Supporting Information

for

"Effects of Porphyrin Core Saddling, *Meso*-Phenyl Twisting, and Counterions on the Optical Properties of *Meso*-Tetraphenylporphyrin Diacids: the $[H_4TPP](X)_2$ (X = F, Cl, Br, I) Series as a Case Study"

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1. Optimized Structures

Tables of the Cartesian coordinates (Å) for the following optimized structures:

H_4TPP^{2+} (D_{4h})

Atom	x	y	z
N	-1.52997	-1.52997	0.00000
N	1.52997	-1.52997	0.00000
N	1.52997	1.52997	0.00000
N	-1.52997	1.52997	0.00000
C	-1.26386	-2.89149	0.00000
C	-2.89149	-1.26386	0.00000
C	2.89149	1.26386	0.00000
C	1.26386	2.89149	0.00000
C	1.26386	-2.89149	0.00000
C	2.89149	-1.26386	0.00000
C	-2.89149	1.26386	0.00000
C	-1.26386	2.89149	0.00000
C	-2.55046	-3.52244	0.00000
C	-3.52244	-2.55046	0.00000
C	3.52244	2.55046	0.00000
C	2.55046	3.52244	0.00000
C	2.55046	-3.52244	0.00000
C	3.52244	-2.55046	0.00000
C	-3.52244	2.55046	0.00000
C	-2.55046	3.52244	0.00000
C	0.00000	-3.51972	0.00000
C	-3.51972	0.00000	0.00000
C	0.00000	3.51972	0.00000
C	3.51972	0.00000	0.00000
H	-2.69776	-4.59644	0.00000
H	-4.59644	-2.69776	0.00000
H	4.59644	2.69776	0.00000
H	2.69776	4.59644	0.00000
H	2.69776	-4.59644	0.00000
H	4.59644	-2.69776	0.00000
H	-4.59644	2.69776	0.00000
H	-2.69776	4.59644	0.00000
C	0.00000	-5.01891	0.00000
C	-5.01891	0.00000	0.00000
C	0.00000	5.01891	0.00000
C	5.01891	0.00000	0.00000
C	0.00000	-5.72167	-1.21332
C	0.00000	-7.11863	-1.20936
C	0.00000	-7.81757	0.00000
C	0.00000	-5.72167	1.21332
C	0.00000	-7.11863	1.20936
H	0.00000	-5.17854	-2.15846
H	0.00000	-7.65875	-2.15463
H	0.00000	-8.90656	0.00000
H	0.00000	-5.17854	2.15846
H	0.00000	-7.65875	2.15463
C	5.72167	0.00000	1.21332
C	7.11863	0.00000	1.20936
C	7.81757	0.00000	0.00000
C	5.72167	0.00000	-1.21332
C	7.11863	0.00000	-1.20936

H	5.17854	0.00000	2.15846
H	7.65875	0.00000	2.15463
H	8.90656	0.00000	0.00000
H	5.17854	0.00000	-2.15846
H	7.65875	0.00000	-2.15463
C	0.00000	5.72167	-1.21332
C	0.00000	7.11863	-1.20936
C	0.00000	7.81757	0.00000
C	0.00000	5.72167	1.21332
C	0.00000	7.11863	1.20936
H	0.00000	5.17854	-2.15846
H	0.00000	7.65875	-2.15463
H	0.00000	8.90656	0.00000
H	0.00000	5.17854	2.15846
H	0.00000	7.65875	2.15463
C	-5.72167	0.00000	1.21332
C	-7.11863	0.00000	1.20936
C	-7.81757	0.00000	0.00000
C	-5.72167	0.00000	-1.21332
C	-7.11863	0.00000	-1.20936
H	-5.17854	0.00000	2.15846
H	-7.65875	0.00000	2.15463
H	-8.90656	0.00000	0.00000
H	-5.17854	0.00000	-2.15846
H	-7.65875	0.00000	-2.15463
H	0.82418	-0.82418	0.00000
H	-0.82418	0.82418	0.00000
H	0.82418	0.82418	0.00000
H	-0.82418	-0.82418	0.00000

$[H_4TPP](F)_2$ (D_{4h})

Atom	x	y	z
N	-1.55278	-1.55278	0.00000
N	1.55278	-1.55278	0.00000
N	1.55278	1.55278	0.00000
N	-1.55278	1.55278	0.00000
C	-1.28264	-2.88760	0.00000
C	-2.88760	-1.28264	0.00000
C	2.88760	1.28264	0.00000
C	1.28264	2.88760	0.00000
C	1.28264	-2.88760	0.00000
C	2.88760	-1.28264	0.00000
C	-2.88760	1.28264	0.00000
C	-1.28264	2.88760	0.00000
C	-2.57575	-3.54482	0.00000
C	-3.54482	-2.57575	0.00000
C	3.54482	2.57575	0.00000
C	2.57575	3.54482	0.00000
C	2.57575	-3.54482	0.00000
C	3.54482	-2.57575	0.00000
C	-3.54482	2.57575	0.00000
C	-2.57575	3.54482	0.00000
C	0.00000	-3.49800	0.00000
C	-3.49800	0.00000	0.00000
C	0.00000	3.49800	0.00000
C	3.49800	0.00000	0.00000
H	-2.72560	-4.61829	0.00000
H	-4.61829	-2.72560	0.00000
H	4.61829	2.72560	0.00000
H	2.72560	4.61829	0.00000

H	2.72560	-4.61829	0.00000
H	4.61829	-2.72560	0.00000
H	-4.61829	2.72560	0.00000
H	-2.72560	4.61829	0.00000
C	0.00000	-5.00001	0.00000
C	-5.00001	0.00000	0.00000
C	0.00000	5.00001	0.00000
C	5.00001	0.00000	0.00000
C	0.00000	-5.71097	-1.20788
C	0.00000	-7.10833	-1.20792
C	0.00000	-7.81026	0.00000
C	0.00000	-5.71097	1.20788
C	0.00000	-7.10833	1.20792
H	0.00000	-5.16129	-2.14930
H	0.00000	-7.64752	-2.15464
H	0.00000	-8.90000	0.00000
H	0.00000	-5.16129	2.14930
H	0.00000	-7.64752	2.15464
C	5.71097	0.00000	1.20788
C	7.10833	0.00000	1.20792
C	7.81026	0.00000	0.00000
C	5.71097	0.00000	-1.20788
C	7.10833	0.00000	-1.20792
H	5.16129	0.00000	2.14930
H	7.64752	0.00000	2.15464
H	8.90000	0.00000	0.00000
H	5.16129	0.00000	-2.14930
H	7.64752	0.00000	-2.15464
C	0.00000	5.71097	-1.20788
C	0.00000	7.10833	-1.20792
C	0.00000	7.81026	0.00000
C	0.00000	5.71097	1.20788
C	0.00000	7.10833	1.20792
H	0.00000	5.16129	-2.14930
H	0.00000	7.64752	-2.15464
H	0.00000	8.90000	0.00000
H	0.00000	5.16129	2.14930
H	0.00000	7.64752	2.15464
C	-5.71097	0.00000	1.20788
C	-7.10833	0.00000	1.20792
C	-7.81026	0.00000	0.00000
C	-5.71097	0.00000	-1.20788
C	-7.10833	0.00000	-1.20792
H	-5.16129	0.00000	2.14930
H	-7.64752	0.00000	2.15464
H	-8.90000	0.00000	0.00000
H	-5.16129	0.00000	-2.14930
H	-7.64752	0.00000	-2.15464
H	0.82288	-0.82288	0.00000
H	-0.82288	0.82288	0.00000
H	0.82288	0.82288	0.00000
H	-0.82288	-0.82288	0.00000
F	0.00000	0.00000	1.30488
F	0.00000	0.00000	-1.30488

$[H_4TPP](Cl)_2$ (D_{4h})

Atom	x	y	z
Cl	0.00000	0.00000	2.08594
Cl	0.00000	0.00000	-2.08594

N	-1.55600	-1.55600	0.00000
N	1.55600	-1.55600	0.00000
N	1.55600	1.55600	0.00000
N	-1.55600	1.55600	0.00000
C	-1.27987	-2.89266	0.00000
C	-2.89266	-1.27987	0.00000
C	2.89266	1.27987	0.00000
C	1.27987	2.89266	0.00000
C	1.27987	-2.89266	0.00000
C	2.89266	-1.27987	0.00000
C	-2.89266	1.27987	0.00000
C	-1.27987	2.89266	0.00000
C	-2.57321	-3.54276	0.00000
C	-3.54276	-2.57321	0.00000
C	3.54276	2.57321	0.00000
C	2.57321	3.54276	0.00000
C	2.57321	-3.54276	0.00000
C	3.54276	-2.57321	0.00000
C	-3.54276	2.57321	0.00000
C	-2.57321	3.54276	0.00000
C	0.00000	-3.50329	0.00000
C	-3.50329	0.00000	0.00000
C	0.00000	3.50329	0.00000
C	3.50329	0.00000	0.00000
H	-2.72344	-4.61600	0.00000
H	-4.61600	-2.72344	0.00000
H	4.61600	2.72344	0.00000
H	2.72344	4.61600	0.00000
H	2.72344	-4.61600	0.00000
H	4.61600	-2.72344	0.00000
H	-4.61600	2.72344	0.00000
H	-2.72344	4.61600	0.00000
C	0.00000	-5.00491	0.00000
C	-5.00491	0.00000	0.00000
C	0.00000	5.00491	0.00000
C	5.00491	0.00000	0.00000
C	0.00000	-5.71431	-1.20868
C	0.00000	-7.11166	-1.20819
C	0.00000	-7.81313	0.00000
C	0.00000	-5.71431	1.20868
C	0.00000	-7.11166	1.20819
H	0.00000	-5.16406	-2.14973
H	0.00000	-7.65104	-2.15471
H	0.00000	-8.90284	0.00000
H	0.00000	-5.16406	2.14973
H	0.00000	-7.65104	2.15471
C	5.71431	0.00000	1.20868
C	7.11166	0.00000	1.20819
C	7.81313	0.00000	0.00000
C	5.71431	0.00000	-1.20868
C	7.11166	0.00000	-1.20819
H	5.16406	0.00000	2.14973
H	7.65104	0.00000	2.15471
H	8.90284	0.00000	0.00000
H	5.16406	0.00000	-2.14973
H	7.65104	0.00000	-2.15471
C	0.00000	5.71431	-1.20868
C	0.00000	7.11166	-1.20819
C	0.00000	7.81313	0.00000
C	0.00000	5.71431	1.20868
C	0.00000	7.11166	1.20819
H	0.00000	5.16406	-2.14973

