Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Bromination of tetrapyrrolic scaffolds: a sustainable approach

Giuseppe Pomarico, Federica Sabuzi, Valeria Conte and Pierluca Galloni

Contents

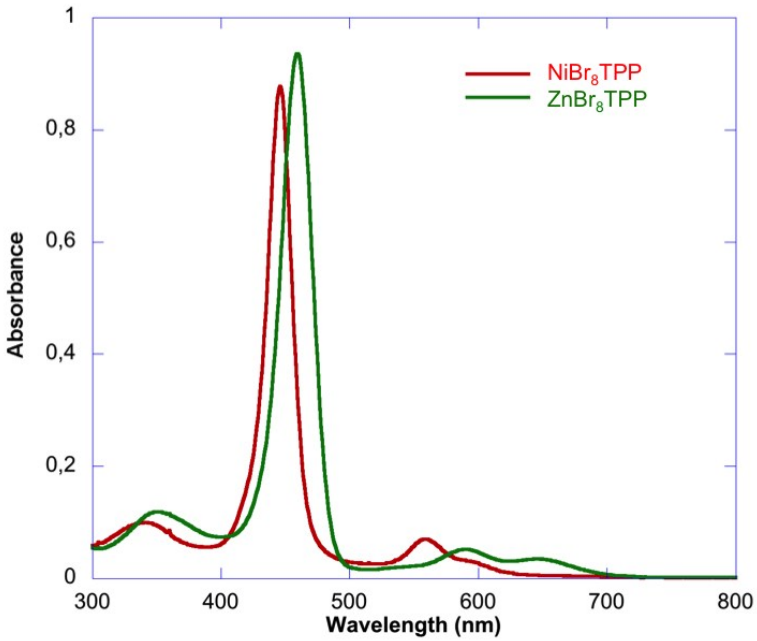


Figure S1: UV-vis spectra (CH_2Cl_2) of $NiBr_8TPP$ (red line) and $ZnBr_8TPP$ (green line).

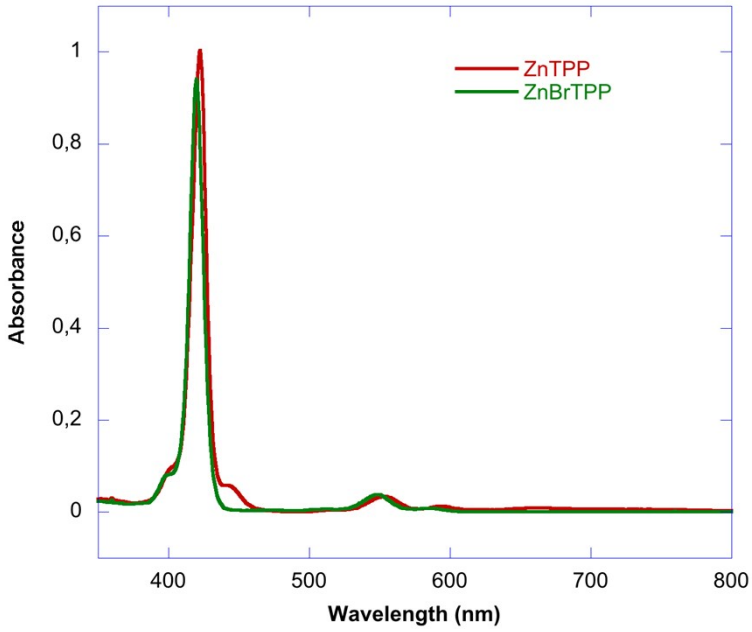


Figure S2: UV-vis spectra (CH_2Cl_2) of ZnTPP (red line) and ZnBrTPP (green line).

