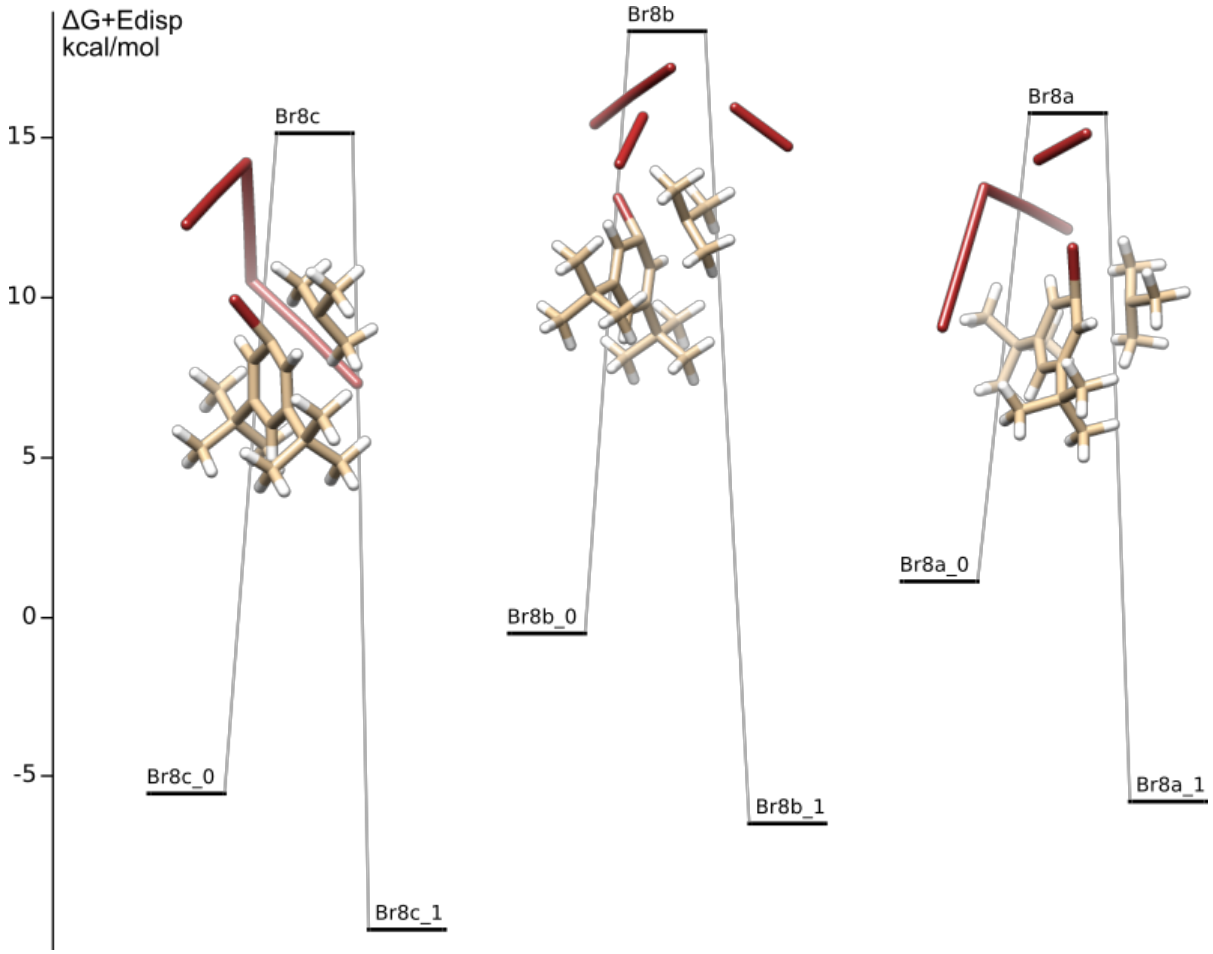
Energy -16146.08142535  Dipole 8.907920  ZPE 0.422692  G(298.15) 214.57  Edisp -47.99
 C    -1.86141370  -1.32315764   0.09792072
 C    -1.66497361   0.97202489   0.79048695
 C    -2.19198967   0.02599101  -0.10194141
 C    -0.83092038   0.62966279   1.86604848
 C    -1.03119765  -1.66760240   1.16241278
 C    -0.51054461  -0.72495673   2.04534562
 H    -2.24579427  -2.10489652  -0.55713217
 H    -1.92095469   2.02490853   0.64551985
 H     0.13631692  -1.05048491   2.85970385
 Br    5.63990351  -1.14528231   0.38292486
 Br    7.29330131  -2.96407383  -0.61828105
 Br    5.60714990  -3.84399472  -2.58736419
 Br    3.92609973  -4.51688939  -4.33704443
 Br    3.99449331   0.61019471   1.31755215
 C    -0.31185762   1.72396674   2.81648514
 C     2.44082301  -1.36711104  -1.84493166
 C     0.47737136   2.78010061   2.00884538
 H     1.35653868   2.32638859   1.52243360
 H    -0.14306942   3.25105945   1.23029991
 H     0.83451187   3.57676532   2.68224000
 C     1.81199468  -0.30689199  -1.10741406
```

H	0.92278568	-0.60451270	-0.53241348
H	2.59076767	-0.04084068	-0.28404539
H	1.68725127	0.63004285	-1.66761910
C	-1.51996219	2.40119263	3.50561740
H	-2.09548619	1.66919370	4.09457268
H	-1.16801823	3.19351605	4.18710649
H	-2.20199240	2.86177957	2.77379086
C	0.61625715	1.15981384	3.90720887
H	1.51118218	0.68146884	3.47629123
H	0.95830187	1.98299933	4.55486363
H	0.09686596	0.42813844	4.54732459
C	2.31858209	-2.76306095	-1.40805401
H	2.10600732	-3.41597154	-2.27910363
H	3.32935271	-3.11189726	-1.09989497
H	1.59650378	-2.91731833	-0.59622016
C	3.30767198	-1.07484888	-2.99360278
H	3.05644238	-1.74499396	-3.84103675
H	3.30455083	-0.02021586	-3.29441024
H	4.33996749	-1.40304070	-2.73896367
C	-3.10765181	0.48091416	-1.25308978
C	-4.34558615	1.19780489	-0.66584074
H	-4.91523888	0.51978568	-0.01049374
H	-4.06386312	2.08381309	-0.07616028
H	-5.00997992	1.53100758	-1.48054988
C	-2.33191292	1.45782156	-2.16698010
H	-1.98268848	2.34389675	-1.61443625
H	-1.45298783	0.96312398	-2.61210658
H	-2.98200795	1.80497077	-2.98732364
C	-3.59775229	-0.69807274	-2.11275504
H	-4.24836317	-0.31816837	-2.91675820
H	-2.76057915	-1.23530824	-2.58782451
H	-4.18514607	-1.41828716	-1.52053375
Br	-0.57906227	-3.53046752	1.41933063

PES I→II, n=4 (DFT/PBE/L1+ΔG+D3)



Br8c (point 15.2 on Fig.8 of the paper)
Energy -21293.680336774 Dipole 13.443430 ZPE 0.427254 G(298.15) 215.72 Edisp -55.02

C	-1.14271961	0.63025082	0.38624533
C	-0.88127456	-0.66223225	-0.18091283
C	0.24534857	-1.39270118	0.17004844
C	1.10569199	-0.81441559	1.12854467
C	0.87623043	0.42146657	1.77455776
C	-0.27322463	1.10984506	1.42085529
C	-0.92829648	1.92233919	-1.11459923
C	0.55474729	-2.79004349	-0.38778670
C	1.86525262	0.92105573	2.83899457
C	3.25800406	1.09607051	2.19009531
C	1.43045132	2.26960417	3.43901914
C	1.94940037	-0.11886448	3.98066118
C	0.52624912	1.82752572	-1.51470454
C	-1.89396183	1.43841200	-2.16725963
C	-1.31382461	3.25557161	-0.51292838
C	1.94967738	-2.78284895	-1.05456049
C	0.54359085	-3.79621896	0.78820781
C	-0.48802828	-3.23637837	-1.42694468
H	-1.59660684	-1.05291635	-0.90659725
H	2.00195988	-1.37630691	1.40726335
H	-0.53926186	2.04673864	1.91237065
H	3.98064203	1.44152214	2.94707363
H	3.64022124	0.15252188	1.76953199
H	3.22701052	1.84223047	1.37983748
H	2.16854781	2.58613152	4.19261871
H	0.45233725	2.19914080	3.94214602
H	1.37851058	3.06207567	2.67429176
H	2.66087626	0.22764056	4.74768879
H	2.29898903	-1.09984312	3.62192125
H	0.96714126	-0.25916344	4.45919898
H	0.67727142	2.53432742	-2.35132160

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 H    1.20639440   2.12454216  -0.70353238
 H    0.80712499   0.83587422  -1.89481281
 H   -1.95110829   2.22632860  -2.94099250
 H   -2.91666826   1.30855253  -1.77926401
 H   -1.55515503   0.52075030  -2.66744110
 H   -1.36656094   3.98042850  -1.34539526
 H   -0.56985152   3.62651446   0.20679151
 H   -2.30971213   3.22742204  -0.04561281
 H    2.17604212  -3.79106449  -1.43760210
 H    2.74776595  -2.51435642  -0.34293066
 H    1.98879939  -2.08025519  -1.90246467
 H    0.77074246  -4.80585304   0.40959746
 H   -0.44414692  -3.82517332   1.27566348
 H    1.29809221  -3.54960001   1.55293946
 H   -0.22784945  -4.24406597  -1.78720564
 H   -1.50096667  -3.29304705  -0.99537496
 H   -0.50736437  -2.57033398  -2.30469034
 Br  -3.06628278   0.79580520   0.90980512
 Br  -6.09148971   1.19555712   1.18016335
 Br  -6.18795450   1.32278239  -1.35635200
 Br  -6.22831594   1.47413718  -4.04246361
 Br  -4.36618353  -0.24771103  -4.77132785
 Br  -2.59670678  -1.97345089  -5.54233355
 Br  -0.06809825  -1.03207856  -4.89513087
 Br   2.25850098  -0.31424214  -4.33359004
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Br8c_0

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Energy -21293.71534758  Dipole 8.690092  ZPE 0.430128  G(298.15) 216.22  Edisp -54.20
 C    0.06548974   1.22951578  -0.33644316
 C   -0.42175296  -0.10241637  -0.58211938
 C   -0.00852245  -1.20944908   0.24323803
 C    0.77921141  -0.92513919   1.34894291
 C    1.21282102   0.38202339   1.65393831
 C    0.84872600   1.43345747   0.79775909
 C   -0.20376724   2.38558803  -1.30655958
 C   -0.37801259  -2.65902202  -0.09759312
 C    2.07433760   0.61024249   2.90168667
 C    3.36565444  -0.23647922   2.78813164
 C    2.47712609   2.08423442   3.08629881
 C    1.27054132   0.16468322   4.14826648
 C    1.16359855   2.82745492  -1.89397140
 C   -1.12347979   1.99584364  -2.47824948
 C   -0.84454879   3.57155579  -0.54649182
 C    0.93874478  -3.42399363  -0.39302861
 C   -1.09446313  -3.31159433   1.10895193
 C   -1.28851893  -2.77772024  -1.33370909
 H   -0.82602404  -0.32466621  -1.57106310
 H    1.08894625  -1.74588596   1.99899895
 H    1.20730088   2.43993372   1.01285550
 H    3.98675476  -0.08213657   3.68568810
 H    3.14928495  -1.31269227   2.70936719
 H    3.95401896   0.06033729   1.90538054
 H    3.08691475   2.18059915   3.99864440
 H    1.59775185   2.73784041   3.20378425
 H    3.08216690   2.45313941   2.24234667
 H    1.87970741   0.31907461   5.05405193
 H    0.99603211  -0.90017788   4.10166363