H	0.00000	7.65104	-2.15471
H	0.00000	8.90284	0.00000
H	0.00000	5.16406	2.14973
H	0.00000	7.65104	2.15471
C	-5.71431	0.00000	1.20868
C	-7.11166	0.00000	1.20819
C	-7.81313	0.00000	0.00000
C	-5.71431	0.00000	-1.20868
C	-7.11166	0.00000	-1.20819
H	-5.16406	0.00000	2.14973
H	-7.65104	0.00000	2.15471
H	-8.90284	0.00000	0.00000
H	-5.16406	0.00000	-2.14973
H	-7.65104	0.00000	-2.15471
H	0.83940	-0.83940	0.00000
H	-0.83940	0.83940	0.00000
H	0.83940	0.83940	0.00000
H	-0.83940	-0.83940	0.00000

$[H_4TPP](Br)_2$ (D_{4h})

Atom	x	y	z
Br	0.00000	0.00000	2.32980
Br	0.00000	0.00000	-2.32980
N	-1.55297	-1.55297	0.00000
N	1.55297	-1.55297	0.00000
N	1.55297	1.55297	0.00000
N	-1.55297	1.55297	0.00000
C	-1.27730	-2.89140	0.00000
C	-2.89140	-1.27730	0.00000
C	2.89140	1.27730	0.00000
C	1.27730	2.89140	0.00000
C	1.27730	-2.89140	0.00000
C	2.89140	-1.27730	0.00000
C	-2.89140	1.27730	0.00000
C	-1.27730	2.89140	0.00000
C	-2.56962	-3.53907	0.00000
C	-3.53907	-2.56962	0.00000
C	3.53907	2.56962	0.00000
C	2.56962	3.53907	0.00000
C	2.56962	-3.53907	0.00000
C	3.53907	-2.56962	0.00000
C	-3.53907	2.56962	0.00000
C	-2.56962	3.53907	0.00000
C	0.00000	-3.50316	0.00000
C	-3.50316	0.00000	0.00000
C	0.00000	3.50316	0.00000
C	3.50316	0.00000	0.00000
H	-2.71958	-4.61207	0.00000
H	-4.61207	-2.71958	0.00000
H	4.61207	2.71958	0.00000
H	2.71958	4.61207	0.00000
H	2.71958	-4.61207	0.00000
H	4.61207	-2.71958	0.00000
H	-4.61207	2.71958	0.00000
H	-2.71958	4.61207	0.00000
C	0.00000	-5.00432	0.00000
C	-5.00432	0.00000	0.00000
C	0.00000	5.00432	0.00000
C	5.00432	0.00000	0.00000

C	0.00000	-5.71304	-1.20882
C	0.00000	-7.11017	-1.20808
C	0.00000	-7.81143	0.00000
C	0.00000	-5.71304	1.20882
C	0.00000	-7.11017	1.20808
H	0.00000	-5.16260	-2.14963
H	0.00000	-7.64956	-2.15444
H	0.00000	-8.90107	0.00000
H	0.00000	-5.16260	2.14963
H	0.00000	-7.64956	2.15444
C	5.71304	0.00000	1.20882
C	7.11017	0.00000	1.20808
C	7.81143	0.00000	0.00000
C	5.71304	0.00000	-1.20882
C	7.11017	0.00000	-1.20808
H	5.16260	0.00000	2.14963
H	7.64956	0.00000	2.15444
H	8.90107	0.00000	0.00000
H	5.16260	0.00000	-2.14963
H	7.64956	0.00000	-2.15444
C	0.00000	5.71304	-1.20882
C	0.00000	7.11017	-1.20808
C	0.00000	7.81143	0.00000
C	0.00000	5.71304	1.20882
C	0.00000	7.11017	1.20808
H	0.00000	5.16260	-2.14963
H	0.00000	7.64956	-2.15444
H	0.00000	8.90107	0.00000
H	0.00000	5.16260	2.14963
H	0.00000	7.64956	2.15444
C	-5.71304	0.00000	1.20882
C	-7.11017	0.00000	1.20808
C	-7.81143	0.00000	0.00000
C	-5.71304	0.00000	-1.20882
C	-7.11017	0.00000	-1.20808
H	-5.16260	0.00000	2.14963
H	-7.64956	0.00000	2.15444
H	-8.90107	0.00000	0.00000
H	-5.16260	0.00000	-2.14963
H	-7.64956	0.00000	-2.15444
H	0.83801	-0.83801	0.00000
H	-0.83801	0.83801	0.00000
H	0.83801	0.83801	0.00000
H	-0.83801	-0.83801	0.00000

$[H_4TPP](I)_2$ (D_{4h})

Atom	x	y	z
I	0.00000	0.00000	-2.66290
I	0.00000	0.00000	2.66290
N	-1.55006	-1.55006	0.00000
N	1.55006	-1.55006	0.00000
N	1.55006	1.55006	0.00000
N	-1.55006	1.55006	0.00000
C	-1.27485	-2.89171	0.00000
C	-2.89171	-1.27485	0.00000
C	2.89171	1.27485	0.00000
C	1.27485	2.89171	0.00000
C	1.27485	-2.89171	0.00000

C	2.89171	-1.27485	0.00000
C	-2.89171	1.27485	0.00000
C	-1.27485	2.89171	0.00000
C	-2.56620	-3.53607	0.00000
C	-3.53607	-2.56620	0.00000
C	3.53607	2.56620	0.00000
C	2.56620	3.53607	0.00000
C	2.56620	-3.53607	0.00000
C	3.53607	-2.56620	0.00000
C	-3.53607	2.56620	0.00000
C	-2.56620	3.53607	0.00000
C	0.00000	-3.50521	0.00000
C	-3.50521	0.00000	0.00000
C	0.00000	3.50521	0.00000
C	3.50521	0.00000	0.00000
H	-2.71571	-4.60900	0.00000
H	-4.60900	-2.71571	0.00000
H	4.60900	2.71571	0.00000
H	2.71571	4.60900	0.00000
H	2.71571	-4.60900	0.00000
H	4.60900	-2.71571	0.00000
H	-4.60900	2.71571	0.00000
H	-2.71571	4.60900	0.00000
C	0.00000	-5.00614	0.00000
C	-5.00614	0.00000	0.00000
C	0.00000	5.00614	0.00000
C	5.00614	0.00000	0.00000
C	0.00000	-5.71413	-1.20929
C	0.00000	-7.11127	-1.20828
C	0.00000	-7.81227	0.00000
C	0.00000	-5.71413	1.20929
C	0.00000	-7.11127	1.20828
H	0.00000	-5.16370	-2.15020
H	0.00000	-7.65074	-2.15474
H	0.00000	-8.90194	0.00000
H	0.00000	-5.16370	2.15020
H	0.00000	-7.65074	2.15474
C	5.71413	0.00000	1.20929
C	7.11127	0.00000	1.20828
C	7.81227	0.00000	0.00000
C	5.71413	0.00000	-1.20929
C	7.11127	0.00000	-1.20828
H	5.16370	0.00000	2.15020
H	7.65074	0.00000	2.15474
H	8.90194	0.00000	0.00000
H	5.16370	0.00000	-2.15020
H	7.65074	0.00000	-2.15474
C	0.00000	5.71413	-1.20929
C	0.00000	7.11127	-1.20828
C	0.00000	7.81227	0.00000
C	0.00000	5.71413	1.20929
C	0.00000	7.11127	1.20828
H	0.00000	5.16370	-2.15020
H	0.00000	7.65074	-2.15474
H	0.00000	8.90194	0.00000
H	0.00000	5.16370	2.15020
H	0.00000	7.65074	2.15474
C	-5.71413	0.00000	1.20929
C	-7.11127	0.00000	1.20828
C	-7.81227	0.00000	0.00000
C	-5.71413	0.00000	-1.20929
C	-7.11127	0.00000	-1.20828

H	-5.16370	0.00000	2.15020
H	-7.65074	0.00000	2.15474
H	-8.90194	0.00000	0.00000
H	-5.16370	0.00000	-2.15020
H	-7.65074	0.00000	-2.15474
H	0.83698	-0.83698	0.00000
H	-0.83698	0.83698	0.00000
H	0.83698	0.83698	0.00000
H	-0.83698	-0.83698	0.00000

H_4TPP^{2+}-*stepo* (C_{2h})