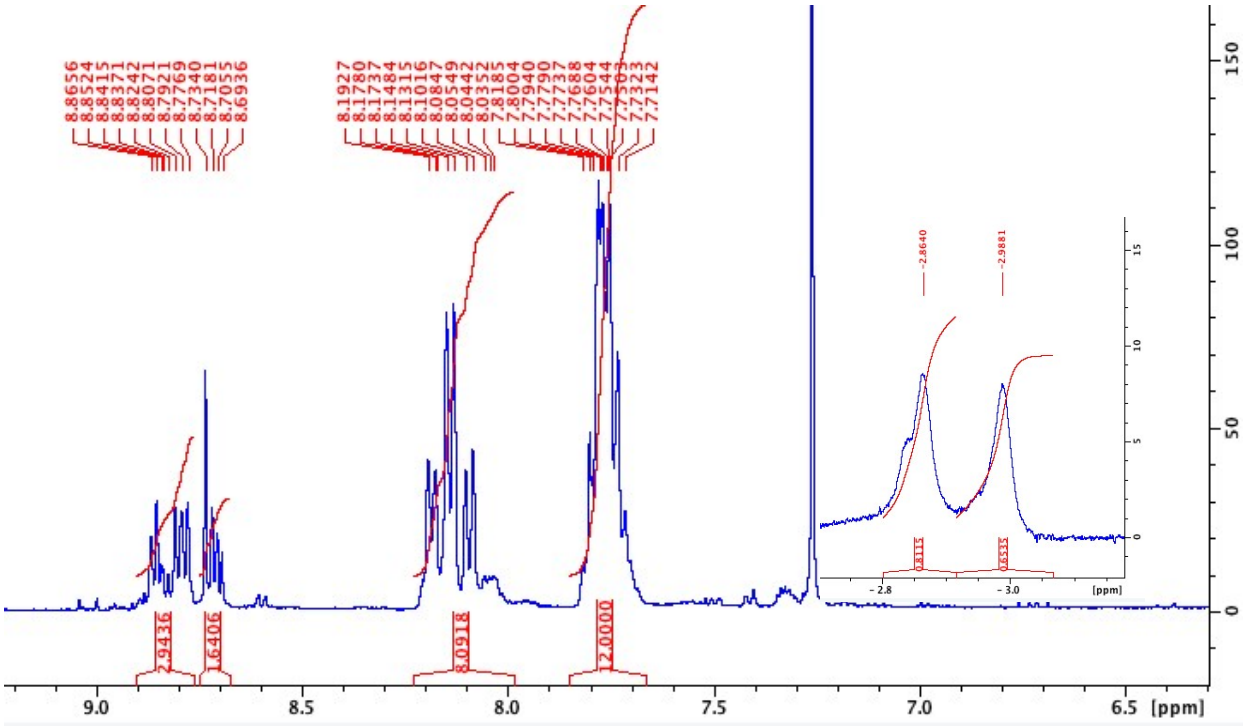


Figure S3: ^{1}H NMR spectrum of H_2Br_3TPP; inset: inner protons

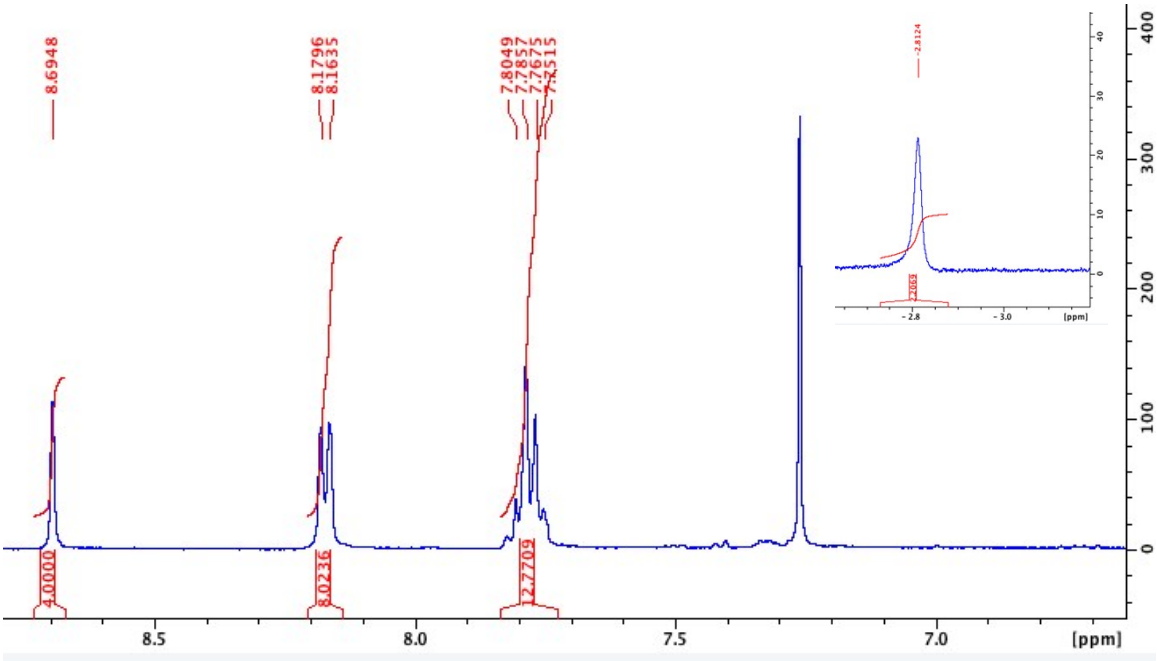


Figure S4: ^{1}H NMR spectrum of H_2Br_4TPP

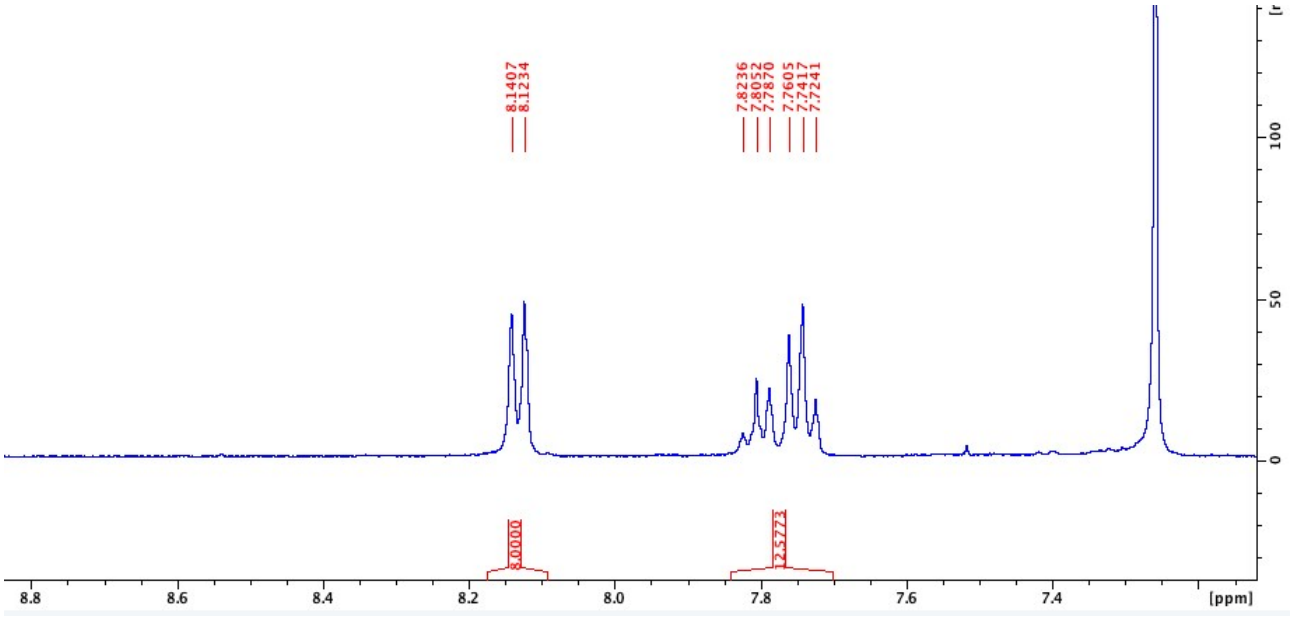


Figure S5: ^{1}H NMR spectrum of $ZnBr_8TPP$

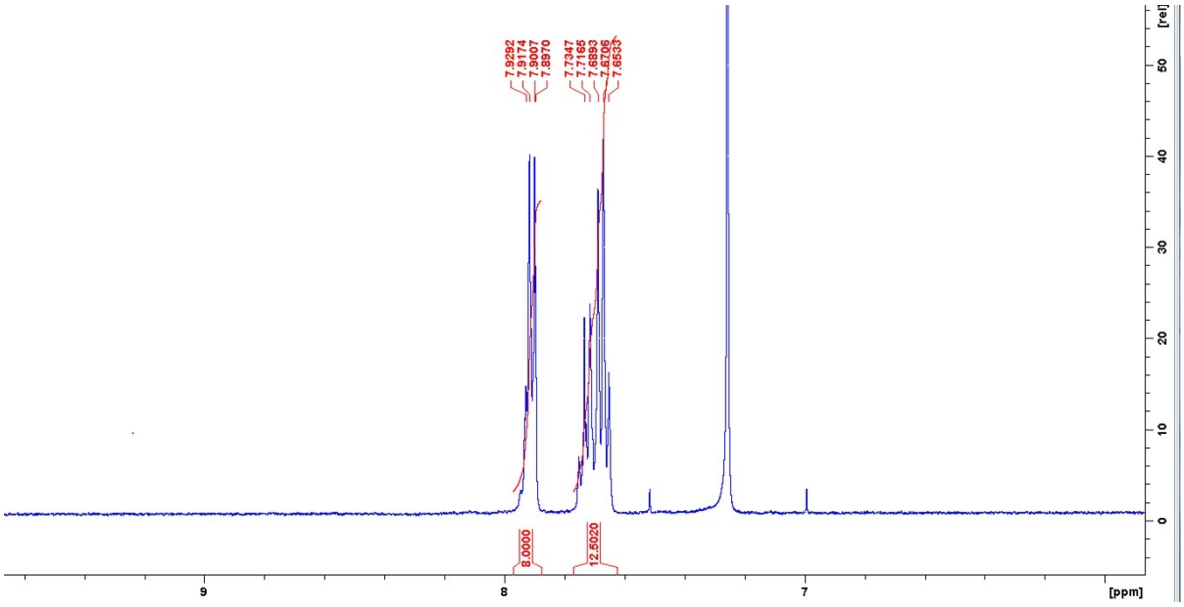