 H    0.34447569   0.75256519   4.24962624
 H    0.99924044   3.65749782  -2.60060961
 H    1.85232295   3.17657915  -1.10888782
 H    1.64231801   1.99812020  -2.43863671
 H   -1.27623684   2.87978687  -3.11751445
 H   -2.11297151   1.65928608  -2.13244758
 H   -0.68010379   1.21123891  -3.11162993
 H   -1.01154798   4.40483746  -1.24801501
 H   -0.19966977   3.94164156   0.26565082
 H   -1.81477258   3.28031005  -0.11516403
 H    0.70036399  -4.47109392  -0.64236720
 H    1.61526413  -3.42513872   0.47601245
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 H    1.46796886  -2.97583355  -1.24900799
 H   -1.33971150  -4.35792598   0.86494254
 H   -2.03042047  -2.78046542   1.34177444
 H   -0.46402801  -3.31685261   2.01185608
 H   -1.51980631  -3.84134718  -1.50275291
 H   -2.24326630  -2.24697969  -1.19634337
 H   -0.79941749  -2.40373133  -2.24716496
 Br  -2.58723684   0.22351856   0.36708565
 Br  -5.12646265   0.45421863   1.05717799
 Br  -6.01152323  -0.20309644  -1.38615080
 Br  -6.75973165  -0.83859398  -3.73476590
 Br  -4.41239536  -1.12442448  -5.11090973
 Br  -2.34670139  -1.41930265  -6.51803497
 Br  -0.01968449  -1.15455690  -4.93714835
 Br   2.09769423  -0.94440836  -3.68734118
Energy -21293.71235028  Dipole 6.510253  ZPE 0.424087  G(298.15) 208.86  Edisp -53.02
 C   -0.99897108  -0.25746820   2.11336427
 C   -0.76600842  -1.43199642   1.40086458
 C    0.53389253  -1.71783818   0.95407552
 C    1.54824977  -0.79423737   1.24904865
 C    1.32181204   0.38705126   1.97146548
 C    0.01409095   0.65273998   2.40792399
 C   -2.08815147   1.74349377  -1.78236425
 C    0.86821575  -3.00809916   0.18407886
 C    2.49307979   1.33970085   2.27309775
 C    3.12528880   1.81518129   0.94462950
 C    2.04917469   2.58060641   3.06833766
 C    3.55491135   0.58549736   3.10734353
 C   -0.90353235   2.18283541  -1.07935826
 C   -2.76439995   0.50835246  -1.38452331
 C   -2.66512002   2.56758813  -2.84835152
 C    1.51242018  -2.65102563  -1.17494000
 C    1.86309041  -3.84457084   1.02308758
 C   -0.37917065  -3.86891229  -0.08526492
 H   -1.59252090  -2.11759490   1.21252704
 H    2.56308736  -1.00907842   0.90507898
 H   -0.22222114   1.55019190   2.97977935
 H    3.97815240   2.48298013   1.15133405
 H    3.49367659   0.97249531   0.33970170
 H    2.39342285   2.37160081   0.33643425
 H    2.92263501   3.22559977   3.25558992
 H    1.62041765   2.30790432   4.04627940
 H    1.30652199   3.17848401   2.51478220
 H    4.40315213   1.25398384   3.33052438
 H    3.94770724  -0.29155161   2.57014683
 H    3.12787832   0.23773911   4.06155930
 H   -0.03323533   1.86090510  -1.74990987
 H   -0.80556322   3.27867509  -1.04089566
 H   -0.73730213   1.68905098  -0.11097251
 H   -3.33414244   0.03906605  -2.19932972
 H   -3.52065815   0.84882498  -0.62859942
 H   -2.09836900  -0.19077558  -0.85858646
 H   -2.88408055   1.95400558  -3.74163642
 H   -2.06501389   3.45134364  -3.09796215
 H   -3.68029082   2.87656950  -2.50464996
 H    1.76953783  -3.57463288  -1.71972014
 H    2.43645800  -2.06542147  -1.05248902
 H    0.82277333  -2.06437444  -1.80247317
 H    2.11997586  -4.77268715   0.48577412
 H    1.42373297  -4.11789916   1.99593925
 H    2.79737360  -3.29370620   1.21340033
 H   -0.08362489  -4.77346071  -0.64043454
 H   -0.86263839  -4.19614327   0.84963259
 H   -1.12231380  -3.33253017  -0.69783858
 Br  -2.79677582   0.12870336   2.70510700
 Br  -5.67440877   2.45663135   0.25610291
 Br  -6.22416398   1.94546616  -2.11027517
 Br  -6.59074456   1.28272515  -4.80999055
 Br  -4.41210061  -0.08079660  -5.07719986
```

```
 Br  -2.19771226  -1.51944745  -5.31103361
 Br  -0.20326147  -0.04534128  -4.21558633
 Br   1.69576663   1.26359633  -3.18262556
```

Br8c_1

```
Energy -21293.71235028  Dipole 6.510253  ZPE 0.424087  G(298.15) 208.86  Edisp -53.02
 C   -0.99897108  -0.25746820   2.11336427
 C   -0.76600842  -1.43199642   1.40086458
 C    0.53389253  -1.71783818   0.95407552
 C    1.54824977  -0.79423737   1.24904865
 C    1.32181204   0.38705126   1.97146548
 C    0.01409095   0.65273998   2.40792399
 C   -2.08815147   1.74349377  -1.78236425
 C    0.86821575  -3.00809916   0.18407886
 C    2.49307979   1.33970085   2.27309775
 C    3.12528880   1.81518129   0.94462950
 C    2.04917469   2.58060641   3.06833766
 C    3.55491135   0.58549736   3.10734353
 C   -0.90353235   2.18283541  -1.07935826
 C   -2.76439995   0.50835246  -1.38452331
 C   -2.66512002   2.56758813  -2.84835152
 C    1.51242018  -2.65102563  -1.17494000
 C    1.86309041  -3.84457084   1.02308758
 C   -0.37917065  -3.86891229  -0.08526492
 H   -1.59252090  -2.11759490   1.21252704
 H    2.56308736  -1.00907842   0.90507898
 H   -0.22222114   1.55019190   2.97977935
 H    3.97815240   2.48298013   1.15133405
 H    3.49367659   0.97249531   0.33970170
 H    2.39342285   2.37160081   0.33643425
 H    2.92263501   3.22559977   3.25558992
 H    1.62041765   2.30790432   4.04627940
 H    1.30652199   3.17848401   2.51478220
 H    4.40315213   1.25398384   3.33052438
 H    3.94770724  -0.29155161   2.57014683
 H    3.12787832   0.23773911   4.06155930
 H   -0.03323533   1.86090510  -1.74990987
 H   -0.80556322   3.27867509  -1.04089566
 H   -0.73730213   1.68905098  -0.11097251
 H   -3.33414244   0.03906605  -2.19932972
 H   -3.52065815   0.84882498  -0.62859942
 H   -2.09836900  -0.19077558  -0.85858646
 H   -2.88408055   1.95400558  -3.74163642
 H   -2.06501389   3.45134364  -3.09796215
 H   -3.68029082   2.87656950  -2.50464996
 H    1.76953783  -3.57463288  -1.71972014
 H    2.43645800  -2.06542147  -1.05248902
 H    0.82277333  -2.06437444  -1.80247317
 H    2.11997586  -4.77268715   0.48577412
 H    1.42373297  -4.11789916   1.99593925
 H    2.79737360  -3.29370620   1.21340033
 H   -0.08362489  -4.77346071  -0.64043454
 H   -0.86263839  -4.19614327   0.84963259
 H   -1.12231380  -3.33253017  -0.69783858
 Br  -2.79677582   0.12870336   2.70510700
 Br  -5.67440877   2.45663135   0.25610291
 Br  -6.22416398   1.94546616  -2.11027517
 Br  -6.59074456   1.28272515  -4.80999055
 Br  -4.41210061  -0.08079660  -5.07719986
 Br  -2.19771226  -1.51944745  -5.31103361