Atom	x	y	z
N	2.05175	-0.52978	0.00000
N	0.00000	0.00000	2.15812
N	-2.05175	0.52978	0.00000
N	0.00000	0.00000	-2.15812
C	2.86458	-0.33710	1.14654
C	2.86458	-0.33710	-1.14654
C	-2.86458	0.33710	1.14654
C	-2.86458	0.33710	-1.14654
C	1.12704	-0.15141	2.94493
C	-1.12704	0.15141	2.94493
C	1.12704	-0.15141	-2.94493
C	-1.12704	0.15141	-2.94493
C	4.16216	-0.01698	0.68714
C	4.16216	-0.01698	-0.68714
C	-4.16216	0.01698	0.68714
C	-4.16216	0.01698	-0.68714
C	0.67877	-0.10088	4.30064
C	-0.67877	0.10088	4.30064
C	0.67877	-0.10088	-4.30064
C	-0.67877	0.10088	-4.30064
C	2.45909	-0.26286	2.49684
C	2.45909	-0.26286	-2.49684
C	-2.45909	0.26286	-2.49684
C	-2.45909	0.26286	2.49684
H	4.97961	0.28494	1.33141
H	4.97961	0.28494	-1.33141
H	-4.97961	-0.28494	1.33141
H	-4.97961	-0.28494	-1.33141
H	1.32347	-0.21030	5.16357
H	-1.32347	0.21030	5.16357
H	1.32347	-0.21030	-5.16357
H	-1.32347	0.21030	-5.16357
C	3.53157	-0.15111	3.51900
C	3.53157	-0.15111	-3.51900
C	-3.53157	0.15111	-3.51900
C	-3.53157	0.15111	3.51900
C	3.58132	0.97570	4.36299
C	4.60408	1.11188	5.29906
C	5.58168	0.11983	5.41780
C	4.52654	-1.13785	3.63812
C	5.53787	-1.00519	4.58910
H	2.83687	1.76429	4.25618
H	4.64323	1.99879	5.92926
H	6.37833	0.22623	6.15262
H	4.49121	-2.02098	3.00096
H	6.29287	-1.78322	4.68549
C	4.52654	-1.13785	-3.63812
C	5.53787	-1.00519	-4.58910

C	5.58168	0.11983	-5.41780
C	3.58132	0.97570	-4.36299
C	4.60408	1.11188	-5.29906
H	4.49121	-2.02098	-3.00096
H	6.29287	-1.78322	-4.68549
H	6.37833	0.22623	-6.15262
H	2.83687	1.76429	-4.25618
H	4.64323	1.99879	-5.92926
C	-3.58132	-0.97570	4.36299
C	-4.60408	-1.11188	5.29906
C	-5.58168	-0.11983	5.41780
C	-4.52654	1.13785	3.63812
C	-5.53787	1.00519	4.58910
H	-2.83687	-1.76429	4.25618
H	-4.64323	-1.99879	5.92926
H	-6.37833	-0.22623	6.15262
H	-4.49121	2.02098	3.00096
H	-6.29287	1.78322	4.68549
C	-4.52654	1.13785	-3.63812
C	-5.53787	1.00519	-4.58910
C	-5.58168	-0.11983	-5.41780
C	-3.58132	-0.97570	-4.36299
C	-4.60408	-1.11188	-5.29906
H	-4.49121	2.02098	-3.00096
H	-6.29287	1.78322	-4.68549
H	-6.37833	-0.22623	-6.15262
H	-2.83687	-1.76429	-4.25618
H	-4.64323	-1.99879	-5.92926
H	1.40819	-1.32153	0.00000
H	-1.40819	1.32153	0.00000
H	0.00000	0.00000	1.14882
H	0.00000	0.00000	-1.14882

[H_4TPP]($F)_2$-*stepo* (C_{2h})

Atom	x	y	z
N	2.04123	-0.25027	0.00000
N	0.00000	0.00000	2.11377
N	-2.04123	0.25027	0.00000
N	0.00000	0.00000	-2.11377
C	2.86655	-0.13032	1.09706
C	2.86655	-0.13032	-1.09706
C	-2.86655	0.13032	1.09706
C	-2.86655	0.13032	-1.09706
C	1.12921	-0.05625	2.89476
C	-1.12921	0.05625	2.89476
C	1.12921	-0.05625	-2.89476
C	-1.12921	0.05625	-2.89476
C	4.24602	0.02630	0.68035
C	4.24602	0.02630	-0.68035
C	-4.24602	-0.02630	0.68035
C	-4.24602	-0.02630	-0.68035
C	0.68450	-0.03231	4.25891
C	-0.68450	0.03231	4.25891
C	0.68450	-0.03231	-4.25891
C	-0.68450	0.03231	-4.25891
C	2.45672	-0.10125	2.44410
C	2.45672	-0.10125	-2.44410
C	-2.45672	0.10125	-2.44410
C	-2.45672	0.10125	2.44410
H	5.09406	0.15002	1.34450

H	5.09406	0.15002	-1.34450
H	-5.09406	-0.15002	1.34450
H	-5.09406	-0.15002	-1.34450
H	1.34332	-0.06645	5.11821
H	-1.34332	0.06645	5.11821
H	1.34332	-0.06645	-5.11821
H	-1.34332	0.06645	-5.11821
C	3.51974	-0.05332	3.50081
C	3.51974	-0.05332	-3.50081
C	-3.51974	0.05332	-3.50081
C	-3.51974	0.05332	3.50081
C	3.96980	1.17738	3.99921
C	4.95897	1.22561	4.98460
C	5.50552	0.04253	5.48825
C	4.07494	-1.23531	4.00884
C	5.06021	-1.18777	4.99880
H	3.54146	2.09959	3.60596
H	5.30122	2.19011	5.35844
H	6.27528	0.07940	6.25890
H	3.72815	-2.19473	3.62469
H	5.47980	-2.11539	5.38666
C	4.07494	-1.23531	-4.00884
C	5.06021	-1.18777	-4.99880
C	5.50552	0.04253	-5.48825
C	3.96980	1.17738	-3.99921
C	4.95897	1.22561	-4.98460
H	3.72815	-2.19473	-3.62469
H	5.47980	-2.11539	-5.38666
H	6.27528	0.07940	-6.25890
H	3.54146	2.09959	-3.60596
H	5.30122	2.19011	-5.35844
C	-3.96980	-1.17738	3.99921
C	-4.95897	-1.22561	4.98460
C	-5.50552	-0.04253	5.48825
C	-4.07494	1.23531	4.00884
C	-5.06021	1.18777	4.99880
H	-3.54146	-2.09959	3.60596
H	-5.30122	-2.19011	5.35844
H	-6.27528	-0.07940	6.25890
H	-3.72815	2.19473	3.62469
H	-5.47980	2.11539	5.38666
C	-4.07494	1.23531	-4.00884
C	-5.06021	1.18777	-4.99880
C	-5.50552	-0.04253	-5.48825
C	-3.96980	-1.17738	-3.99921
C	-4.95897	-1.22561	-4.98460
H	-3.72815	2.19473	-3.62469
H	-5.47980	2.11539	-5.38666
H	-6.27528	-0.07940	-6.25890
H	-3.54146	-2.09959	-3.60596
H	-5.30122	-2.19011	-5.35844
H	1.20592	-1.68409	0.00000
H	-1.20592	1.68409	0.00000
H	0.00000	0.00000	1.09805
H	0.00000	0.00000	-1.09805
F	0.70891	-2.52601	0.00000
F	-0.70891	2.52601	0.00000

$[H_4TPP](Cl)_2$-*stepo* (C_{2h})

Atom	x	y	z
Cl	-0.06736	-2.36120	0.00000
Cl	0.06736	2.36120	0.00000
N	2.12522	-0.44389	0.00000
N	0.00000	0.00000	2.16242
N	-2.12522	0.44389	0.00000
N	0.00000	0.00000	-2.16242
C	2.88550	-0.19577	1.12252
C	2.88550	-0.19577	-1.12252
C	-2.88550	0.19577	1.12252
C	-2.88550	0.19577	-1.12252
C	1.12681	-0.10621	2.93031
C	-1.12681	0.10621	2.93031
C	1.12681	-0.10621	-2.93031
C	-1.12681	0.10621	-2.93031
C	4.19629	0.19755	0.68342
C	4.19629	0.19755	-0.68342
C	-4.19629	-0.19755	0.68342
C	-4.19629	-0.19755	-0.68342
C	0.68032	-0.07317	4.29888
C	-0.68032	0.07317	4.29888
C	0.68032	-0.07317	-4.29888
C	-0.68032	0.07317	-4.29888
C	2.45864	-0.17456	2.47134
C	2.45864	-0.17456	-2.47134
C	-2.45864	0.17456	-2.47134
C	-2.45864	0.17456	2.47134
H	4.99649	0.52252	1.33737
H	4.99649	0.52252	-1.33737
H	-4.99649	-0.52252	1.33737
H	-4.99649	-0.52252	-1.33737
H	1.32880	-0.15435	5.16183
H	-1.32880	0.15435	5.16183
H	1.32880	-0.15435	-5.16183
H	-1.32880	0.15435	-5.16183
C	3.53557	-0.11058	3.50062
C	3.53557	-0.11058	-3.50062
C	-3.53557	0.11058	-3.50062
C	-3.53557	0.11058	3.50062
C	3.62806	0.97629	4.38642
C	4.65351	1.03868	5.33088
C	5.60177	0.01499	5.40780
C	4.49783	-1.13047	3.58284
C	5.52023	-1.06978	4.53097
H	2.90339	1.78642	4.31143
H	4.71700	1.89531	6.00096
H	6.40269	0.06465	6.14502
H	4.43071	-1.97923	2.90281
H	6.25336	-1.87368	4.58525
C	4.49783	-1.13047	-3.58284
C	5.52023	-1.06978	-4.53097
C	5.60177	0.01499	-5.40780
C	3.62806	0.97629	-4.38642
C	4.65351	1.03868	-5.33088
H	4.43071	-1.97923	-2.90281
H	6.25336	-1.87368	-4.58525
H	6.40269	0.06465	-6.14502
H	2.90339	1.78642	-4.31143
H	4.71700	1.89531	-6.00096

C	-3.62806	-0.97629	4.38642
C	-4.65351	-1.03868	5.33088
C	-5.60177	-0.01499	5.40780
C	-4.49783	1.13047	3.58284
C	-5.52023	1.06978	4.53097
H	-2.90339	-1.78642	4.31143
H	-4.71700	-1.89531	6.00096
H	-6.40269	-0.06465	6.14502
H	-4.43071	1.97923	2.90281
H	-6.25336	1.87368	4.58525
C	-4.49783	1.13047	-3.58284
C	-5.52023	1.06978	-4.53097
C	-5.60177	-0.01499	-5.40780
C	-3.62806	-0.97629	-4.38642
C	-4.65351	-1.03868	-5.33088
H	-4.43071	1.97923	-2.90281
H	-6.25336	1.87368	-4.58525
H	-6.40269	-0.06465	-6.14502
H	-2.90339	-1.78642	-4.31143
H	-4.71700	-1.89531	-6.00096
H	1.27954	-1.17170	0.00000
H	-1.27954	1.17170	0.00000
H	0.00000	0.00000	1.14603
H	0.00000	0.00000	-1.14603