Figure S6: ^{1}H NMR spectrum of $NiBr_8TPP$

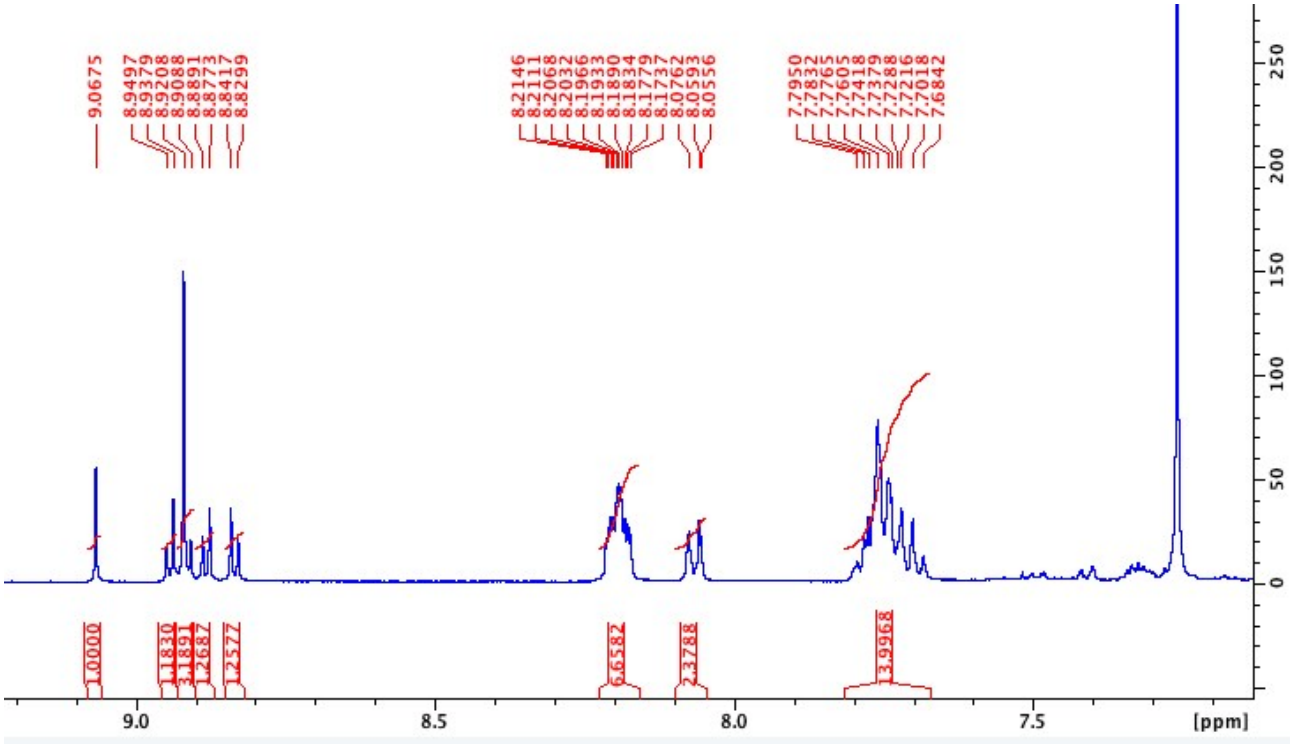


Figure S7: ^{1}H NMR spectrum of ZnBrTPP

Table S1. E-factor calculation for the brominated porphyrin derivatives investigated in this work. We considered all the substances used in the reaction and in the following work-up, not the materials for the chromatographic purification.