 Br  -0.20326147  -0.04534128  -4.21558633
 Br   1.69576663   1.26359633  -3.18262556
```

Br8a

```
Energy -21293.6729827  Dipole 15.505511  ZPE 0.427286  G(298.15) 216.24  Edisp -59.53
 C   -0.62589645  -0.95614302  -1.18771558
 C   -1.26548527   0.38668809   0.68522716
 C   -1.63702389  -0.34176224  -0.47599802
 C    0.04808857   0.50031383   1.17060855
```

```
 C    0.74194915  -0.81743453  -0.78179553
 C    1.04548118  -0.16275673   0.45163593
 H   -0.83867179  -1.56652754  -2.06571710
 H   -2.06187040   0.87195062   1.25277502
 H    2.07980278  -0.19208072   0.80930997
 Br   4.54619489  -1.27274842   1.69164156
 Br   3.70630703  -3.91351714   2.01690802
 Br   3.88172390  -5.00631306  -0.64342780
 Br   4.06666375  -5.96240116  -2.89382299
 Br   5.19467034   1.12062493   1.39464104
 C    0.38845541   1.27918069   2.45425299
 C    1.45071446   0.65365411  -2.11668801
 C    1.31293268   2.46471475   2.09123267
 H    2.26095209   2.12375313   1.64428288
 H    0.81545150   3.16403908   1.39796256
 H    1.56756116   3.02326208   3.00673846
 C    0.70135885   1.91357545  -1.78553093
 H   -0.38733852   1.76146463  -1.73961782
 H    1.05146003   2.37934863  -0.85596646
 H    0.89124274   2.62230908  -2.61397056
 C   -0.87362962   1.83057557   3.14226467
 H   -1.56056715   1.02137802   3.44000407
 H   -0.57486961   2.36385229   4.05820594
 H   -1.41726601   2.54981268   2.50625522
 C    1.11496077   0.34730903   3.45052062
 H    2.06016796  -0.04390188   3.04514567
 H    1.35474147   0.91425938   4.36480904
 H    0.47800011  -0.50764727   3.72393888
 C    1.09387320   0.03578934  -3.44607809
 H    1.63230182   0.61319783  -4.22094059
 H    1.44325481  -1.00542892  -3.52177162
 H    0.01838975   0.09054567  -3.66372738
 C    2.92565066   0.68563825  -1.83291944
 H    3.38410000   1.29904784  -2.63291651
 H    3.18330924   1.14614827  -0.86920491
 H    3.38454703  -0.31244161  -1.89606278
 C   -3.12021010  -0.45197771  -0.85929046
 C   -3.90108170  -1.07129102   0.32373846
 H   -3.49570269  -2.05996134   0.58974794
 H   -3.85880593  -0.43805963   1.22370845
 H   -4.96146526  -1.18611954   0.04592221
 C   -3.67167431   0.96024706  -1.16467911
 H   -3.56797167   1.63834783  -0.30264827
 H   -3.15109826   1.41382835  -2.02441068
 H   -4.74381998   0.89574202  -1.41173899
 C   -3.32770798  -1.34037242  -2.09812372
 H   -4.40273946  -1.39292831  -2.33128274
 H   -2.81679441  -0.93519714  -2.98756425
 H   -2.97414173  -2.36962667  -1.92513084
 Br   1.83654681  -2.39141565  -1.16825381
 Br   0.97686177  -3.43125375   2.51796711
 Br  -1.40188373  -2.94129111   3.01754994
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Br8a_0

```
Energy -21293.70316351  Dipole 10.717824  ZPE 0.430132  G(298.15) 218.42  Edisp -57.42
 C   -0.21173236  -0.35241294  -1.40615201
 C   -1.31230691  -0.00977423   0.73692824
 C   -1.31421441  -0.64082730  -0.49599023
 C   -0.33885632   0.94833949   1.09042957
 C    0.74205886   0.70831649  -1.09663463
 C    0.67081808   1.28495863   0.15593701
 H   -0.39016721  -0.55358680  -2.46480900
 H   -2.09613344  -0.24883098   1.45515098
 H    1.40896021   2.03885854   0.43422435
 Br   4.08016494  -0.95625529   2.01405640
 Br   3.03282787  -3.61326005   2.09398979
 Br   2.68472035  -4.42197756  -0.55773182
 Br   2.50968552  -5.32725972  -2.86792990
 Br   4.93465405   1.34534000   2.03916134
```

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 C   -0.35345204   1.63661129   2.45252608
 C    1.76855258   1.18228294  -2.13066410
 C   -0.30527098   3.17365947   2.26118734
 H    0.60976795   3.50677413   1.74925158
 H   -1.17672748   3.53117843   1.68931122
 H   -0.32322634   3.65468203   3.25219134
 C    1.54551296   2.70062573  -2.36092598
 H    0.52803166   2.90461632  -2.73173761
 H    1.70295665   3.28292966  -1.44074354
 H    2.26548046   3.05749183  -3.11526381
 C   -1.60045705   1.29051766   3.28588740
 H   -1.65427630   0.21658115   3.52666876
 H   -1.55121923   1.83746966   4.24062229
 H   -2.53084012   1.59386601   2.77727796
 C    0.90885787   1.17205759   3.22794797
 H    1.84082914   1.45034999   2.71290212
 H    0.90867911   1.65199072   4.22045838
 H    0.90634744   0.08027998   3.36853076
 C    1.63015816   0.46802965  -3.48865580
 H    2.40265171   0.85374700  -4.17204618
 H    1.77848874  -0.61924797  -3.40041885
 H    0.65249983   0.66232249  -3.96127223
 C    3.20072350   0.95480805  -1.58914307
 H    3.92894836   1.33437355  -2.32425935
 H    3.37626102   1.47717711  -0.63675926
 H    3.39427380  -0.11564317  -1.42581331
 C   -2.45355616  -1.58252785  -0.89463705
 C   -2.50973381  -2.77995929   0.08599066
 H   -1.58980436  -3.37988468   0.02456512
 H   -2.63359077  -2.45878754   1.13120447
 H   -3.36568621  -3.42180942  -0.17878079
 C   -3.78216300  -0.78482990  -0.80038201
 H   -3.98061366  -0.43680479   0.22416912
 H   -3.77284385   0.09012332  -1.47019716
 H   -4.61384146  -1.44173954  -1.10287371
 C   -2.32013904  -2.11977155  -2.33208703
 H   -3.16714496  -2.79230744  -2.53900367
 H   -2.35722996  -1.31102844  -3.08136289
 H   -1.39457437  -2.69897771  -2.47224338
 Br   1.05469178  -2.12377150  -0.98362118
 Br   0.42830555  -3.14905880   3.14807439
 Br  -1.79610636  -2.75002442   4.12349490
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Br8a_1

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Energy -21293.7068881  Dipole 8.170769  ZPE 0.424044  G(298.15) 209.96  Edisp -53.54
 C   -2.27076606  -0.81931948  -0.98203178
 C   -1.87556786   1.06694950   0.46200902
 C   -2.41902680   0.54903100  -0.72930268
 C   -1.20179074   0.27628776   1.39900249
 C   -1.59328161  -1.60946577  -0.05183287
 C   -1.05837657  -1.09869505   1.12265737
 H   -2.67606060  -1.27970276  -1.88296054
 H   -1.99105913   2.13290498   0.66412061
 H   -0.53628772  -1.76251038   1.81617788
 Br   4.81821766   0.55786483   0.68746786
 Br   6.07982199  -1.60591209   1.85443274
 Br   6.28510109  -3.12668768  -0.53881566
 Br   6.23575916  -4.39694978  -2.64897054
 Br   3.57822672   2.42840612  -0.40989215
 C   -0.62129576   0.84602865   2.70533856
 C    2.63003980  -1.49627440  -1.66202055
 C    0.91188430   0.64714972   2.71393910