[H_4TPP]($Br)_2$-*stepo* (C_{2h})

Atom	x	y	z
Br	-.117663	-2.588687	.000000
Br	.117663	2.588687	.000000
N	2.125327	-.455294	.000000
N	.000000	.000000	2.154953
N	-2.125327	.455294	.000000
N	.000000	.000000	-2.154953
C	2.890787	-.219925	1.125645
C	2.890787	-.219925	-1.125645
C	-2.890787	.219925	1.125645
C	-2.890787	.219925	-1.125645
C	1.127565	-.111980	2.925093
C	-1.127565	.111980	2.925093
C	1.127565	-.111980	-2.925093
C	-1.127565	.111980	-2.925093
C	4.203870	.155434	.683876
C	4.203870	.155434	-.683876
C	-4.203870	-.155434	.683876
C	-4.203870	-.155434	-.683876
C	.680152	-.074448	4.292419
C	-.680152	.074448	4.292419
C	.680152	-.074448	-4.292419
C	-.680152	.074448	-4.292419
C	2.461357	-.190846	2.472432
C	2.461357	-.190846	-2.472432
C	-2.461357	.190846	-2.472432
C	-2.461357	.190846	2.472432
H	5.009481	.466704	1.337427
H	5.009481	.466704	-1.337427
H	-5.009481	-.466704	1.337427
H	-5.009481	-.466704	-1.337427
H	1.329250	-.156800	5.154747
H	-1.329250	.156800	5.154747
H	1.329250	-.156800	-5.154747

H	-1.329250	.156800	-5.154747
C	3.537597	-.112053	3.505411
C	3.537597	-.112053	-3.505411
C	-3.537597	.112053	-3.505411
C	-3.537597	.112053	3.505411
C	3.639336	1.006341	4.349643
C	4.664737	1.096004	5.291854
C	5.604637	.068874	5.409510
C	4.490588	-1.136652	3.629309
C	5.515159	-1.047418	4.575191
H	2.922547	1.819666	4.242419
H	4.735081	1.977110	5.928189
H	6.405236	.138937	6.145057
H	4.415445	-2.011968	2.984650
H	6.239577	-1.856356	4.663635
C	4.490588	-1.136652	-3.629309
C	5.515159	-1.047418	-4.575191
C	5.604637	.068874	-5.409510
C	3.639336	1.006341	-4.349643
C	4.664737	1.096004	-5.291854
H	4.415445	-2.011968	-2.984650
H	6.239577	-1.856356	-4.663635
H	6.405236	.138937	-6.145057
H	2.922547	1.819666	-4.242419
H	4.735081	1.977110	-5.928189
C	-3.639336	-1.006341	4.349643
C	-4.664737	-1.096004	5.291854
C	-5.604637	-.068874	5.409510
C	-4.490588	1.136652	3.629309
C	-5.515159	1.047418	4.575191
H	-2.922547	-1.819666	4.242419
H	-4.735081	-1.977110	5.928189
H	-6.405236	-.138937	6.145057
H	-4.415445	2.011968	2.984650
H	-6.239577	1.856356	4.663635
C	-4.490588	1.136652	-3.629309
C	-5.515159	1.047418	-4.575191
C	-5.604637	-.068874	-5.409510
C	-3.639336	-1.006341	-4.349643
C	-4.664737	-1.096004	-5.291854
H	-4.415445	2.011968	-2.984650
H	-6.239577	1.856356	-4.663635
H	-6.405236	-.138937	-6.145057
H	-2.922547	-1.819666	-4.242419
H	-4.735081	-1.977110	-5.928189
H	1.310729	-1.187156	.000000
H	-1.310729	1.187156	.000000
H	.000000	.000000	1.139717
H	.000000	.000000	-1.139717

$[H_4TPP](I)_2$-*stepo* (C_{2h})

Atom	x	y	z
I	-0.14475	-2.90001	0.00000
I	0.14475	2.90001	0.00000
N	-1.45672	0.31640	-1.55583
N	1.45672	-0.31640	-1.55583
N	1.45672	-0.31640	1.55583
N	-1.45672	0.31640	1.55583
C	-1.24721	0.03413	-2.88894
C	-2.79866	0.19586	-1.26338

C	2.79866	-0.19586	1.26338
C	1.24721	-0.03413	2.88894
C	1.24721	-0.03413	-2.88894
C	2.79866	-0.19586	-1.26338
C	-2.79866	0.19586	1.26338
C	-1.24721	0.03413	2.88894
C	-2.51977	-0.27892	-3.46726
C	-3.46441	-0.17145	-2.48284
C	3.46441	0.17145	2.48284
C	2.51977	0.27892	3.46726
C	2.51977	0.27892	-3.46726
C	3.46441	0.17145	-2.48284
C	-3.46441	-0.17145	2.48284
C	-2.51977	-0.27892	3.46726
C	0.00000	0.00000	-3.54509
C	-3.41789	0.23879	0.00000
C	0.00000	0.00000	3.54509
C	3.41789	-0.23879	0.00000
H	-2.66826	-0.61090	-4.48730
H	-4.52168	-0.39138	-2.56348
H	4.52168	0.39138	2.56348
H	2.66826	0.61090	4.48730
H	2.66826	0.61090	-4.48730
H	4.52168	0.39138	-2.56348
H	-4.52168	-0.39138	2.56348
H	-2.66826	-0.61090	4.48730
C	0.00000	0.00000	-5.02886
C	-4.91659	0.14616	0.00000
C	0.00000	0.00000	5.02886
C	4.91659	-0.14616	0.00000
C	-0.71334	0.97658	-5.74606
C	-0.70963	0.97806	-7.14064
C	0.00000	0.00000	-7.84253
C	0.71334	-0.97658	-5.74606
C	0.70963	-0.97806	-7.14064
H	-1.25105	1.75033	-5.19942
H	-1.25618	1.75063	-7.67990
H	0.00000	0.00000	-8.93214
H	1.25105	-1.75033	-5.19942
H	1.25618	-1.75063	-7.67990
C	5.69278	-1.31191	0.00000
C	7.08784	-1.23076	0.00000
C	7.71873	0.01520	0.00000
C	5.55470	1.10192	0.00000
C	6.94921	1.18144	0.00000
H	5.19858	-2.28346	0.00000
H	7.68043	-2.14479	0.00000
H	8.80658	0.07762	0.00000
H	4.95009	2.00909	0.00000
H	7.43293	2.15741	0.00000
C	-0.71334	0.97658	5.74606
C	-0.70963	0.97806	7.14064
C	0.00000	0.00000	7.84253
C	0.71334	-0.97658	5.74606
C	0.70963	-0.97806	7.14064
H	-1.25105	1.75033	5.19942
H	-1.25618	1.75063	7.67990
H	0.00000	0.00000	8.93214
H	1.25105	-1.75033	5.19942
H	1.25618	-1.75063	7.67990
C	-5.55470	-1.10192	0.00000
C	-6.94921	-1.18144	0.00000

C	-7.71873	-0.01520	0.00000
C	-5.69278	1.31191	0.00000
C	-7.08784	1.23076	0.00000
H	-4.95009	-2.00909	0.00000
H	-7.43293	-2.15741	0.00000
H	-8.80658	-0.07762	0.00000
H	-5.19858	2.28346	0.00000
H	-7.68043	2.14479	0.00000
H	0.81552	-0.96491	-1.02414
H	-0.81552	0.96491	1.02414
H	0.81552	-0.96491	1.02414
H	-0.81552	0.96491	-1.02414

H_4TPP^{2+}-*stepa* (C_{2h})

Atom	x	y	z
N	-1.43856	0.19552	-1.55834
N	1.43856	-0.19552	-1.55834
N	1.43856	-0.19552	1.55834
N	-1.43856	0.19552	1.55834
C	-1.24405	-0.01575	-2.92591
C	-2.80279	0.11687	-1.26303
C	2.80279	-0.11687	1.26303
C	1.24405	0.01575	2.92591
C	1.24405	0.01575	-2.92591
C	2.80279	-0.11687	-1.26303
C	-2.80279	0.11687	1.26303
C	-1.24405	-0.01575	2.92591
C	-2.52110	-0.29418	-3.48607
C	-3.46278	-0.19777	-2.48842
C	3.46278	0.19777	2.48842
C	2.52110	0.29418	3.48607
C	2.52110	0.29418	-3.48607
C	3.46278	0.19777	-2.48842
C	-3.46278	-0.19777	2.48842
C	-2.52110	-0.29418	3.48607
C	0.00000	0.00000	-3.59378
C	-3.42457	0.15872	0.00000
C	0.00000	0.00000	3.59378
C	3.42457	-0.15872	0.00000
H	-2.68788	-0.58603	-4.51602
H	-4.52645	-0.38695	-2.57410
H	4.52645	0.38695	2.57410
H	2.68788	0.58603	4.51602
H	2.68788	0.58603	-4.51602
H	4.52645	0.38695	-2.57410
H	-4.52645	-0.38695	2.57410
H	-2.68788	-0.58603	4.51602
C	0.00000	0.00000	-5.07218
C	-4.92524	0.13085	0.00000
C	0.00000	0.00000	5.07218
C	4.92524	-0.13085	0.00000
C	-0.75944	0.94735	-5.78707
C	-0.74941	0.95112	-7.17995
C	0.00000	0.00000	-7.87920
C	0.75944	-0.94735	-5.78707
C	0.74941	-0.95112	-7.17995
H	-1.32574	1.70502	-5.24635
H	-1.32067	1.70304	-7.72147
H	0.00000	0.00000	-8.96821
H	1.32574	-1.70502	-5.24635