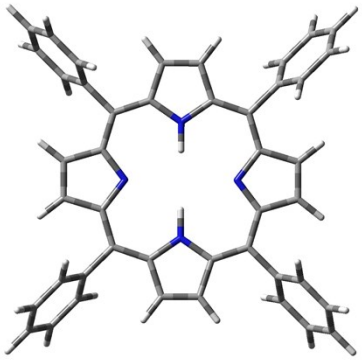
	H_2Br_3TPP	H_2Br_4TPP	ZnBrTPP	$ZnBr_8TPP$	$NiBr_8TPP$	$CuBr_8TPP$[a)]
Sustainable method	3411	3029	5194	2607	5270	718
Classical methods	2897	413	4700	6285[a]	50	1107

a) Multi steps procedure via $ZnBr_8TPP$ followed by demetalation and re-metalation with Cu

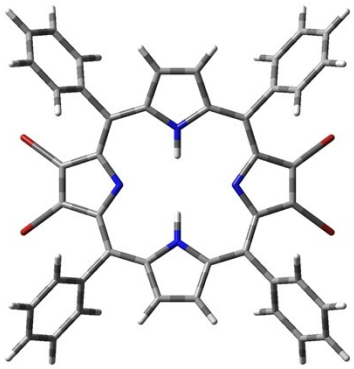
DFT CALCULATIONS

DFT geometry optimizations have been performed with Gaussian 16 rev. A.03, using B3LYP functional and a 6-31G (d) basis set.

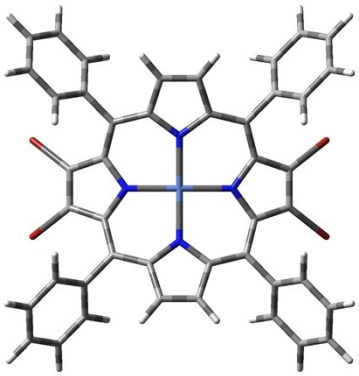
H_2TPP



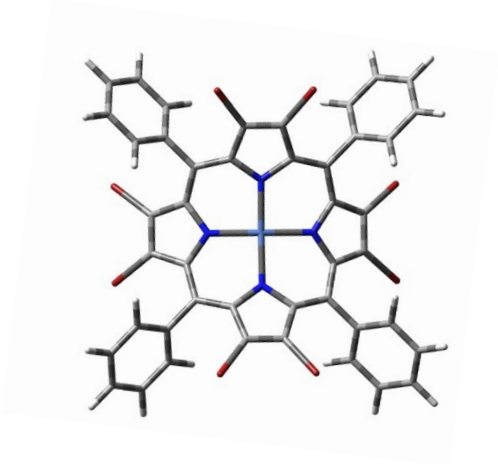
H_2Br_4TPP - 3



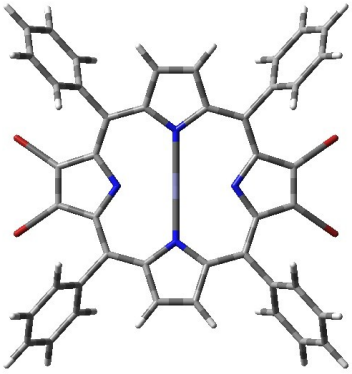
$NiBr_4$TPP



$NiBr_8$TPP



$ZnBr_4$TPP



$ZnBr_8$TPP

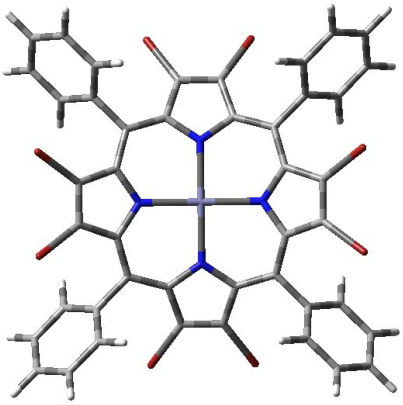


Figure S8: DFT optimized geometry for H_2TPP and brominated porphyrins, front view. Bromine atom is represented in red; nitrogen in blue; carbon atoms are in grey and hydrogen in white.

Optimized cartesian coordinates (in Angstroms) are listed below:

- **H_2TPP**

Total Energies: -1913.750636Hartrees
Stoichiometry C44H30N4
Framework group C1[X(C44H30N4)]
Deg. of freedom 228
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.011931	-2.109873	-0.050735
2	7	0	2.038824	-0.008373	0.023696
3	7	0	0.009022	2.109355	0.020311
4	7	0	-2.041102	0.009109	-0.015898
5	6	0	-1.147874	-2.884571	0.008541
6	6	0	-0.706173	-4.245234	0.109127
7	6	0	0.663167	-4.251520	0.106200
8	6	0	1.117260	-2.894956	0.003073
9	6	0	2.450617	-2.450773	-0.016967
10	6	0	2.859723	-1.099432	-0.037396
11	6	0	4.257797	-0.694407	-0.153395
12	6	0	4.263773	0.659404	-0.148646
13	6	0	2.869495	1.075686	-0.030085
14	6	0	2.472819	2.430433	-0.007563
15	6	0	1.144485	2.887073	0.019402
16	6	0	0.701648	4.251323	0.041330
17	6	0	-0.667576	4.256468	0.033589
18	6	0	-1.120474	2.895540	0.025501
19	6	0	-2.452685	2.450976	-0.000644
20	6	0	-2.863190	1.100974	-0.025754
21	6	0	-4.266401	0.697710	-0.037588
22	6	0	-4.273469	-0.655992	-0.042757
23	6	0	-2.874590	-1.074156	-0.016437
24	6	0	-2.477078	-2.428347	0.004398
25	1	0	-1.364478	-5.097131	0.189613
26	1	0	1.313591	-5.109561	0.184868
27	1	0	5.103155	-1.360656	-0.246989
28	1	0	5.114961	1.319171	-0.235632
29	1	0	1.359213	5.107415	0.055350
30	1	0	-1.319215	5.117273	0.032248
31	1	0	-5.115777	1.365473	-0.040239
32	1	0	-5.129836	-1.314388	-0.062412
33	1	0	0.005549	1.094253	0.024437
34	1	0	-0.008408	-1.095452	-0.085897
35	6	0	3.542280	3.480943	-0.020619
36	6	0	4.382220	3.659717	1.089770
37	6	0	3.727691	4.307057	-1.140243
38	6	0	5.378422	4.636719	1.081277
39	1	0	4.245436	3.029156	1.963818
40	6	0	4.724346	5.283920	-1.149637
41	1	0	3.090326	4.172296	-2.009800
42	6	0	5.552567	5.452181	-0.038511
43	1	0	6.016410	4.762491	1.952195
44	1	0	4.856221	5.909956	-2.028298