 H    1.18709015  -0.41682346   2.64970561
 H    1.38680890   1.18306489   1.87606597
 H    1.33540080   1.04199831   3.65241018
 C    2.46240801  -2.67057771  -0.81659274
 H    1.39893148  -2.94268380  -0.68536048
 H    3.08773490  -3.52254655  -1.11467336
 H    2.79641807  -2.38321798   0.21953608
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C	-0.91573418	2.34831888	2.86738351
H	-1.99856833	2.55399440	2.89038993
H	-0.48859516	2.69870517	3.82059463
H	-0.45834723	2.94478245	2.06117804
C	-1.24285518	0.09686615	3.90725532
H	-1.00723070	-0.97829801	3.88474351
H	-0.84226536	0.50672223	4.84922622
H	-2.33895553	0.21059617	3.91846519
C	3.79899555	-1.40285995	-2.53614779
H	3.83095296	-0.49687019	-3.15325768
H	4.69810343	-1.45095013	-1.87475891
H	3.91482253	-2.32278091	-3.14189839
C	1.68806874	-0.38723712	-1.59675836
H	1.41618006	-0.05793663	-2.61631437
H	0.80086695	-0.57143985	-0.97829288
H	2.25004265	0.50910217	-1.20139902
C	-3.15384134	1.48601749	-1.70456602
C	-4.34854669	2.14446048	-0.97598352
H	-5.06029257	1.38075931	-0.62384944
H	-4.02201285	2.73299709	-0.10484880
H	-4.88086440	2.82346061	-1.66290363
C	-2.17834973	2.58361450	-2.18954509
H	-1.77950998	3.17511684	-1.35105082
H	-1.32602698	2.13965957	-2.72966115
H	-2.69729007	3.27420889	-2.87510086
C	-3.69476911	0.74076626	-2.93782034
H	-4.21174209	1.45496194	-3.59872800
H	-2.88522378	0.27280481	-3.52175132
H	-4.42031495	-0.03980274	-2.65690052
Br	-1.38665828	-3.49943614	-0.43212969
Br	3.57921852	-2.75532816	2.66831484
Br	1.41041292	-3.71329445	3.29570530

Br8b

Energy -21293.674075927 Dipole 16.966138 ZPE 0.427158 G(298.15) 215.57 Edisp -55.66

C	-1.13057339	-0.44531934	-0.13194234
C	-0.35180267	-1.63308131	-0.29905331
C	0.86131110	-1.79416953	0.35549435
C	1.24792106	-0.77126467	1.24936221
C	0.47238612	0.37229329	1.54045803
C	-0.73147699	0.50367868	0.86269222
C	-0.89355217	0.53606158	-1.85585127
C	1.75901544	-3.02803674	0.17096801
C	0.96280192	1.39057946	2.58165441
C	2.27033859	2.03756396	2.06783322
C	-0.07407672	2.49921074	2.83403044
C	1.23392268	0.66192793	3.91870697
C	0.59442088	0.76828756	-1.99312906
C	-1.46255293	-0.39181068	-2.89893273
C	-1.69545610	1.79213121	-1.65545282
C	3.13940310	-2.57688782	-0.36029604
C	1.93272955	-3.73391190	1.53614301
C	1.15524336	-4.03388408	-0.82466844
H	-0.72927289	-2.39661600	-0.98070436
H	2.20291826	-0.88450472	1.77096330
H	-1.39436926	1.34896517	1.05407035
H	2.64959653	2.75302313	2.81527906
H	3.05911730	1.28875729	1.88918462
H	2.09709756	2.58751722	1.12881063
H	0.31687110	3.19214194	3.59566540
H	-1.02376515	2.09034058	3.21593860
H	-0.28918245	3.09359006	1.93096909
H	1.58130383	1.38899389	4.67027008
H	2.01159500	-0.11275087	3.82412783
H	0.31711716	0.18514080	4.30038208
H	0.72897158	1.37724712	-2.90582683
H	1.01442787	1.33983407	-1.15370591
H	1.15995364	-0.16415334	-2.12780371
H	-1.47533428	0.17708668	-3.85115523

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 H   -2.50373449  -0.67374485  -2.68609000
 H   -0.84754740  -1.29038056  -3.05191058
 H   -1.80590847   2.26874676  -2.64809843
 H   -1.21095019   2.51233363  -0.98210042
 H   -2.72278954   1.59033232  -1.31503262
 H    3.79583475  -3.45363926  -0.48228091
 H    3.64026723  -1.87880598   0.32913494
 H    3.04528935  -2.08160920  -1.34020075
 H    2.57910604  -4.61867203   1.41796201
 H    0.96094540  -4.06722911   1.93359283
 H    2.40175615  -3.07644441   2.28521723
 H    1.83070112  -4.89817494  -0.92256548
 H    0.17861257  -4.41355440  -0.48300154
 H    1.03167197  -3.59594344  -1.82882550
 Br  -3.10390358  -0.80925029  -0.04933194
 Br  -6.21868955  -0.79206979  -0.32046981
 Br  -5.96490007   1.35854336  -1.59383835
 Br  -5.55107824   3.70586005  -2.95352306
 Br  -3.61798531   2.72100012  -4.78445472
 Br  -1.83457264   1.79942221  -6.22734020
 Br  -3.65899108   4.76490000  -1.08316421
 Br  -1.94018266   5.51039844   0.51183964
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Br8b_0

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Energy -21293.70684035  Dipole 11.205808  ZPE 0.429846  G(298.15) 215.36  Edisp -53.72
 C    0.22298989   0.13046378  -0.94966944
 C    0.86443069  -1.10513582  -0.86790307
 C    1.15985424  -1.71422833   0.36186931
 C    0.81006163  -1.04419104   1.55275542
 C    0.16382604   0.18473311   1.55204784
 C   -0.18576968   0.74982068   0.27860576
 C    0.01666469   0.81144088  -2.30823843
 C    1.85593962  -3.07851615   0.44878733
 C   -0.11672892   0.92214524   2.86963319
 C    1.24351109   1.21780649   3.55153800
 C   -0.85304501   2.25933023   2.66523679
 C   -0.97002967   0.02604580   3.79849094
 C    1.41393641   1.05125414  -2.93809528
 C   -0.80733771  -0.11100379  -3.23969719
 C   -0.69908659   2.16941678  -2.19819410
 C    3.17738947  -2.92716683   1.24076303
 C    0.91976611  -4.06653474   1.18735048
 C    2.18627231  -3.66691979  -0.93458856
 H    1.15889733  -1.60357246  -1.79155953
 H    1.06775595  -1.50412482   2.50921928
 H   -0.51075241   1.79055788   0.24401391
 H    1.06864430   1.75136856   4.50023521
 H    1.79857966   0.29403399   3.77697740
 H    1.87680992   1.85289052   2.91168116
 H   -1.03085888   2.72371354   3.64806344
 H   -1.83139706   2.12206898   2.17948270
 H   -0.26253358   2.97453861   2.06994327
 H   -1.15109268   0.55023613   4.75097441
 H   -0.46602322  -0.92548654   4.02883043
 H   -1.94262585  -0.20051717   3.33524346
 H    1.28653589   1.54710231  -3.91407177
 H    2.03097377   1.70272556  -2.29858601
 H    1.95941103   0.10888396  -3.10183977
 H   -0.93829855   0.38022707  -4.21740700
 H   -1.80439751  -0.30390863  -2.81576795
 H   -0.30693402  -1.07775857  -3.40767154
 H   -0.82827899   2.59077581  -3.20688654
 H   -0.11857125   2.89942135  -1.61022019
 H   -1.70256459   2.07647623  -1.75611228
 H    3.67822579  -3.90654616   1.31281839
 H    3.00668946  -2.56079878   2.26456800
 H    3.86078651  -2.22657359   0.73496767
 H    1.40715082  -5.05270448   1.26049101
 H   -0.02984271  -4.18935846   0.64276650
```

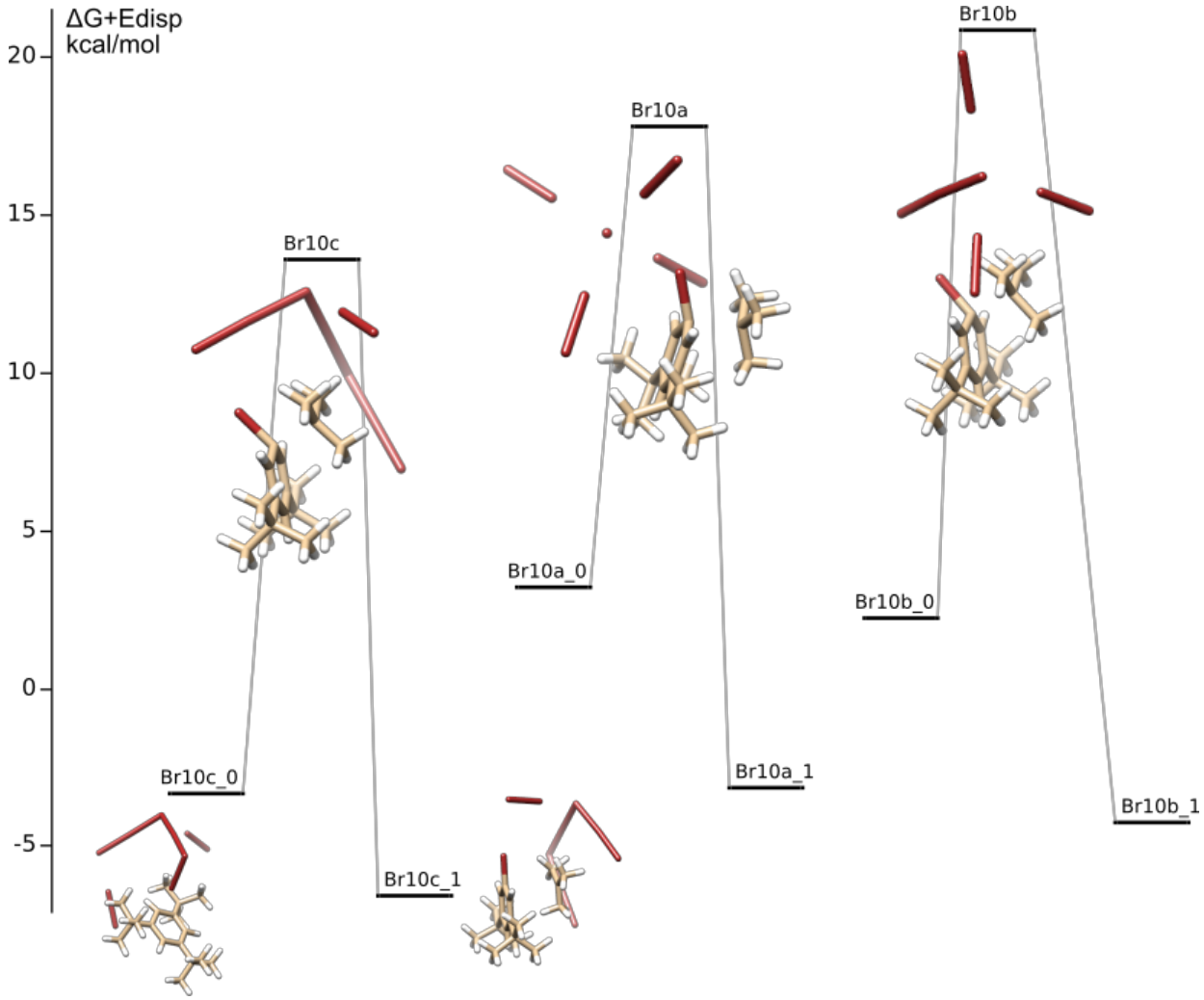
```
 H    0.68678908  -3.72689403   2.20817024
 H    2.67771343  -4.64412698  -0.80387103
 H    1.27882644  -3.82935750  -1.53813768