H	1.32067	-1.70304	-7.72147
C	5.63803	-1.33772	0.00000
C	7.03503	-1.32447	0.00000
C	7.72563	-0.11090	0.00000
C	5.62076	1.08684	0.00000
C	7.01751	1.09357	0.00000
H	5.10232	-2.28705	0.00000
H	7.58128	-2.26619	0.00000
H	8.81449	-0.10313	0.00000
H	5.07043	2.02807	0.00000
H	7.55109	2.04260	0.00000
C	-0.75944	0.94735	5.78707
C	-0.74941	0.95112	7.17995
C	0.00000	0.00000	7.87920
C	0.75944	-0.94735	5.78707
C	0.74941	-0.95112	7.17995
H	-1.32574	1.70502	5.24635
H	-1.32067	1.70304	7.72147
H	0.00000	0.00000	8.96821
H	1.32574	-1.70502	5.24635
H	1.32067	-1.70304	7.72147
C	-5.62076	-1.08684	0.00000
C	-7.01751	-1.09357	0.00000
C	-7.72563	0.11090	0.00000
C	-5.63803	1.33772	0.00000
C	-7.03503	1.32447	0.00000
H	-5.07043	-2.02807	0.00000
H	-7.55109	-2.04260	0.00000
H	-8.81449	0.10313	0.00000
H	-5.10232	2.28705	0.00000
H	-7.58128	2.26619	0.00000
H	0.79362	-0.79064	-1.05025
H	-0.79362	0.79064	1.05025
H	0.79362	-0.79064	1.05025
H	-0.79362	0.79064	-1.05025

[H_4TPP]($F)_2$-*stepa* (C_{2h})

Atom	x	y	z
N	-1.45387	0.33159	-1.56342
N	1.45387	-0.33159	-1.56342
N	1.45387	-0.33159	1.56342
N	-1.45387	0.33159	1.56342
C	-1.25195	0.06269	-2.89130
C	-2.78997	0.21286	-1.27174
C	2.78997	-0.21286	1.27174
C	1.25195	-0.06269	2.89130
C	1.25195	-0.06269	-2.89130
C	2.78997	-0.21286	-1.27174
C	-2.78997	0.21286	1.27174
C	-1.25195	0.06269	2.89130
C	-2.53499	-0.21257	-3.48697
C	-3.47578	-0.11241	-2.50042
C	3.47578	0.11241	2.50042
C	2.53499	0.21257	3.48697
C	2.53499	0.21257	-3.48697
C	3.47578	0.11241	-2.50042
C	-3.47578	-0.11241	2.50042
C	-2.53499	-0.21257	3.48697
C	0.00000	0.00000	-3.54649
C	-3.40425	0.24505	0.00000

C	0.00000	0.00000	3.54649
C	3.40425	-0.24505	0.00000
H	-2.69149	-0.50855	-4.51723
H	-4.53904	-0.30194	-2.58684
H	4.53904	0.30194	2.58684
H	2.69149	0.50855	4.51723
H	2.69149	0.50855	-4.51723
H	4.53904	0.30194	-2.58684
H	-4.53904	-0.30194	2.58684
H	-2.69149	-0.50855	4.51723
C	0.00000	0.00000	-5.03141
C	-4.90485	0.15708	0.00000
C	0.00000	0.00000	5.03141
C	4.90485	-0.15708	0.00000
C	-0.70189	0.98303	-5.75180
C	-0.70012	0.98421	-7.14678
C	0.00000	0.00000	-7.84994
C	0.70189	-0.98303	-5.75180
C	0.70012	-0.98421	-7.14678
H	-1.23411	1.76090	-5.20552
H	-1.24089	1.76151	-7.68559
H	0.00000	0.00000	-8.93966
H	1.23411	-1.76090	-5.20552
H	1.24089	-1.76151	-7.68559
C	5.67904	-1.32469	0.00000
C	7.07473	-1.25166	0.00000
C	7.71259	-0.00903	0.00000
C	5.55238	1.08635	0.00000
C	6.94763	1.16029	0.00000
H	5.18058	-2.29415	0.00000
H	7.66271	-2.16887	0.00000
H	8.80083	0.04830	0.00000
H	4.95352	1.99730	0.00000
H	7.43624	2.13415	0.00000
C	-0.70189	0.98303	5.75180
C	-0.70012	0.98421	7.14678
C	0.00000	0.00000	7.84994
C	0.70189	-0.98303	5.75180
C	0.70012	-0.98421	7.14678
H	-1.23411	1.76090	5.20552
H	-1.24089	1.76151	7.68559
H	0.00000	0.00000	8.93966
H	1.23411	-1.76090	5.20552
H	1.24089	-1.76151	7.68559
C	-5.55238	-1.08635	0.00000
C	-6.94763	-1.16029	0.00000
C	-7.71259	0.00903	0.00000
C	-5.67904	1.32469	0.00000
C	-7.07473	1.25166	0.00000
H	-4.95352	-1.99730	0.00000
H	-7.43624	-2.13415	0.00000
H	-8.80083	-0.04830	0.00000
H	-5.18058	2.29415	0.00000
H	-7.66271	2.16887	0.00000
H	0.74694	-0.89595	-0.90778
H	-0.74694	0.89595	0.90778
H	0.74694	-0.89595	0.90778
H	-0.74694	0.89595	-0.90778
F	0.09349	-1.65925	0.00000
F	-0.09349	1.65925	0.00000

$[H_4TPP](Cl)_2$-*stepa* (C_{2h})

Atom	x	y	z
N	-1.45899	0.33669	-1.55786
N	1.45899	-0.33669	-1.55786
N	1.45899	-0.33669	1.55786
N	-1.45899	0.33669	1.55786
C	-1.24903	0.04791	-2.88496
C	-2.79667	0.21087	-1.26536
C	2.79667	-0.21087	1.26536
C	1.24903	-0.04791	2.88496
C	1.24903	-0.04791	-2.88496
C	2.79667	-0.21087	-1.26536
C	-2.79667	0.21087	1.26536
C	-1.24903	0.04791	2.88496
C	-2.52351	-0.26050	-3.46991
C	-3.46787	-0.15321	-2.48653
C	3.46787	0.15321	2.48653
C	2.52351	0.26050	3.46991
C	2.52351	0.26050	-3.46991
C	3.46787	0.15321	-2.48653
C	-3.46787	-0.15321	2.48653
C	-2.52351	-0.26050	3.46991
C	0.00000	0.00000	-3.53969
C	-3.41546	0.25050	0.00000
C	0.00000	0.00000	3.53969
C	3.41546	-0.25050	0.00000
H	-2.67183	-0.58701	-4.49207
H	-4.52646	-0.36841	-2.56839
H	4.52646	0.36841	2.56839
H	2.67183	0.58701	4.49207
H	2.67183	0.58701	-4.49207
H	4.52646	0.36841	-2.56839
H	-4.52646	-0.36841	2.56839
H	-2.67183	-0.58701	4.49207
C	0.00000	0.00000	-5.02422
C	-4.91496	0.15730	0.00000
C	0.00000	0.00000	5.02422
C	4.91496	-0.15730	0.00000
C	-0.69600	0.98858	-5.74224
C	-0.69219	0.99048	-7.13718
C	0.00000	0.00000	-7.83944
C	0.69600	-0.98858	-5.74224
C	0.69219	-0.99048	-7.13718
H	-1.22151	1.77060	-5.19517
H	-1.22512	1.77272	-7.67646
H	0.00000	0.00000	-8.92911
H	1.22151	-1.77060	-5.19517
H	1.22512	-1.77272	-7.67646
C	5.69060	-1.32377	0.00000
C	7.08604	-1.24603	0.00000
C	7.71996	-0.00141	0.00000
C	5.55719	1.08903	0.00000
C	6.95222	1.16622	0.00000
H	5.19447	-2.29438	0.00000
H	7.67664	-2.16149	0.00000
H	8.80800	0.05876	0.00000
H	4.95495	1.99779	0.00000
H	7.43828	2.14133	0.00000
C	-0.69600	0.98858	5.74224
C	-0.69219	0.99048	7.13718

C	0.00000	0.00000	7.83944
C	0.69600	-0.98858	5.74224
C	0.69219	-0.99048	7.13718
H	-1.22151	1.77060	5.19517
H	-1.22512	1.77272	7.67646
H	0.00000	0.00000	8.92911
H	1.22151	-1.77060	5.19517
H	1.22512	-1.77272	7.67646
C	-5.55719	-1.08903	0.00000
C	-6.95222	-1.16622	0.00000
C	-7.71996	0.00141	0.00000
C	-5.69060	1.32377	0.00000
C	-7.08604	1.24603	0.00000
H	-4.95495	-1.99779	0.00000
H	-7.43828	-2.14133	0.00000
H	-8.80800	-0.05876	0.00000
H	-5.19447	2.29438	0.00000
H	-7.67664	2.16149	0.00000
H	0.79548	-0.96334	-0.99467
H	-0.79548	0.96334	0.99467
H	0.79548	-0.96334	0.99467
H	-0.79548	0.96334	-0.99467
Cl	-0.08484	-2.37727	0.00000
Cl	0.08484	2.37727	0.00000

[H_4TPP]($Br)_2$-*stepa* (C_{2h})

Atom	x	y	z
Br	-0.12751	-2.58825	0.00000
Br	0.12751	2.58825	0.00000
N	-1.45837	0.32708	-1.55862
N	1.45837	-0.32708	-1.55862
N	1.45837	-0.32708	1.55862
N	-1.45837	0.32708	1.55862
C	-1.24832	0.04129	-2.88763
C	-2.79689	0.20193	-1.26470
C	2.79689	-0.20193	1.26470
C	1.24832	-0.04129	2.88763
C	1.24832	-0.04129	-2.88763
C	2.79689	-0.20193	-1.26470
C	-2.79689	0.20193	1.26470
C	-1.24832	0.04129	2.88763
C	-2.52195	-0.27020	-3.46925
C	-3.46588	-0.16400	-2.48508
C	3.46588	0.16400	2.48508
C	2.52195	0.27020	3.46925
C	2.52195	0.27020	-3.46925
C	3.46588	0.16400	-2.48508
C	-3.46588	-0.16400	2.48508
C	-2.52195	-0.27020	3.46925
C	0.00000	0.00000	-3.54255
C	-3.41517	0.24217	0.00000
C	0.00000	0.00000	3.54255
C	3.41517	-0.24217	0.00000
H	-2.67072	-0.59894	-4.49036
H	-4.52356	-0.38253	-2.56623
H	4.52356	0.38253	2.56623
H	2.67072	0.59894	4.49036
H	2.67072	0.59894	-4.49036
H	4.52356	0.38253	-2.56623
H	-4.52356	-0.38253	2.56623
H	-2.67072	-0.59894	4.49036