45	1	0	6.328779	6.212733	-0.045515
46	6	0	-3.510253	3.514767	-0.005498
47	6	0	-3.759858	4.284001	1.141412
48	6	0	-4.269499	3.765233	-1.158972
49	6	0	-4.742222	5.275458	1.135943
50	1	0	-3.183132	4.094581	2.042607
51	6	0	-5.252196	4.756014	-1.164957
52	1	0	-4.081381	3.179421	-2.054440
53	6	0	-5.491463	5.514443	-0.017432
54	1	0	-4.924495	5.857747	2.035436
55	1	0	-5.828256	4.937359	-2.068627
56	1	0	-6.256732	6.286028	-0.021973
57	6	0	-3.542522	-3.482346	0.039001
58	6	0	-4.351094	-3.649381	1.174343
59	6	0	-3.750511	-4.328746	-1.061309
60	6	0	-5.340248	-4.632965	1.207635
61	1	0	-4.195006	-3.004936	2.034899
62	6	0	-4.740165	-5.312198	-1.028926
63	1	0	-3.135790	-4.205001	-1.948643
64	6	0	-5.538141	-5.467488	0.105921
65	1	0	-5.953694	-4.749347	2.097279
66	1	0	-4.889916	-5.953958	-1.893270
67	1	0	-6.308812	-6.233253	0.131670
68	6	0	3.508260	-3.511847	-0.009511
69	6	0	3.662377	-4.382644	-1.100034
70	6	0	4.367433	-3.659959	1.091100
71	6	0	4.647323	-5.371115	-1.091472
72	1	0	3.010134	-4.272867	-1.961986
73	6	0	5.351392	-4.649076	1.100871
74	1	0	4.253932	-2.996652	1.943886
75	6	0	5.494770	-5.507897	0.009442
76	1	0	4.755075	-6.031075	-1.948327
77	1	0	6.003663	-4.750726	1.964316
78	1	0	6.261694	-6.277806	0.016653

Rotational constants (GHZ): 0.0583458 0.0577754 0.0300906

- **H_2Br_4TPP - 3**

Total Energies: -12198.136944 Hartrees
Stoichiometry C44H26Br4N4
Framework group C1[X(C44H26Br4N4)]
Deg. of freedom 228
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000118	2.068000	0.329012
2	7	0	-2.095391	0.000026	0.256641
3	7	0	-0.000111	-2.068004	0.329068
4	7	0	2.095375	-0.000044	0.256551
5	6	0	1.134235	2.827013	0.513658

6	6	0	0.683964	4.139480	0.880563
7	6	0	-0.683805	4.139505	0.880345
8	6	0	-1.134022	2.827035	0.513369
9	6	0	-2.467909	2.427804	0.318705
10	6	0	-2.875856	1.100447	0.044452
11	6	0	-4.192760	0.681036	-0.432814
12	6	0	-4.192835	-0.680947	-0.432609
13	6	0	-2.875960	-1.100362	0.044733
14	6	0	-2.468117	-2.427719	0.319174
15	6	0	-1.134228	-2.827037	0.513604
16	6	0	-0.683963	-4.139541	0.880396
17	6	0	0.683801	-4.139561	0.880230
18	6	0	1.134031	-2.827063	0.513351
19	6	0	2.467916	-2.427821	0.318702
20	6	0	2.875873	-1.100462	0.044448
21	6	0	4.192775	-0.681055	-0.432818
22	6	0	4.192832	0.680934	-0.432648
23	6	0	2.875976	1.100346	0.044726
24	6	0	2.468134	2.427702	0.319212
25	1	0	1.337067	4.966001	1.114371
26	1	0	-1.336954	4.966051	1.113937
27	1	0	-1.337071	-4.966086	1.114106
28	1	0	1.336946	-4.966124	1.113773
29	1	0	-0.000167	-1.070477	0.161328
30	1	0	0.000198	1.070484	0.161207
31	6	0	-3.495578	-3.502699	0.485033
32	6	0	-4.395823	-3.450172	1.559942
33	6	0	-3.564596	-4.587831	-0.401557
34	6	0	-5.345356	-4.454450	1.740271
35	1	0	-4.346047	-2.615957	2.254081
36	6	0	-4.519953	-5.588193	-0.225890
37	1	0	-2.877734	-4.632430	-1.241986
38	6	0	-5.414040	-5.523458	0.844772
39	1	0	-6.034049	-4.400608	2.579167
40	1	0	-4.569403	-6.415701	-0.928678
41	1	0	-6.158290	-6.303362	0.981890
42	6	0	3.495272	-3.502987	0.484143
43	6	0	4.395638	-3.450924	1.558972
44	6	0	3.564019	-4.587858	-0.402780
45	6	0	5.345037	-4.455400	1.738891
46	1	0	4.346061	-2.616910	2.253369
47	6	0	4.519251	-5.588418	-0.227526
48	1	0	2.877037	-4.632115	-1.243129
49	6	0	5.413464	-5.524145	0.843054
50	1	0	6.033827	-4.401922	2.577732
51	1	0	4.568483	-6.415726	-0.930566
52	1	0	6.157617	-6.304198	0.979850
53	6	0	3.495565	3.502706	0.485070
54	6	0	4.395870	3.450204	1.559930
55	6	0	3.564485	4.587877	-0.401486
56	6	0	5.345347	4.454534	1.740250
57	1	0	4.346177	2.615965	2.254049
58	6	0	4.519789	5.588291	-0.225832
59	1	0	2.877580	4.632470	-1.241881
60	6	0	5.413928	5.523579	0.844787
61	1	0	6.034077	4.400700	2.579117
62	1	0	4.569141	6.415828	-0.928595
63	1	0	6.158142	6.303519	0.981899
64	6	0	-3.495258	3.502965	0.484143
65	6	0	-3.563994	4.587827	-0.402799

66	6	0	-4.395622	3.450926	1.558971
67	6	0	-4.519221	5.588392	-0.227567
68	1	0	-2.877005	4.632063	-1.243143
69	6	0	-5.345016	4.455413	1.738871
70	1	0	-4.346055	2.616926	2.253385
71	6	0	-5.413437	5.524140	0.843016
72	1	0	-4.568455	6.415685	-0.930623
73	1	0	-6.033805	4.401953	2.577713
74	1	0	-6.157586	6.304199	0.979798
75	35	0	-5.604323	1.721830	-1.109583
76	35	0	-5.604549	-1.721786	-1.108998
77	35	0	5.604511	1.721770	-1.109115
78	35	0	5.604395	-1.721826	-1.109499