 H    2.87670432  -3.02123868  -1.50104601
 Br  -2.49106405  -0.04143419   0.21572082
 Br  -5.04047471  -0.52389718   0.03364730
 Br  -5.43716321   1.72555512  -1.40556337
 Br  -5.52692186   3.88649211  -2.72047335
 Br  -3.72809085   3.06791363  -4.95325683
 Br  -2.20467427   2.38710921  -6.69972165
 Br  -3.30606825   5.11760290  -1.12929207
 Br  -1.46450981   5.97984412   0.17297792
```

Br8b_1

```
Energy -21293.7067225  Dipole 10.092069  ZPE 0.423661  G(298.15) 210.09  Edisp -54.46
 C   -1.24790288  -1.44069067   1.31077153
 C   -0.39298762  -2.19468819   0.50806200
 C    0.95508027  -1.82111088   0.40156569
 C    1.38326188  -0.69402750   1.12409242
 C    0.53194716   0.05621289   1.95326214
 C   -0.81490826  -0.33110637   2.03335264
 C   -1.83631222   0.57591184  -1.69729657
 C    1.96194554  -2.61864643  -0.44734625
 C    1.09539779   1.23223078   2.77174308
 C    1.78020118   2.25213703   1.83333440
 C    0.00183847   1.96827956   3.56658720
 C    2.13560156   0.67460414   3.77288291
 C   -0.52663920   1.22409599  -1.58139315
 C   -1.96806319  -0.61206516  -2.54715579
 C   -2.98409768   1.09594242  -0.98976292
 C    2.59820970  -1.69200117  -1.50900155
 C    3.06933770  -3.17263974   0.48036620
 C    1.30518621  -3.80610282  -1.17358880
 H   -0.78205686  -3.07012264  -0.01254191
 H    2.43416106  -0.40075983   1.05737471
 H   -1.52264529   0.21450708   2.65731259
 H    2.22661106   3.06381913   2.43109793
 H    2.58730731   1.79340642   1.24094079
 H    1.05229387   2.70713446   1.14239697
 H    0.45939212   2.79745501   4.12953070
 H   -0.49128770   1.30617182   4.29681328
 H   -0.76465706   2.40167224   2.90331023
 H    2.55289302   1.49798565   4.37584638
 H    2.97059057   0.17496890   3.25705715
 H    1.67127644  -0.05405558   4.45659818
 H   -0.61480861   2.28857902  -1.31526018
 H   -0.01649471   0.72142181  -0.72392137
 H    0.10130799   1.06513191  -2.47214810
 H   -1.61287178  -0.35532630  -3.57367754
 H   -2.98114818  -1.03228293  -2.56650369
 H   -1.24107650  -1.37209711  -2.20313427
 H   -3.62619902   1.59834761  -1.77969478
 H   -2.74902985   1.85958506  -0.23773146
 H   -3.64556142   0.29438755  -0.61584514
 H    3.34223730  -2.25261261  -2.09850137
 H    3.11181080  -0.83270463  -1.05088816
 H    1.83760388  -1.30370609  -2.20635570
 H    3.80095525  -3.74863693  -0.11011744
 H    2.64136300  -3.83882603   1.24629777
 H    3.61158398  -2.36483053   0.99561131
 H    2.06719550  -4.33920977  -1.76402230
 H    0.86700974  -4.52831237  -0.46595695
 H    0.51720173  -3.47827974  -1.87221164
 Br  -3.10154508  -1.96922726   1.43801206
 Br  -6.88538464   0.60631575  -2.26677888
 Br  -5.46957166   2.43555393  -3.09623481
 Br  -3.64852102   4.44558244  -3.98913370
 Br  -1.82837252   2.53344142  -4.83356298
 Br  -0.21635545   0.74331619  -5.48266977
```

Br	-2.39627359	4.79697764	-1.45348942
Br	-1.30603006	4.89889359	0.75170637

PES I→II, n=5 (DFT/PBE/L1+ΔG+D3)



Br10c (point 13.6 on Fig.8 of the paper)
Energy -26441.306053914 Dipole 14.668281 ZPE 0.428668 G(298.15) 211.29 Edisp -59.67

C	-1.07977004	0.35118845	0.54632129
C	-0.77203014	-0.93220016	-0.01302579
C	0.39615684	-1.60243466	0.32229246
C	1.23857832	-0.97934737	1.26868180
C	0.95515938	0.24434307	1.91549802
C	-0.23456263	0.87142761	1.57835695
C	-0.83512047	1.62238424	-0.96768409
C	0.76005684	-2.98945651	-0.22915081
C	1.92783501	0.79489657	2.97002765
C	3.30378022	1.03966820	2.30790144
C	1.43043003	2.12024036	3.57289364
C	2.07580354	-0.23875246	4.11095907
C	0.62391105	1.53551089	-1.35107429
C	-1.77850607	1.10987810	-2.02377788
C	-1.23750395	2.95828768	-0.38990804
C	2.15719596	-2.93921189	-0.88845140
C	0.77682264	-3.98874698	0.95283735
C	-0.25932483	-3.47731403	-1.27328523
H	-1.47970503	-1.36098873	-0.72408424
H	2.16410805	-1.49597015	1.53932521
H	-0.54586302	1.79150179	2.07439779
H	4.01516761	1.42007242	3.05866110
H	3.72871177	0.11656491	1.88281989
H	3.22876381	1.78475844	1.49950618
H	2.15988445	2.47746084	4.31654532
H	0.46370890	2.00011177	4.08846970
H	1.32712899	2.90667647	2.80721455
H	2.77567130	0.14466576	4.87098887
H	2.47227552	-1.20077969	3.74955649

```
 H    1.10669141  -0.42878588   4.59901849
 H    0.76719682   2.25349293  -2.17959111
 H    1.29721946   1.83497552  -0.53557357
 H    0.91170543   0.54849587  -1.73835306
 H   -1.85137153   1.90138366  -2.79367144
 H   -2.80280097   0.96651838  -1.64689157
 H   -1.41605406   0.19781168  -2.51713854
 H   -1.27722787   3.67145712  -1.23667126
 H   -0.50841939   3.34258473   0.33778625
 H   -2.24386999   2.93823720   0.05345991
 H    2.42688620  -3.94558867  -1.24751124
 H    2.94037508  -2.62134846  -0.18098778
 H    2.16595574  -2.25795679  -1.75430925
 H    1.03984630  -4.99250941   0.58192382
 H   -0.21154563  -4.04757219   1.43629208
 H    1.51872121  -3.71098597   1.71916532
 H    0.04618846  -4.47088452  -1.63702617
 H   -1.26976578  -3.58138261  -0.84460354
 H   -0.30815296  -2.80910621  -2.14848040
 Br  -3.01869742   0.49952400   1.01554672
 Br  -6.17569575   0.95173240   1.13871722
 Br  -6.03800472   1.57284880  -1.25810297
 Br  -5.77567751   2.26011880  -3.95610083
 Br  -3.60045702   4.14076072  -3.67136791
 Br  -1.70373997   5.65412632  -3.35996618
 Br  -4.36251898   0.12053568  -4.81936984
 Br  -3.03994886  -1.89254711  -5.61390267
 Br  -0.37229818  -1.31870884  -4.94086519
 Br   1.99669642  -0.86166208  -4.37423826
```

Br10c_0

```
Energy -26441.33517472  Dipole 10.535840  ZPE 0.431188  G(298.15) 211.71  Edisp -58.71
 C    0.17555466   0.92281149  -0.21914307
 C   -0.33302027  -0.41640188  -0.42494713
 C    0.07372019  -1.50529680   0.43859278
 C    0.84965578  -1.19104236   1.54197424
 C    1.28865623   0.12420960   1.81037488
 C    0.94594627   1.15261182   0.91683792
 C   -0.06929659   2.04568537  -1.23032429
 C   -0.29588784  -2.96169115   0.13258199
 C    2.13479759   0.38517816   3.06064889
 C    3.41897230  -0.47789353   2.99250503
 C    2.54938218   1.86043472   3.20399501
 C    1.30768622  -0.01325870   4.30858557
 C    1.31398446   2.45449240  -1.80783058
 C   -0.97056771   1.62577247  -2.40476610
 C   -0.70981813   3.26423892  -0.52110526
 C    1.02388024  -3.73673323  -0.12305845