C	0.00000	0.00000	-5.02649
C	-4.91412	0.14718	0.00000
C	0.00000	0.00000	5.02649
C	4.91412	-0.14718	0.00000
C	-0.70371	0.98316	-5.74393
C	-0.69971	0.98506	-7.13856
C	0.00000	0.00000	-7.84054
C	0.70371	-0.98316	-5.74393
C	0.69971	-0.98506	-7.13856
H	-1.23465	1.76126	-5.19689
H	-1.23843	1.76317	-7.67779
H	0.00000	0.00000	-8.93007
H	1.23465	-1.76126	-5.19689
H	1.23843	-1.76317	-7.67779
C	5.69145	-1.31222	0.00000
C	7.08650	-1.23125	0.00000
C	7.71739	0.01471	0.00000
C	5.55282	1.10063	0.00000
C	6.94741	1.18062	0.00000
H	5.19722	-2.28369	0.00000
H	7.67919	-2.14524	0.00000
H	8.80524	0.07738	0.00000
H	4.94839	2.00786	0.00000
H	7.43120	2.15664	0.00000
C	-0.70371	0.98316	5.74393
C	-0.69971	0.98506	7.13856
C	0.00000	0.00000	7.84054
C	0.70371	-0.98316	5.74393
C	0.69971	-0.98506	7.13856
H	-1.23465	1.76126	5.19689
H	-1.23843	1.76317	7.67779
H	0.00000	0.00000	8.93007
H	1.23465	-1.76126	5.19689
H	1.23843	-1.76317	7.67779
C	-5.55282	-1.10063	0.00000
C	-6.94741	-1.18062	0.00000
C	-7.71739	-0.01471	0.00000
C	-5.69145	1.31222	0.00000
C	-7.08650	1.23125	0.00000
H	-4.94839	-2.00786	0.00000
H	-7.43120	-2.15664	0.00000
H	-8.80524	-0.07738	0.00000
H	-5.19722	2.28369	0.00000
H	-7.67919	2.14524	0.00000
H	0.80307	-0.95940	-1.00903
H	-0.80307	0.95940	1.00903
H	0.80307	-0.95940	1.00903
H	-0.80307	0.95940	-1.00903

[H_4TPP](I)$_2$-*stepa* (C_{2h})

Atom	x	y	z
I	-0.14475	-2.90001	0.00000
I	0.14475	2.90001	0.00000
N	-1.45672	0.31640	-1.55583
N	1.45672	-0.31640	-1.55583
N	1.45672	-0.31640	1.55583
N	-1.45672	0.31640	1.55583
C	-1.24721	0.03413	-2.88894
C	-2.79866	0.19586	-1.26338
C	2.79866	-0.19586	1.26338

C	1.24721	-0.03413	2.88894
C	1.24721	-0.03413	-2.88894
C	2.79866	-0.19586	-1.26338
C	-2.79866	0.19586	1.26338
C	-1.24721	0.03413	2.88894
C	-2.51977	-0.27892	-3.46726
C	-3.46441	-0.17145	-2.48284
C	3.46441	0.17145	2.48284
C	2.51977	0.27892	3.46726
C	2.51977	0.27892	-3.46726
C	3.46441	0.17145	-2.48284
C	-3.46441	-0.17145	2.48284
C	-2.51977	-0.27892	3.46726
C	0.00000	0.00000	-3.54509
C	-3.41789	0.23879	0.00000
C	0.00000	0.00000	3.54509
C	3.41789	-0.23879	0.00000
H	-2.66826	-0.61090	-4.48730
H	-4.52168	-0.39138	-2.56348
H	4.52168	0.39138	2.56348
H	2.66826	0.61090	4.48730
H	2.66826	0.61090	-4.48730
H	4.52168	0.39138	-2.56348
H	-4.52168	-0.39138	2.56348
H	-2.66826	-0.61090	4.48730
C	0.00000	0.00000	-5.02886
C	-4.91659	0.14616	0.00000
C	0.00000	0.00000	5.02886
C	4.91659	-0.14616	0.00000
C	-0.71334	0.97658	-5.74606
C	-0.70963	0.97806	-7.14064
C	0.00000	0.00000	-7.84253
C	0.71334	-0.97658	-5.74606
C	0.70963	-0.97806	-7.14064
H	-1.25105	1.75033	-5.19942
H	-1.25618	1.75063	-7.67990
H	0.00000	0.00000	-8.93214
H	1.25105	-1.75033	-5.19942
H	1.25618	-1.75063	-7.67990
C	5.69278	-1.31191	0.00000
C	7.08784	-1.23076	0.00000
C	7.71873	0.01520	0.00000
C	5.55470	1.10192	0.00000
C	6.94921	1.18144	0.00000
H	5.19858	-2.28346	0.00000
H	7.68043	-2.14479	0.00000
H	8.80658	0.07762	0.00000
H	4.95009	2.00909	0.00000
H	7.43293	2.15741	0.00000
C	-0.71334	0.97658	5.74606
C	-0.70963	0.97806	7.14064
C	0.00000	0.00000	7.84253
C	0.71334	-0.97658	5.74606
C	0.70963	-0.97806	7.14064
H	-1.25105	1.75033	5.19942
H	-1.25618	1.75063	7.67990
H	0.00000	0.00000	8.93214
H	1.25105	-1.75033	5.19942
H	1.25618	-1.75063	7.67990
C	-5.55470	-1.10192	0.00000
C	-6.94921	-1.18144	0.00000
C	-7.71873	-0.01520	0.00000

C	-5.69278	1.31191	0.00000
C	-7.08784	1.23076	0.00000
H	-4.95009	-2.00909	0.00000
H	-7.43293	-2.15741	0.00000
H	-8.80658	-0.07762	0.00000
H	-5.19858	2.28346	0.00000
H	-7.68043	2.14479	0.00000
H	0.81552	-0.96491	-1.02414
H	-0.81552	0.96491	1.02414
H	0.81552	-0.96491	1.02414
H	-0.81552	0.96491	-1.02414

H_2TPP-*planar* (D_{2h})

Atom	x	y	z
N	.000000	-2.104834	.000000
N	2.024542	.000000	.000000
N	.000000	2.104834	.000000
N	-2.024542	.000000	.000000
C	1.130049	-2.889788	.000000
C	-1.130049	-2.889788	.000000
C	1.130049	2.889788	.000000
C	-1.130049	2.889788	.000000
C	2.857874	-1.087936	.000000
C	2.857874	1.087936	.000000
C	-2.857874	-1.087936	.000000
C	-2.857874	1.087936	.000000
C	.685752	-4.252823	.000000
C	-.685752	-4.252823	.000000
C	.685752	4.252823	.000000
C	-.685752	4.252823	.000000
C	4.257195	-.678452	.000000
C	4.257195	.678452	.000000
C	-4.257195	-.678452	.000000
C	-4.257195	.678452	.000000
C	2.456295	-2.437685	.000000
C	-2.456295	-2.437685	.000000
C	-2.456295	2.437685	.000000
C	2.456295	2.437685	.000000
H	1.345424	-5.112299	.000000
H	-1.345424	-5.112299	.000000
H	1.345424	5.112299	.000000
H	-1.345424	5.112299	.000000
H	5.112430	-1.345366	.000000
H	5.112430	1.345366	.000000
H	-5.112430	-1.345366	.000000
H	-5.112430	1.345366	.000000
C	3.518599	-3.496407	.000000
C	-3.518599	-3.496407	.000000
C	-3.518599	3.496407	.000000
C	3.518599	3.496407	.000000
C	4.020290	-4.003808	-1.206449
C	5.002833	-4.997326	-1.207451
C	5.496501	-5.497385	.000000
C	4.020290	-4.003808	1.206449
C	5.002833	-4.997326	1.207451
H	3.634629	-3.613281	-2.148377
H	5.381822	-5.380596	-2.154398
H	6.262158	-6.272912	.000000
H	3.634629	-3.613281	2.148377
H	5.381822	-5.380596	2.154398
C	4.020290	4.003808	1.206449

C	5.002833	4.997326	1.207451
C	5.496501	5.497385	.000000
C	4.020290	4.003808	-1.206449
C	5.002833	4.997326	-1.207451
H	3.634629	3.613281	2.148377
H	5.381822	5.380596	2.154398
H	6.262158	6.272912	.000000
H	3.634629	3.613281	-2.148377
H	5.381822	5.380596	-2.154398
C	-4.020290	4.003808	-1.206449
C	-5.002833	4.997326	-1.207451
C	-5.496501	5.497385	.000000
C	-4.020290	4.003808	1.206449
C	-5.002833	4.997326	1.207451
H	-3.634629	3.613281	-2.148377
H	-5.381822	5.380596	-2.154398
H	-6.262158	6.272912	.000000
H	-3.634629	3.613281	2.148377
H	-5.381822	5.380596	2.154398
C	-4.020290	-4.003808	1.206449
C	-5.002833	-4.997326	1.207451
C	-5.496501	-5.497385	.000000
C	-4.020290	-4.003808	-1.206449
C	-5.002833	-4.997326	-1.207451
H	-3.634629	-3.613281	2.148377
H	-5.381822	-5.380596	2.154398
H	-6.262158	-6.272912	.000000
H	-3.634629	-3.613281	-2.148377
H	-5.381822	-5.380596	-2.154398
H	.000000	1.085216	.000000
H	.000000	-1.085216	.000000