Rotational constants (GHZ): 0.0496973 0.0267743 0.0184643

- **$NiBr_4TPP$**

Total Energies: -13705.208223 Hartrees
Stoichiometry C44H24Br4N4Ni
Framework group C1[X(C44H24Br4N4Ni)]
Deg. of freedom 225
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.000291	1.900452	0.556541
2	7	0	-1.929528	-0.000202	0.219853
3	7	0	0.000305	-1.900582	0.556052
4	7	0	1.929564	0.000159	0.219785
5	6	0	1.095674	2.705313	0.792697
6	6	0	0.678684	3.980409	1.317983
7	6	0	-0.679176	3.980116	1.318907
8	6	0	-1.096300	2.704901	0.794015
9	6	0	-2.404337	2.393447	0.424718
10	6	0	-2.727417	1.106597	-0.017566
11	6	0	-3.969914	0.681560	-0.614973
12	6	0	-3.969473	-0.681742	-0.616211
13	6	0	-2.726863	-1.107066	-0.019209
14	6	0	-2.403484	-2.394287	0.421806
15	6	0	-1.095646	-2.705535	0.791998
16	6	0	-0.678622	-3.980789	1.316866
17	6	0	0.679231	-3.980498	1.317698
18	6	0	1.096329	-2.705114	0.793191
19	6	0	2.404335	-2.393570	0.423865
20	6	0	2.727400	-1.106576	-0.018038
21	6	0	3.969874	-0.681365	-0.615395
22	6	0	3.969509	0.681939	-0.616094
23	6	0	2.726903	1.107096	-0.018976
24	6	0	2.403519	2.394172	0.422413
25	1	0	1.347519	4.771222	1.623015
26	1	0	-1.347933	4.770648	1.624833

27	1	0	-1.347443	-4.771700	1.621677
28	1	0	1.348016	-4.771133	1.623298
29	6	0	-3.449557	-3.449983	0.567906
30	6	0	-4.473692	-3.299162	1.514936
31	6	0	-3.413189	-4.617751	-0.208425
32	6	0	-5.440865	-4.289543	1.678025
33	1	0	-4.506351	-2.400257	2.124246
34	6	0	-4.386038	-5.604439	-0.051407
35	1	0	-2.627272	-4.739864	-0.948172
36	6	0	-5.403073	-5.442592	0.891535
37	1	0	-6.225921	-4.159597	2.418128
38	1	0	-4.351403	-6.498393	-0.668445
39	1	0	-6.160359	-6.212210	1.014737
40	6	0	3.450843	-3.448627	0.571401
41	6	0	4.474635	-3.296239	1.518552
42	6	0	3.415372	-4.617220	-0.203739
43	6	0	5.442307	-4.285914	1.682966
44	1	0	4.506624	-2.396671	2.126918
45	6	0	4.388705	-5.603212	-0.045382
46	1	0	2.629780	-4.740519	-0.943632
47	6	0	5.405372	-5.439818	0.897692
48	1	0	6.227080	-4.154750	2.423154
49	1	0	4.354754	-6.497824	-0.661503
50	1	0	6.163044	-6.208889	1.021926
51	6	0	3.449593	3.449832	0.568797
52	6	0	4.473752	3.298717	1.515753
53	6	0	3.413211	4.617831	-0.207185
54	6	0	5.440932	4.289048	1.679121
55	1	0	4.506422	2.399628	2.124790
56	6	0	4.386064	5.604471	-0.049885
57	1	0	2.627277	4.740170	-0.946876
58	6	0	5.403122	5.442336	0.892982
59	1	0	6.226005	4.158876	2.419165
60	1	0	4.351418	6.498612	-0.666652
61	1	0	6.160413	6.211914	1.016399
62	6	0	-3.450869	3.448436	0.572627
63	6	0	-3.415507	4.617250	-0.202182
64	6	0	-4.474604	3.295715	1.519787
65	6	0	-4.388874	5.603153	-0.043471
66	1	0	-2.629972	4.740799	-0.942094
67	6	0	-5.442309	4.285300	1.684556
68	1	0	-4.506517	2.395965	2.127889
69	6	0	-5.405472	5.439438	0.899622
70	1	0	-4.355006	6.497946	-0.659334
71	1	0	-6.227031	4.153883	2.424753
72	1	0	-6.163170	6.208440	1.024131
73	35	0	-5.309111	1.736507	-1.396797
74	35	0	-5.307898	-1.736142	-1.400091
75	35	0	5.307989	1.736562	-1.399578
76	35	0	5.308952	-1.736070	-1.397750
77	28	0	0.000055	-0.000046	0.397997