 C   -1.03085480  -3.57906196   1.34654346
 C   -1.18657967  -3.11355467  -1.11433078
 H   -0.68549268  -0.66909766  -1.42713361
 H    1.14898308  -1.99209965   2.22058082
 H    1.31289152   2.16142546   1.10419231
 H    4.02866018  -0.29793039   3.89292882
 H    3.19397557  -1.55426037   2.94814360
 H    4.02241892  -0.21622782   2.10888362
 H    3.14675991   1.97957973   4.12172902
 H    1.67524461   2.52594554   3.28801880
 H    3.17055329   2.19659925   2.35818075
 H    1.90583873   0.16567760   5.21701730
 H    1.02430460  -1.07668199   4.29298762
 H    0.38620774   0.58628036   4.37752153
 H    1.16468610   3.26134048  -2.54365222
 H    1.99329642   2.82485780  -1.02428904
 H    1.79413120   1.60452052  -2.31850731
 H   -1.10949081   2.48958658  -3.07286810
 H   -1.96970594   1.31029943  -2.06846946
 H   -0.52203344   0.81873632  -3.00548899
 H   -0.86859076   4.06885137  -1.25690569
```

```
 H   -0.06953944   3.66077353   0.28245953
 H   -1.68621784   2.99535811  -0.08976971
 H    0.78587206  -4.79071414  -0.34160584
 H    1.69189689  -3.71078246   0.75193610
 H    1.56031860  -3.31725822  -0.98870038
 H   -1.27465159  -4.63125265   1.12793487
 H   -1.96879136  -3.03974877   1.55067810
 H   -0.41353073  -3.56027194   2.25817373
 H   -1.41628081  -4.18134629  -1.25696775
 H   -2.14204448  -2.57764020  -1.00661061
 H   -0.68225371  -2.76586058  -2.02991789
 Br  -2.45497570  -0.05724738   0.43356403
 Br  -5.07705766   0.36440585   0.98009518
 Br  -5.53274988   1.10940057  -1.47535034
 Br  -5.78574875   1.84361788  -3.96604174
 Br  -3.92199326   4.20348576  -3.82581018
 Br  -2.38758623   6.05175738  -3.66783310
 Br  -4.04876172   0.02359547  -5.15284226
 Br  -2.51870334  -1.60805358  -6.24690473
 Br  -0.05474976  -1.52559525  -4.82230307
 Br   2.09869935  -1.51452636  -3.63418783
```

Br10c_1

```
Energy -26441.33293811  Dipole 10.993987  ZPE 0.425505  G(298.15) 206.13  Edisp -57.75
 C   -1.37227504  -0.28752055   1.36571437
 C   -0.97004215  -1.40122864   0.62913715
 C    0.38917700  -1.74775762   0.58936270
 C    1.29323395  -0.93834529   1.30267413
 C    0.89483886   0.17619079   2.06121068
 C   -0.46845065   0.50105177   2.08068423
 C   -0.84125601   1.75543349  -1.36190606
 C    0.89047338  -3.00580234  -0.14245811
 C    1.94047188   0.97617634   2.85945956
 C    3.02565603   1.52049222   1.90247467
 C    1.31751386   2.16659845   3.61025345
 C    2.59812017   0.03832545   3.89943582
 C    0.56166715   1.37521407  -1.47993424
 C   -1.87909869   0.96115689  -2.01310837
 C   -1.22024431   2.97920811  -0.66843536
 C    2.09009789  -2.66394556  -1.05449390
 C    1.33773152  -4.03072680   0.92856499
 C   -0.20389867  -3.65137205  -1.01211575
 H   -1.71797760  -1.99231066   0.10012353
 H    2.35270239  -1.20628554   1.28657733
 H   -0.84076167   1.34939748   2.65560691
 H    3.79326152   2.06530402   2.47632856
 H    3.52991261   0.71365632   1.34848003
 H    2.59123781   2.21998342   1.16939459
 H    2.10612350   2.70418968   4.16042178
 H    0.56415917   1.83907770   4.34470114
 H    0.84445338   2.88579631   2.92111887
 H    3.34948982   0.59379813   4.48480042
 H    3.10532547  -0.81241698   3.41861381
 H    1.84465819  -0.36294235   4.59566918
 H    1.26006869   2.16148373  -1.16422891
 H    0.70406988   0.49516343  -0.80285313
 H    0.80635935   0.97231821  -2.48522010
 H   -2.36872116   1.62205465  -2.76637899
 H   -2.69990141   0.74348319  -1.29898523
 H   -1.50982446   0.05934490  -2.51638578
 H   -1.23183473   3.77103036  -1.47866005
 H   -0.47592446   3.31149686   0.06828648
 H   -2.24373840   2.95579321  -0.26583163
 H    2.45282447  -3.58285920  -1.54322528
 H    2.93450813  -2.23746640  -0.49066237
 H    1.80783457  -1.95433660  -1.84888541
 H    1.70234343  -4.94894068   0.43914854
 H    0.49835771  -4.30028227   1.58939232
 H    2.15113606  -3.63129577   1.55488073
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H	0.21426674	-4.53244272	-1.52423573
H	-1.05957924	-3.99751470	-0.41029524
H	-0.57119893	-2.96127167	-1.78926927
Br	-3.24428934	0.17435781	1.41175104
Br	-6.65127413	1.33810510	1.09320851
Br	-6.23620357	1.75598026	-1.26594448
Br	-5.74491303	2.28791675	-4.09738834
Br	-3.55796812	3.97867439	-3.72739916
Br	-1.56244649	5.41201495	-3.31350611
Br	-4.42469194	0.05008394	-4.80410836
Br	-3.14131486	-2.05240967	-5.44090924
Br	-0.51562805	-1.20382628	-4.99494982
Br	1.80138251	-0.40705202	-4.58570108

Br10a

Energy -26441.29230482 Dipole 19.628509 ZPE 0.428205 G(298.15) 208.95 Edisp -61.75

C	-0.89626507	-0.74306247	-1.31858740
C	-1.44076712	0.43495443	0.68994896
C	-1.87319085	-0.25660246	-0.47275162
C	-0.09655469	0.63194865	1.04993506
C	0.49184050	-0.50924983	-1.04385340
C	0.86917935	0.09675003	0.19479255
H	-1.15085632	-1.31878852	-2.20878505
H	-2.20927537	0.81925350	1.36349296
H	1.93410460	0.13562356	0.44579468
Br	4.58043343	-0.73474474	1.00946363
Br	3.94303478	-3.48186919	1.21562552
Br	3.94961727	-4.44697650	-1.55179997
Br	3.95142767	-5.22775975	-3.85618809
Br	5.01051734	1.69577593	0.80160663
C	0.31328919	1.36510729	2.34013675
C	0.93788000	1.07343434	-2.34334829
C	1.09880652	2.64261192	1.96179408
H	2.01831824	2.40806224	1.40125484
H	0.47845821	3.33443471	1.36713000
H	1.40366585	3.16963680	2.88052701
C	0.12866447	2.24863930	-1.86922747
H	-0.93679996	2.00755651	-1.73987889
H	0.52534740	2.68824116	-0.94559709
H	0.19006654	3.01613159	-2.66394765
C	-0.90973530	1.76964083	3.18319986
H	-1.49615374	0.89044288	3.49693172
H	-0.56021673	2.27579616	4.09647204
H	-1.57156149	2.47367322	2.65064591
C	1.21103522	0.44553323	3.19871498
H	2.13661156	0.15780544	2.67777291
H	1.50035507	0.98032275	4.11786533
H	0.67588132	-0.47351144	3.48192750
C	0.49981916	0.50046833	-3.66939498
H	0.90985194	1.16240941	-4.45492303
H	0.92117416	-0.50149605	-3.84339917
H	-0.59302974	0.47640595	-3.77908218
C	2.42749343	1.22157068	-2.20436317
H	2.74861633	1.91255012	-3.00772237
H	2.74209363	1.65498905	-1.24511531
H	2.95930610	0.27281170	-2.37030698
C	-3.37496643	-0.46824811	-0.71495710
C	-3.97930611	-1.21885690	0.49505659
H	-3.47787274	-2.18696273	0.64955312
H	-3.88904477	-0.64050402	1.42786695
H	-5.05176317	-1.40051153	0.31773490