H_2TPP-near-planar triclinic structure (C_2)

Atom	x	y	z
N	-2.10745	0.03476	0.08983
N	0.00000	1.97537	-0.52910
N	2.10745	-0.01486	-0.09471
N	0.00000	-1.95357	0.52370
C	-2.88904	1.10980	-0.27055
C	-2.88934	-1.07709	0.31059
C	2.88904	1.09628	-0.32014
C	2.88934	-1.08820	0.27003
C	-1.08919	2.78131	-0.73599
C	1.08919	2.77670	-0.75287
C	-1.08903	-2.75667	0.74184
C	1.08903	-2.75822	0.73634
C	-4.24509	0.64760	-0.27324
C	-4.24516	-0.67711	0.07854
C	4.24509	0.69725	-0.08669
C	4.24516	-0.62584	0.27104
C	-0.67796	4.13275	-1.09294
C	0.67796	4.12558	-1.11952
C	-0.67790	-4.10495	1.11012
C	0.67790	-4.10998	1.09157
C	-2.44128	2.39360	-0.62399
C	-2.44118	-2.36645	0.64181
C	2.44118	-2.37036	0.62790
C	2.44128	2.38484	-0.65597
H	-5.10043	1.25296	-0.54521

H	-5.10063	-1.33756	0.14262
H	5.10043	1.35742	-0.15382
H	5.10063	-1.22992	0.54579
H	-1.33820	4.96875	-1.29036
H	1.33820	4.94824	-1.36653
H	-1.33812	-4.92876	1.35336
H	1.33812	-4.94505	1.29285
C	-3.50064	3.40527	-0.91887
C	-3.49742	-3.39308	0.89179
C	3.49742	-3.38451	0.92477
C	3.50064	3.40833	-0.90645
C	-4.40237	3.80751	0.07931
C	-5.40097	4.74468	-0.19243
C	-5.51594	5.29791	-1.47008
C	-3.62727	3.96814	-2.19899
C	-4.62466	4.90611	-2.47221
H	-4.30933	3.38390	1.07901
H	-6.08743	5.04573	0.59831
H	-6.29520	6.02924	-1.68350
H	-2.94028	3.65669	-2.98509
H	-4.70844	5.32715	-3.47360
C	4.40237	3.25752	-1.97201
C	5.40097	4.20491	-2.20525
C	5.51594	5.32281	-1.37538
C	3.62727	4.53583	-0.07927
C	4.62466	5.48466	-0.31163
H	4.30933	2.39082	-2.62595
H	6.08743	4.07021	-3.04057
H	6.29520	6.06284	-1.55621
H	2.94028	4.65920	0.75722
H	4.70844	6.34998	0.34506
C	4.39601	-3.79184	-0.07408
C	5.38428	-4.74062	0.19475
C	5.49220	-5.30019	1.47023
C	3.61864	-3.95163	2.20361
C	4.60568	-4.90141	2.47386
H	4.30673	-3.36484	-1.07271
H	6.06703	-5.04681	-0.59724
H	6.26210	-6.04213	1.68080
H	2.93431	-3.63623	2.99052
H	4.68425	-5.32739	3.47359
C	-4.39601	-3.24634	1.96046
C	-5.38428	-4.20235	2.20204
C	-5.49220	-5.32469	1.37724
C	-3.61864	-4.52362	0.06784
C	-4.60568	-5.48119	0.30867
H	-4.30673	-2.37723	2.61177
H	-6.06703	-4.07147	3.04100
H	-6.26210	-6.07243	1.56584
H	-2.93431	-4.64398	-0.77135
H	-4.68425	-6.34998	-0.34410
H	1.08887	-0.02872	-0.14247
H	-1.08887	0.04657	0.13814

H_2TPP-ruffled conformation (C_2)

Atom	x	y	z
N	0.00000	0.00000	-0.00414
N	0.00000	0.00000	-4.19620
N	-0.00456	2.00089	-2.09734
N	0.00456	-2.00089	-2.09734

C	-0.17599	-1.11632	0.78015
C	0.17599	1.11632	0.78015
C	0.18151	-1.11632	-4.97943
C	-0.18151	1.11632	-4.97943
C	-0.12290	-0.67491	2.14277
C	0.12290	0.67491	2.14277
C	0.12769	-0.67418	-6.34184
C	-0.12769	0.67418	-6.34184
C	0.31977	2.43319	0.31957
C	-0.31977	-2.43319	0.31957
C	-0.32683	2.43264	-4.51584
C	0.32683	-2.43264	-4.51584
C	0.18413	2.83367	-1.02485
C	-0.18413	-2.83367	-1.02485
C	-0.18415	2.83284	-3.17081
C	0.18415	-2.83284	-3.17081
C	0.13752	4.23177	-1.43265
C	-0.13752	-4.23177	-1.43265
C	-0.11630	4.23188	-2.76620
C	0.11630	-4.23188	-2.76620
H	-0.24208	-1.32173	3.00325
H	0.24208	1.32173	3.00325
H	0.25269	-1.31912	-7.20278
H	-0.25269	1.31912	-7.20278
H	0.26332	5.08740	-0.77838
H	-0.26332	-5.08740	-0.77838
H	-0.22484	5.08795	-3.42283
H	0.22484	-5.08795	-3.42283
C	-0.63717	3.48333	-5.53582
C	0.63717	-3.48333	-5.53582
C	0.61943	3.47758	1.35089
C	-0.61943	-3.47758	1.35089
C	1.92496	-4.03916	-5.58243
C	-1.92496	4.03916	-5.58243
C	2.24897	-5.01432	-6.52770
C	-2.24897	5.01432	-6.52770
C	1.28694	-5.45299	-7.44080
C	-1.28694	5.45299	-7.44080
C	-0.32106	-3.93067	-6.45668
C	0.32106	3.93067	-6.45668
C	0.00058	-4.90944	-7.40136
C	-0.00058	4.90944	-7.40136
H	2.67556	-3.69508	-4.87097
H	-2.67556	3.69508	-4.87097
H	3.25633	-5.42907	-6.55085
H	-3.25633	5.42907	-6.55085
H	1.53786	-6.21553	-8.17780
H	-1.53786	6.21553	-8.17780
H	-1.32780	-3.51442	-6.42189
H	1.32780	3.51442	-6.42189
H	-0.75819	-5.25225	-8.10420
H	0.75819	5.25225	-8.10420
C	-1.92353	-3.98229	1.46492
C	1.92353	3.98229	1.46492
C	-2.23756	-4.93758	2.43398
C	2.23756	4.93758	2.43398
C	-1.24940	-5.40587	3.30338
C	1.24940	5.40587	3.30338
C	0.36586	-3.95603	2.22644
C	-0.36586	3.95603	2.22644
C	0.05374	-4.91413	3.19544
C	-0.05374	4.91413	3.19544

H	-2.69525	-3.61286	0.78953
H	2.69525	3.61286	0.78953
H	-3.25796	-5.31202	2.51135
H	3.25796	5.31202	2.51135
H	-1.49352	-6.15027	4.06093
H	1.49352	6.15027	4.06093
H	1.38383	-3.57606	2.14060
H	-1.38383	3.57606	2.14060
H	0.83165	-5.27901	3.86544
H	-0.83165	5.27901	3.86544
H	0.00000	0.00000	-3.17649
H	0.00000	0.00000	-1.02526

Table S1. ^{1}HNMR resonances of H_2TPP and $[H_4TPP](X)_2$ diacid derivatives in $CDCl_3$ at 298K.

	δ (p.p.m)			
	NH	H_β pyrrole	H_0	$H_m + H_p$
$[H_4TPP](F)_2$	1.70	8.56	8.58	7.98
$[H_4TPP](Cl)_2$	0.27	8.56	8.60	7.98
$[H_4TPP](Br)_2$	-0.25	8.55	8.62	7.98
$[H_4TPP](I)_2$	-0.60	8.58	8.62	7.80
H_2TPP	-2.78	8.83	8.20	7.74

Table S2. Relative Energy (kcal/mol) of Energy Minimized Stable Conformers for H_4TPP^{2+} and $[H_4TPP](X)_2$ Diacid Derivatives

conformer	H_4TPP^{2+}	$[H_4TPP](F)_2$	$[H_4TPP](Cl)_2$	$[H_4TPP](Br)_2$	$[H_4TPP](I)_2$
sad	0.0	0.3	0.0	0.7	0.7
sadruf	0.5	0.0	0.3	0.0	0.0
stepa	14.5	5.5	9.3	9.4	9.7
stepo	14.4	9.3	17.1	17.7	15.1
planar	31.6	40.3	40.3	39.7	38.2

Table S3. Hydrogen Bond Energy Terms for *sad* and *sadruf* $[H_4TPP](X)_2$ (X = F, Cl, Br, I) Conformers

Bond energy decomposition		X = F	X = Cl	X = Br	X = I
	sad	195.6	106.7	95.6	83.3
ΔE_{Pauli}	*sadruf*	197.8	106.3	95.4	83.3
	sad	–348.0	–262.9	–250.2	–235.2
ΔV_{elstat}	*sadruf*	–349.4	–262.9	–250.0	–235.4
	sad	**–152.4**	**–156.2**	**–154.6**	**–151.9**
$\Delta E_{Pauli} + \Delta V_{elstat}$	*sadruf*	**–151.6**	**–156.7**	**–154.6**	**–152.1**
	sad	–216.5	–116.4	–104.3	–92.3
ΔE_{oi}	*sadruf*	–217.7	–116.0	–122.5	–92.3
	sad	**–368.9**	**–272.6**	**–258.9**	**–244.2**
ΔE_{int} ($\Delta E_{Pauli} + \Delta V_{elstat} + \Delta E_{oi}$)	*sadruf*	**–369.3**	**–272.6**	**–277.1**	**–244.4**
	Halide Charge (electrons)				
	sad	**–0.727**	**–0.797**	**–0.823**	**–0.826**
Hirshfeld[81]	*sadruf*	**–0.727**	**–0.797**	**–0.823**	**–0.826**

Table S4. Calculated Excitation Energies and Oscillator strengths (*f*) for the Optically Allowed ^{1}B Excited States of H_2TPP in the C_2 Near-planar Triclinic Conformation[a]

state	composition	E (eV)	*f*	assignment
1^1B	69 (79b→83a) 30 (82a→80b)	2.00	0.031	Q_x
1^1A	67 (79b→80b) 31 (82a→83a)	2.12	0.061	Q_y
3^1B	55 (77b→83a) 32 (82a→70b) 10 (79b→83a)	2.83	0.270	B tail
3^1A	77 (77b→80b) 13 (82a→83a) 7 (79b→80b)	2.87	0.123	
4^1A	46 (82a→83a) 21 (77b→80b) 17 (79b→80b)	3.04	0.8995	B
4^1B	40 (77b→83a) 28 (82a→80b) 15 (79b→83a)	3.08	0.8679	

[a] The major one-electron transitions contributing to the BP/ALDA solution vectors are also given; the excited states with negligible intensity are omitted.