Rotational constants (GHZ): 0.0496194 0.0281570 0.0195420

- **$ZnBr_4TPP$**

Total Energies: -13976.167483 Hartrees
Stoichiometry C44H24Br4N4Zn
Framework group C1[X(C44H24Br4N4Zn)]
Deg. of freedom 225
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.000050	1.991018	0.290459
2	7	0	-2.093962	-0.000019	0.159667
3	7	0	-0.000070	-1.991109	0.289925
4	7	0	2.093825	-0.000050	0.159556
5	6	0	1.105949	2.801889	0.434470
6	6	0	0.679459	4.145881	0.748575
7	6	0	-0.679553	4.145880	0.748585
8	6	0	-1.106045	2.801896	0.434449
9	6	0	-2.450827	2.432232	0.249753
10	6	0	-2.886737	1.114605	0.002431
11	6	0	-4.216502	0.683755	-0.381912
12	6	0	-4.216524	-0.683640	-0.382030
13	6	0	-2.886780	-1.114594	0.002259
14	6	0	-2.450860	-2.432290	0.249150
15	6	0	-1.106060	-2.802045	0.433617
16	6	0	-0.679571	-4.146179	0.747131
17	6	0	0.679447	-4.146188	0.747071
18	6	0	1.105924	-2.802055	0.433543
19	6	0	2.450719	-2.432315	0.249046
20	6	0	2.886656	-1.114626	0.002185
21	6	0	4.216484	-0.683653	-0.381785
22	6	0	4.216486	0.683743	-0.381520
23	6	0	2.886620	1.114576	0.002465
24	6	0	2.450729	2.432201	0.249802
25	1	0	1.338271	4.978869	0.941250
26	1	0	-1.338365	4.978868	0.941255
27	1	0	-1.338347	-4.979282	0.939417
28	1	0	1.338228	-4.979299	0.939309
29	6	0	-3.458162	-3.533790	0.382673
30	6	0	-4.281658	-3.598492	1.515645
31	6	0	-3.572798	-4.532023	-0.595312
32	6	0	-5.206239	-4.631733	1.662660
33	1	0	-4.195173	-2.831869	2.280801
34	6	0	-4.502703	-5.561329	-0.452325
35	1	0	-2.938975	-4.488382	-1.476551
36	6	0	-5.323864	-5.612450	0.676014
37	1	0	-5.837057	-4.669038	2.546810
38	1	0	-4.588001	-6.321903	-1.223960
39	1	0	-6.048098	-6.414950	0.787777
40	6	0	3.458012	-3.533840	0.382457
41	6	0	4.281722	-3.598498	1.515272
42	6	0	3.572436	-4.532126	-0.595499
43	6	0	5.206303	-4.631759	1.662167
44	1	0	4.195405	-2.831830	2.280402
45	6	0	4.502328	-5.561459	-0.452626

46	1	0	2.938445	-4.488514	-1.476618
47	6	0	5.323703	-5.612541	0.675559
48	1	0	5.837290	-4.669033	2.546198
49	1	0	4.587455	-6.322081	-1.224233
50	1	0	6.047936	-6.415055	0.787229
51	6	0	3.458016	3.533672	0.383616
52	6	0	4.281756	3.597987	1.516423
53	6	0	3.572427	4.532228	-0.594065
54	6	0	5.206374	4.631173	1.663571
55	1	0	4.195458	2.831083	2.281321
56	6	0	4.502358	5.561496	-0.450936
57	1	0	2.938385	4.488893	-1.475160
58	6	0	5.323777	5.612225	0.677228
59	1	0	5.837389	4.668187	2.547593
60	1	0	4.587479	6.322340	-1.222325
61	1	0	6.048028	6.414694	0.789108
62	6	0	-3.458046	3.533781	0.383444
63	6	0	-3.572604	4.532055	-0.594507
64	6	0	-4.281503	3.598513	1.516435
65	6	0	-4.502439	5.561424	-0.451484
66	1	0	-2.938763	4.488410	-1.475732
67	6	0	-5.206016	4.631807	1.663480
68	1	0	-4.195074	2.831844	2.281553
69	6	0	-5.323592	5.612556	0.676856
70	1	0	-4.587688	6.322038	-1.223086
71	1	0	-5.836817	4.669139	2.547641
72	1	0	-6.047764	6.415107	0.788658
73	35	0	-5.689814	1.712053	-0.929796
74	35	0	-5.689787	-1.711836	-0.930212
75	35	0	5.690015	1.712129	-0.928645
76	35	0	5.689940	-1.711862	-0.929422
77	30	0	-0.000061	-0.000060	0.218751

Rotational constants (GHZ): 0.0497665 0.0268272 0.0183011

- **$ZnBr_8TPP$ - 5**

Total Energies: -24260.543517 Hartrees
Stoichiometry C44H20Br8N4Zn
Framework group C1[X(C44H20Br8N4Zn)]
Deg. of freedom 225
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.026754	2.021932	-0.131085
2	7	0	2.021904	0.026758	0.131124
3	7	0	0.026760	-2.021919	-0.131094
4	7	0	-2.021903	-0.026757	0.131137
5	6	0	-1.153856	2.762211	-0.406989
6	6	0	-0.737361	3.997573	-1.042141
7	6	0	0.631863	4.015826	-1.041416

8	6	0	1.080490	2.791924	-0.405980
9	6	0	2.390043	2.454255	0.000895
10	6	0	2.762191	1.153855	0.407011
11	6	0	3.997565	0.737359	1.042139
12	6	0	4.015818	-0.631868	1.041409
13	6	0	2.791906	-1.080490	0.406000
14	6	0	2.454247	-2.390046	-0.000872
15	6	0	1.153853	-2.762204	-0.406988
16	6	0	0.737358	-3.997554	-1.042163
17	6	0	-0.631871	-4.015798	-1.041437
18	6	0	-1.080484	-2.791904	-0.405980
19	6	0	-2.390041	-2.454247	0.000910
20	6	0	-2.762196	-1.153859	0.407025
21	6	0	-3.997562	-0.737361	1.042159
22	6	0	-4.015813	0.631865	1.041424
23	6	0	-2.791896	1.080486	0.406011
24	6	0	-2.454243	2.390049	-0.000879
25	6	0	3.524248	-3.431828	-0.001627
26	6	0	4.586232	-3.357615	-0.913346
27	6	0	3.479313	-4.496048	0.909405
28	6	0	5.580364	-4.333325	-0.918826
29	1	0	4.623581	-2.536170	-1.623339
30	6	0	4.481455	-5.463532	0.913499
31	1	0	2.659720	-4.555953	1.619989
32	6	0	5.532314	-5.386511	-0.003014
33	1	0	6.394691	-4.270600	-1.635610
34	1	0	4.441233	-6.279714	1.629789
35	1	0	6.311060	-6.144553	-0.003541
36	6	0	-3.431821	-3.524252	0.001665
37	6	0	-4.496066	-3.479295	-0.909335
38	6	0	-3.357584	-4.586255	0.913360
39	6	0	-5.463559	-4.481429	-0.913415
40	1	0	-4.555987	-2.659689	-1.619903
41	6	0	-4.333302	-5.580380	0.918853
42	1	0	-2.536117	-4.623623	1.623326
43	6	0	-5.386518	-5.532304	0.003077
44	1	0	-6.279763	-4.441187	-1.629679
45	1	0	-4.270562	-6.394720	1.635620
46	1	0	-6.144566	-6.311045	0.003616
47	6	0	-3.524254	3.431822	-0.001645
48	6	0	-4.586268	3.357561	-0.913323
49	6	0	-3.479306	4.496075	0.909349
50	6	0	-5.580418	4.333253	-0.918801
51	1	0	-4.623629	2.536089	-1.623285
52	6	0	-4.481462	5.463543	0.913443
53	1	0	-2.659692	4.556015	1.619906
54	6	0	-5.532353	5.386473	-0.003029
55	1	0	-6.394769	4.270489	-1.635554
56	1	0	-4.441229	6.279751	1.629704
57	1	0	-6.311114	6.144500	-0.003555
58	6	0	3.431834	3.524248	0.001660
59	6	0	3.357620	4.586236	0.913375
60	6	0	4.496085	3.479284	-0.909333
61	6	0	4.333356	5.580343	0.918887
62	1	0	2.536155	4.623605	1.623344
63	6	0	5.463598	4.481397	-0.913393
64	1	0	4.555995	2.659685	-1.619911
65	6	0	5.386574	5.532262	0.003113
66	1	0	4.270629	6.394672	1.635668
67	1	0	6.279805	4.441149	-1.629653