C	-4.06237351	0.90852121	-0.86961409
H	-3.92463501	1.54083408	0.02193427
H	-3.66932734	1.45436576	-1.74332232
H	-5.14576773	0.76874821	-1.01540190
C	-3.63964933	-1.29655010	-1.98413920
H	-4.72561173	-1.42550193	-2.11351402
H	-3.25672590	-0.79809895	-2.89035448
H	-3.19153982	-2.30101742	-1.91639566

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 Br    1.65783706  -1.96818443  -1.63082862
 Br    5.69414998  -4.89408198   3.21496153
 Br    7.08833113  -6.03024862   4.80896646
 Br    1.22601335  -3.28543926   2.07510027
 Br   -1.10023084  -3.02678409   2.83059251
```

Br10a_0

```
Energy -26441.32184568  Dipole 14.563290  ZPE 0.431071  G(298.15) 210.87  Edisp -59.69
 C    -0.43428832  -0.22033335  -1.50431830
 C    -1.48458953   0.07105696   0.67191780
 C    -1.46064364  -0.60042505  -0.53910675
 C    -0.61692331   1.14750348   0.95321539
 C     0.39900601   0.95598011  -1.26973563
 C     0.30862938   1.56547740  -0.03432587
 H    -0.63243341  -0.47519282  -2.54797354
 H    -2.20824988  -0.22907257   1.42927960
 H     0.96101294   2.41159869   0.18728046
 Br    4.08000535  -0.13080981   1.76084869
 Br    3.27888934  -2.91094406   1.94781537
 Br    2.95065565  -3.90532149  -0.67912027
 Br    2.79571334  -4.90979147  -2.92753005
 Br    4.64192929   2.23939734   1.66656315
 C    -0.65870502   1.87846262   2.29212376
 C     1.32127085   1.50895695  -2.36091192
 C    -0.80642024   3.40210246   2.04975390
 H     0.03888599   3.82383378   1.48590950
 H    -1.73802907   3.63034352   1.50738706
 H    -0.84168713   3.91389077   3.02470351
 C     0.91171164   2.98181706  -2.62828566
 H    -0.13626113   3.05230562  -2.96152405
 H     1.03495243   3.61140662  -1.73440749
 H     1.55474382   3.39275413  -3.42347523
 C    -1.81844466   1.41612684   3.19234208
 H    -1.73276045   0.35269622   3.46773627
 H    -1.79532389   1.99839507   4.12689146
 H    -2.79926662   1.58835693   2.71853808
 C     0.68197497   1.59869360   3.02349697
 H     1.55073068   1.96667243   2.45692250
 H     0.66548416   2.11301926   3.99837137
 H     0.81767482   0.52077744   3.20092116
 C     1.21562611   0.73576154  -3.68921921
 H     1.90961387   1.18488386  -4.41661811
 H     1.49504288  -0.32288156  -3.57471081
 H     0.20420286   0.79768294  -4.12509992
 C     2.79018575   1.47014727  -1.87364998
 H     3.43982819   1.90440128  -2.65081258
 H     2.93844438   2.04568332  -0.94760405
 H     3.11528644   0.43653747  -1.68405391
 C    -2.49765206  -1.67998679  -0.85888046
 C    -2.37874456  -2.83796455   0.16292554
 H    -1.39865094  -3.33111547   0.08424522
 H    -2.50113105  -2.49250728   1.20054580
 H    -3.16386189  -3.58298198  -0.04454360
 C    -3.90481521  -1.03517535  -0.73556298
 H    -4.10335756  -0.67356292   0.28425405
 H    -4.02137234  -0.19075582  -1.43380359
 H    -4.66601689  -1.79332138  -0.98128478
 C    -2.35803096  -2.25225861  -2.28210589
 H    -3.12927289  -3.02393765  -2.43085857
 H    -2.51675197  -1.48185193  -3.05545393
 H    -1.37812462  -2.72743141  -2.44232619
 Br    1.04262979  -1.81763030  -1.09102996
 Br    5.20138186  -5.01712212   2.96540748
 Br    6.72229508  -6.71378974   3.71439082
 Br    0.65920175  -2.76339460   3.15640756
 Br   -1.54520042  -2.59716287   4.19813873
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Br10a_1

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Energy -26441.32456256  Dipole 12.493995  ZPE 0.425074  G(298.15) 202.65  Edisp -56.10
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C	-2.40976659	-0.41805832	-1.40105272
C	-2.01728940	1.17460619	0.36240977
C	-2.46408741	0.90434387	-0.94583464
C	-1.53533861	0.18273947	1.22406904
C	-1.92167155	-1.40809164	-0.54684406
C	-1.48961450	-1.14277298	0.74539787
H	-2.74475269	-0.68997018	-2.40195278
H	-2.05867308	2.20383534	0.72218754
H	-1.12609465	-1.95807152	1.37612669
Br	4.47373272	-0.13498327	0.90486443
Br	5.26273590	-2.67707353	1.58685955
Br	5.29317438	-3.76877954	-1.07929670
Br	5.10492008	-4.59343393	-3.37541484
Br	3.66043912	2.14526682	0.25803372
C	-1.06465657	0.48366483	2.65810333
C	2.14713124	-1.05123070	-1.80832756
C	0.42773083	0.10465595	2.79926589
H	0.60034356	-0.96505596	2.60392971
H	1.05521503	0.69450825	2.11107628
H	0.77057593	0.30903786	3.82701188
C	1.75268967	-2.17376501	-0.96003431
H	0.83479118	-2.61589347	-1.42436451
H	2.51401388	-2.96471942	-0.89919263
H	1.41745497	-1.84440110	0.03621678
C	-1.22353002	1.97063515	3.02341529
H	-2.27502579	2.29677040	2.96688870
H	-0.88118372	2.12589045	4.05892294
H	-0.61500241	2.62039721	2.37333513
C	-1.90214334	-0.35344607	3.65337926
H	-1.77364089	-1.43415631	3.48738438
H	-1.58211595	-0.13428670	4.68536646
H	-2.97413885	-0.11410390	3.56464363
C	3.22924641	-1.23881058	-2.77979124
H	3.37804994	-0.39036199	-3.45866841
H	4.15669727	-1.43225406	-2.19433031
H	3.10494501	-2.18883155	-3.33565999
C	1.49678759	0.23465610	-1.67518146
H	1.43783708	0.78719605	-2.62556910
H	0.54554141	0.21110739	-1.12519846
H	2.21460249	0.86747358	-1.04743956
C	-3.00217033	2.04966207	-1.82202903
C	-4.22006483	2.69453864	-1.11968616
H	-5.02316734	1.95481846	-0.97316182
H	-3.95259634	3.10657444	-0.13450985
H	-4.61669031	3.51895242	-1.73537324
C	-1.89653565	3.11376385	-2.01296650
H	-1.55228846	3.52433082	-1.05121413
H	-1.02447464	2.68487148	-2.53382971
H	-2.27938850	3.95066112	-2.62035153
C	-3.45005150	1.56333085	-3.21190023
H	-3.82612581	2.41935548	-3.79474796
H	-2.61695162	1.11530423	-3.77820045
H	-4.26418085	0.82381795	-3.14267192
Br	-1.83078674	-3.22682272	-1.21094831
Br	7.86701442	-2.55278092	3.18933009
Br	9.90101326	-2.48132598	4.44508828
Br	2.60713163	-3.59818323	2.47953602
Br	0.36038392	-4.28510211	3.08290143

Br10b

Energy -26441.292904017 Dipole 21.683866 ZPE 0.428298 G(298.15) 208.40 Edisp -57.77

C	-0.78649202	-0.68569331	0.03372979
C	0.06633662	-1.83433695	0.00269072
C	1.25216624	-1.86741712	0.72236530
C	1.53310350	-0.75404315	1.54506604
C	0.67991520	0.36002951	1.70480325
C	-0.49379158	0.36264706	0.96477157
C	-0.51190471	0.16526175	-1.74776984
C	2.22694781	-3.05491591	0.68331669

C	1.05783636	1.48466575	2.68125719
C	2.35552502	2.16259989	2.18253177
C	-0.04880266	2.54834651	2.78833852
C	1.29323632	0.88088933	4.08565241