68	1	0	6.144638	6.310986	0.003667
69	35	0	5.312000	1.782082	1.880353
70	35	0	5.357784	-1.642162	1.878206
71	35	0	-5.357772	1.642162	1.878222
72	35	0	-5.311993	-1.782084	1.880382
73	35	0	-1.782087	5.311978	-1.880400
74	35	0	1.642154	5.357748	-1.878284
75	35	0	1.782085	-5.311972	-1.880405
76	35	0	-1.642184	-5.357720	-1.878286
77	30	0	-0.000008	0.000011	0.000061

Rotational constants (GHZ): 0.0245917 0.0245915 0.0140406

- **$NiBr_8TPP$ - 7**

Total Energies: -23989.589749 Hartrees
Stoichiometry C44H20Br8N4Ni
Framework group C1[X(C44H20Br8N4Ni)]
Deg. of freedom 225
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.878885	-0.251237	-0.203717
2	7	0	-0.250480	1.880157	0.200762
3	7	0	1.881070	0.251749	-0.199867
4	7	0	0.251506	-1.879220	0.201665
5	6	0	-2.488018	-1.451215	-0.517063
6	6	0	-3.707608	-1.182339	-1.244228
7	6	0	-3.888291	0.170712	-1.242043
8	6	0	-2.781933	0.747764	-0.513277
9	6	0	-2.675608	2.045772	0.001342
10	6	0	-1.450382	2.488715	0.514582
11	6	0	-1.182282	3.706700	1.244917
12	6	0	0.170751	3.887639	1.243520
13	6	0	0.748300	2.782649	0.512642
14	6	0	2.046045	2.676949	-0.002641
15	6	0	2.488791	1.451705	-0.516140
16	6	0	3.705465	1.182659	-1.247761
17	6	0	3.886692	-0.170445	-1.245107
18	6	0	2.783163	-0.747163	-0.512070
19	6	0	2.677374	-2.044461	0.004062
20	6	0	1.451627	-2.487353	0.516722
21	6	0	1.182796	-3.706128	1.245545
22	6	0	-0.170083	-3.887933	1.242051
23	6	0	-0.747060	-2.782626	0.511140
24	6	0	-2.044657	-2.676701	-0.004711
25	6	0	2.951122	3.861608	-0.002663
26	6	0	2.667471	4.970985	-0.811115
27	6	0	4.097380	3.879036	0.803748
28	6	0	3.517065	6.075030	-0.816339
29	1	0	1.782850	4.959943	-1.441624

30	6	0	4.939820	4.988726	0.807638
31	1	0	4.320830	3.021687	1.432377
32	6	0	4.653271	6.087899	-0.004548
33	1	0	3.291846	6.926550	-1.452697
34	1	0	5.821606	4.994702	1.442607
35	1	0	5.313139	6.951377	-0.004964
36	6	0	3.862408	-2.949023	0.004464
37	6	0	3.880381	-4.095830	-0.801282
38	6	0	4.971750	-2.664287	0.812554
39	6	0	4.990219	-4.937943	-0.804431
40	1	0	3.023048	-4.319997	-1.429690
41	6	0	6.076036	-3.513684	0.818581
42	1	0	4.960438	-1.779279	1.442504
43	6	0	6.089245	-4.650512	0.007758
44	1	0	4.996598	-5.820203	-1.438740
45	1	0	6.927425	-3.287640	1.454820
46	1	0	6.952864	-5.310194	0.008672
47	6	0	-2.948911	-3.862103	-0.005152
48	6	0	-2.665067	-4.970338	-0.815084
49	6	0	-4.094339	-3.881360	0.802394
50	6	0	-3.513519	-6.075309	-0.820324
51	1	0	-1.781254	-4.957779	-1.446690
52	6	0	-4.935631	-4.991891	0.806173
53	1	0	-4.318039	-3.024773	1.431977
54	6	0	-4.648739	-6.090105	-0.007233
55	1	0	-3.288102	-6.926025	-1.457690
56	1	0	-5.816743	-4.999378	1.442061
57	1	0	-5.307660	-6.954307	-0.007572
58	6	0	-3.859999	2.951275	0.000830
59	6	0	-4.968608	2.669367	0.810886
60	6	0	-3.878243	4.095566	-0.808400
61	6	0	-6.072491	3.519265	0.815505
62	1	0	-4.957236	1.785961	1.443086
63	6	0	-4.987672	4.938288	-0.812782
64	1	0	-3.021589	4.317338	-1.438569
65	6	0	-6.085949	4.653769	0.001390
66	1	0	-6.923405	3.295445	1.453163
67	1	0	-4.994290	5.818682	-1.449679
68	1	0	-6.949216	5.313912	0.001369
69	35	0	-2.388029	4.806483	2.166292
70	35	0	1.046518	5.266074	2.162865
71	35	0	-1.045218	-5.269741	2.157003
72	35	0	2.388206	-4.806145	2.167066
73	28	0	0.000567	0.000307	-0.000059
74	35	0	-4.811378	-2.387437	-2.161789
75	35	0	-5.271369	1.046452	-2.154518
76	35	0	4.805511	2.387909	-2.169594
77	35	0	5.266502	-1.046588	-2.162161

Rotational constants (GHZ): 0.0249464 0.0249429 0.0148894