C	0.96406633	0.48417492	-1.83077995
C	-0.96346541	-0.87956520	-2.73744548
C	-1.39955123	1.37918221	-1.69822243
C	3.60522588	-2.56392760	0.18267565
C	2.36869924	-3.63719029	2.10920218
C	1.73399765	-4.17165696	-0.25334914
H	-0.23264425	-2.67256365	-0.62820558
H	2.46488978	-0.76690698	2.11823293
H	-1.21362366	1.17754887	1.05604952
H	2.65457010	2.95519934	2.88722923
H	3.19173025	1.44874002	2.10612557
H	2.20568115	2.62605512	1.19409031
H	0.26303670	3.32237755	3.50709237
H	-0.99459449	2.11816401	3.15626986
H	-0.24572693	3.05342997	1.82852965
H	1.56109544	1.68365071	4.79119982
H	2.11416490	0.14620775	4.09406311
H	0.38317254	0.38522251	4.45921526
H	1.11120717	1.01999900	-2.78634628
H	1.30052594	1.15273748	-1.02616237
H	1.59356302	-0.41611255	-1.85349718
H	-0.95769833	-0.39186630	-3.73324278
H	-1.99520885	-1.21268969	-2.55462069
H	-0.28635422	-1.74459769	-2.78317796
H	-1.47884778	1.76504769	-2.73230994
H	-0.99903010	2.18171586	-1.06385539
H	-2.43052252	1.13905914	-1.39585947
H	4.31581430	-3.40599508	0.16529459
H	4.02910770	-1.78389234	0.83488761
H	3.53483632	-2.15553779	-0.83842129
H	3.06978929	-4.48730983	2.09544155
H	1.39817713	-3.99663767	2.48639436
H	2.75994388	-2.89472940	2.82269283
H	2.46184583	-4.99801959	-0.24770648
H	0.76437581	-4.58237474	0.07192903
H	1.63844206	-3.82327916	-1.29495726
Br	-2.73287852	-1.16315023	0.05454462
Br	-5.84873240	-1.35742753	-0.37750013
Br	-5.65208984	0.66960920	-1.80885716
Br	-5.25384472	2.94282187	-3.35988243
Br	-3.15634175	1.92833324	-5.04184452
Br	-1.24138090	1.00985728	-6.27307917
Br	-7.77352434	4.11831778	-4.53807035
Br	-9.76629509	5.06817542	-5.48142322
Br	-3.53947146	4.30961293	-1.46450497
Br	-1.95020769	5.25215708	0.13540817

Br10b_0

Energy -26441.32429506 Dipole 14.957988 ZPE 0.430725 G(298.15) 207.67 Edisp -55.96

C	0.63089091	-0.11036101	-0.78564175
C	1.28836284	-1.31350711	-0.53486936
C	1.47465138	-1.80696878	0.76654274
C	0.99491382	-1.04975145	1.85629028
C	0.32460346	0.15352556	1.68764592
C	0.08532390	0.59740816	0.34024359
C	0.54591940	0.44765843	-2.21119688
C	2.18991539	-3.13591558	1.03821436
C	-0.09898230	0.99117940	2.90257402
C	1.18195594	1.38109096	3.68396151
C	-0.83761068	2.28536453	2.51347663
C	-1.02131432	0.15237170	3.81913065
C	1.99418025	0.67709985	-2.71846070
C	-0.15864746	-0.57570265	-3.13540782
C	-0.20786226	1.78721909	-2.29057610
C	3.42493464	-2.87500884	1.93476213

C	1.20968228	-4.08540844	1.77058449
C	2.66539399	-3.83045670	-0.25037118
H	1.68458101	-1.87899806	-1.37830541
H	1.16933141	-1.41901499	2.86908413
H	-0.24330630	1.62624394	0.18576663
H	0.90358705	1.98824136	4.56089136
H	1.72971329	0.49576418	4.04216208
H	1.86297191	1.97700643	3.05556865
H	-1.11959821	2.82567608	3.43085816
H	-1.76109411	2.08096452	1.95020387
H	-0.20551373	2.96416061	1.91817755
H	-1.30495257	0.74975067	4.70075002
H	-0.52344502	-0.76176848	4.17819878
H	-1.93933809	-0.13945960	3.28637924
H	1.95445284	1.08594535	-3.74107710
H	2.52915868	1.39821788	-2.07986699
H	2.57410577	-0.25837239	-2.74651263
H	-0.20230757	-0.17251950	-4.16002644
H	-1.18834140	-0.76444344	-2.79607707
H	0.37882880	-1.53639731	-3.16965676
H	-0.24397176	2.11730807	-3.34008210
H	0.29405433	2.58232112	-1.71478001
H	-1.24825292	1.70054930	-1.94258747
H	3.93882664	-3.82848143	2.13916576
H	3.14795292	-2.42846158	2.90189064
H	4.13757916	-2.19919405	1.43572485
H	1.71097235	-5.04552050	1.97581074
H	0.32005402	-4.28488954	1.15241681
H	0.87201723	-3.66726819	2.73118782
H	3.16323083	-4.77733642	0.01222397
H	1.82449220	-4.07200636	-0.92017660
H	3.39333894	-3.21546207	-0.80384222
Br	-2.16315753	-0.24556371	0.12229959
Br	-4.69319402	-0.80826003	-0.27076884
Br	-4.99871062	1.27573115	-1.89937696
Br	-5.01065288	3.33923114	-3.41372815
Br	-2.99214340	2.33068575	-5.43492165
Br	-1.27526545	1.52430101	-6.91041611
Br	-7.89124623	4.23822117	-3.91852779
Br	-10.09698707	5.03576210	-4.38330523
Br	-2.95278239	4.76319076	-1.69077346
Br	-1.22129926	5.71430793	-0.32085419

Br10b_1

Energy -26441.32438948 Dipole 13.911975 ZPE 0.425015 G(298.15) 201.93 Edisp -56.59

C	-0.74820202	-1.67794936	1.72739990
C	0.17222140	-2.36822061	0.93980503
C	1.44262776	-1.81359746	0.72441436
C	1.72935049	-0.57596566	1.32629673
C	0.81493025	0.11234874	2.14243137
C	-0.45342948	-0.45803495	2.33236696
C	-1.73061480	-0.06967299	-1.40183265
C	2.51879128	-2.53000186	-0.11172887
C	1.23512365	1.42297368	2.83218563
C	1.71015627	2.44905328	1.77803749
C	0.08483530	2.05510760	3.63625981
C	2.39699225	1.11006306	3.80567427
C	-0.54771517	0.79520744	-1.40307005
C	-1.69204918	-1.32617296	-2.15693713
C	-2.92132732	0.30261341	-0.66903962
C	2.96228329	-1.62092131	-1.28107269
C	3.73637679	-2.83114870	0.79432925
C	2.01554635	-3.86113117	-0.69786213
H	-0.10476062	-3.33377532	0.51585448
H	2.72047253	-0.14043017	1.17512861
H	-1.20496406	0.03080259	2.95225804
H	2.05865687	3.36488101	2.28316407
H	2.54640198	2.06492919	1.17311452
H	0.88832205	2.73260069	1.10089218

H	0.43985523	2.98669121	4.10513530
H	-0.26461651	1.39166617	4.44401239
H	-0.77154147	2.31382403	2.99202155
H	2.71417605	2.03344258	4.31782175
H	3.27132564	0.69765825	3.27813744
H	2.08353665	0.38087816	4.56982807
H	-0.80387386	1.84801239	-1.20987300
H	0.07513684	0.45392474	-0.53969789
H	0.06314215	0.67222663	-2.31118231
H	-1.46024806	-1.08681327	-3.22274501
H	-2.60930091	-1.92199134	-2.07394789
H	-0.81448966	-1.91351161	-1.82786657
H	-3.69720466	0.57676233	-1.44689340
H	-2.79757554	1.17119864	-0.01057161
H	-3.38264479	-0.56672254	-0.16486142
H	3.75550225	-2.11852631	-1.86281957
H	3.36090895	-0.65798115	-0.92620229
H	2.12263252	-1.41243093	-1.96471751
H	4.51865234	-3.34678148	0.21316520
H	3.44677660	-3.47960347	1.63644598
H	4.17463109	-1.90994306	1.20825328
H	2.82162870	-4.32924486	-1.28477383
H	1.72245363	-4.57219798	0.09127266
H	1.15685301	-3.71660701	-1.37495599
Br	-2.49360277	-2.45700081	2.00570684
Br	-6.76602680	-0.99561593	-1.68219312
Br	-5.75553432	0.98696119	-2.68921739
Br	-4.31925160	3.24232542	-3.78453582
Br	-2.22486428	1.61152230	-4.65480495
Br	-0.37500330	0.08258187	-5.28477460
Br	-5.52753405	5.08758940	-5.90039351
Br	-6.48846289	6.53832067	-7.54150493
Br	-2.99129598	4.05796230	-1.35780390
Br	-1.81416610	4.51786531	0.73646648