Table S5. Calculated Excitation Energies and Oscillator strengths (*f*) for the Optically Allowed ^1E and $^1B_2$ Excited States of $[H_4TPP](F)_2$ in the *sad* Conformation[a]

state	composition	character	E (eV)	*f*	assignment
1^1E	75 ($24b_2 \rightarrow 43e$) 23 ($20b_1 \rightarrow 43e$)	$\pi\pi^*$	1.89	0.247	Q
1^1B_2	100 ($42e \rightarrow 43e$)	HPCT	2.77	0.0001	
2^1E	67 ($20b_1 \rightarrow 43e$) 20 ($24b_2 \rightarrow 43e$) 5 ($23b_2 \rightarrow 43e$)	$\pi\pi^*$	2.81	1.845	B
3^1E	98 ($27a_1 \rightarrow 43e$)	HPCT	2.92	0.0125	
2^1B_2	73 ($41e \rightarrow 43e$) 26 ($20b_1 \rightarrow 17a_2$)	PhPCT	3.06	~0	

[a] The major one-electron transitions contributing to the BP/ALDA solution vectors as well as the character of the excited states are also given

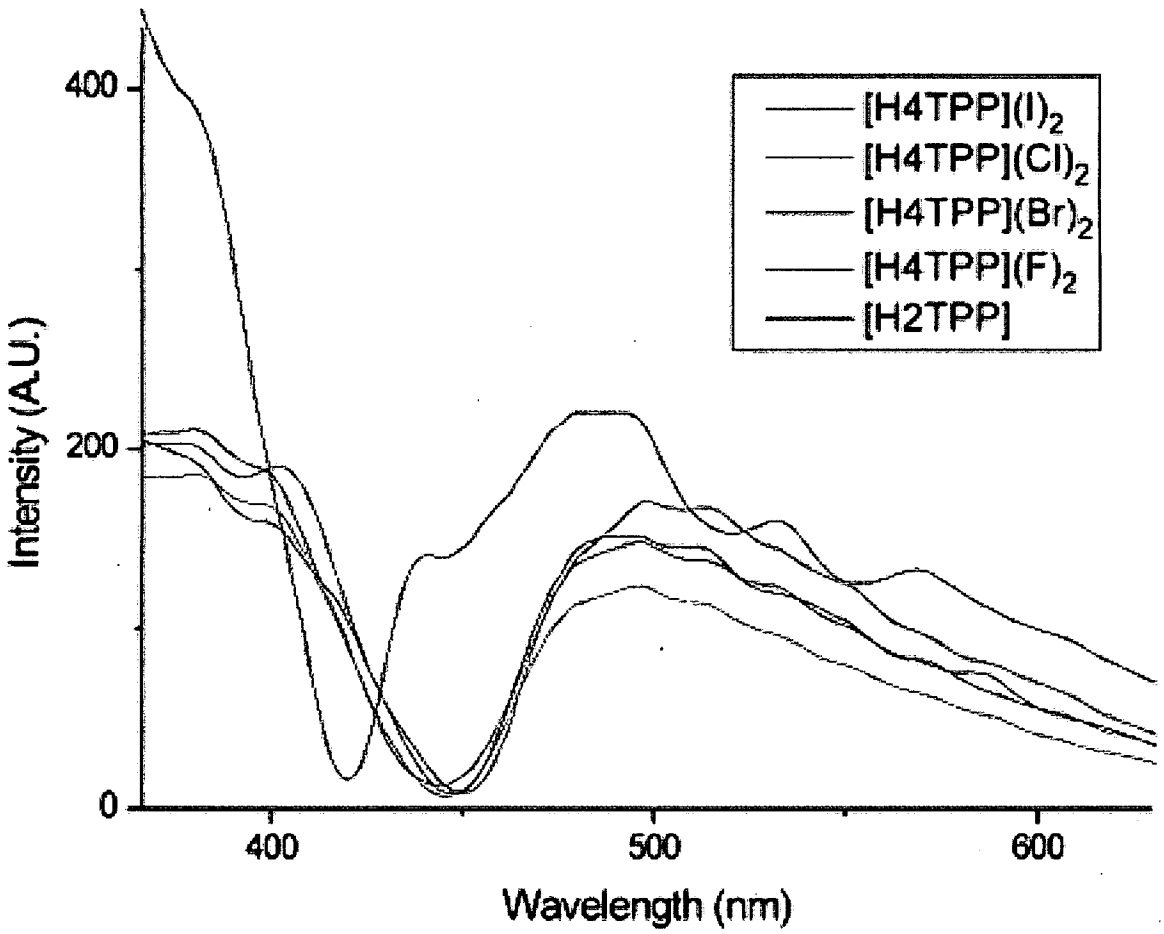

Figure S1. RLS spectra of $[H_4TPP](X)_2$ (X = F, Cl, Br, I) and of H_2TPP in CH_2Cl_2 at 298K.

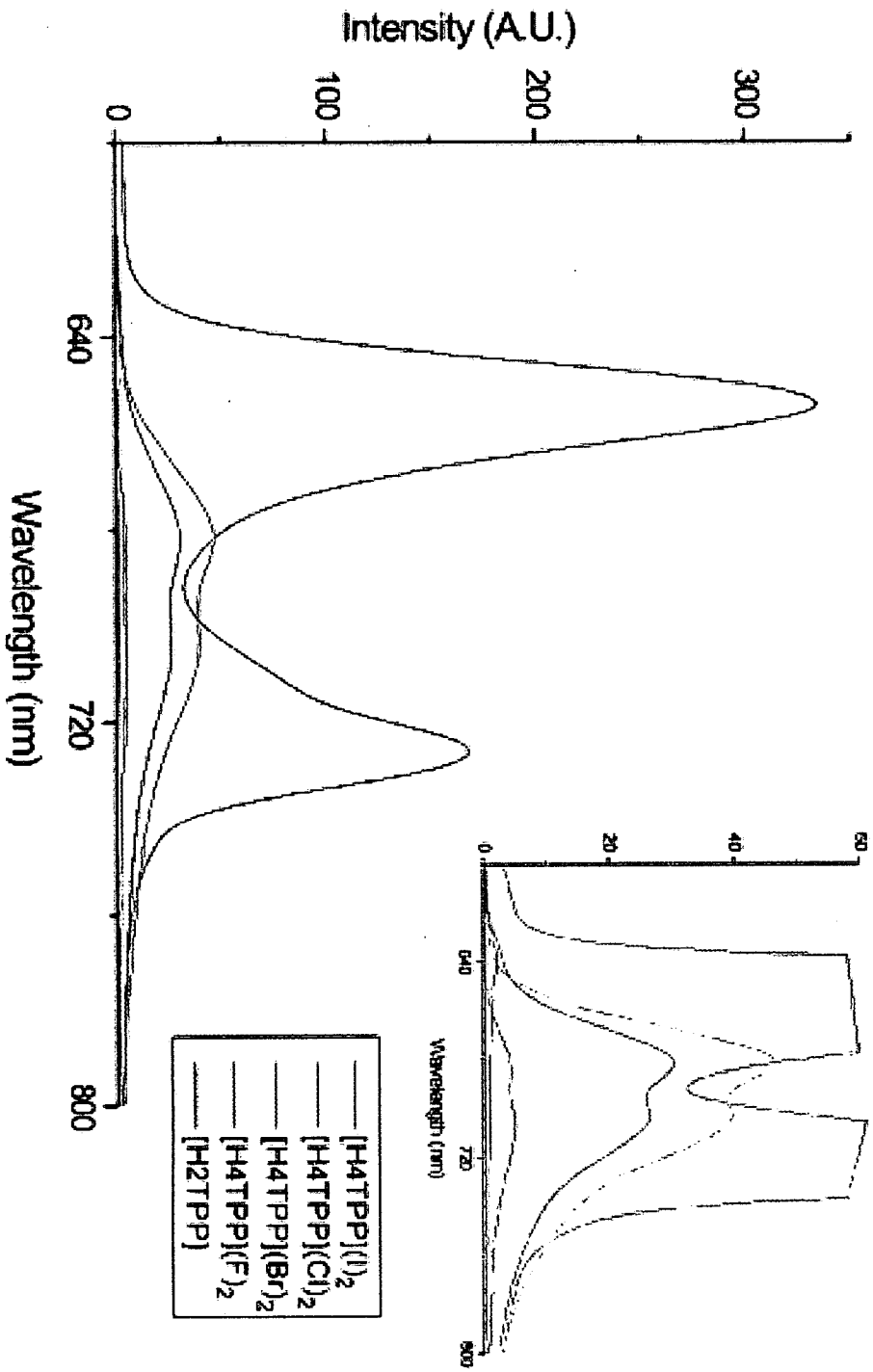

Figure S2. Fluorescence spectra of $[H_4TPP](X)_2$ (X = F, Cl, Br, I) and of H_2TPP in CH_2Cl_2 at 298K.

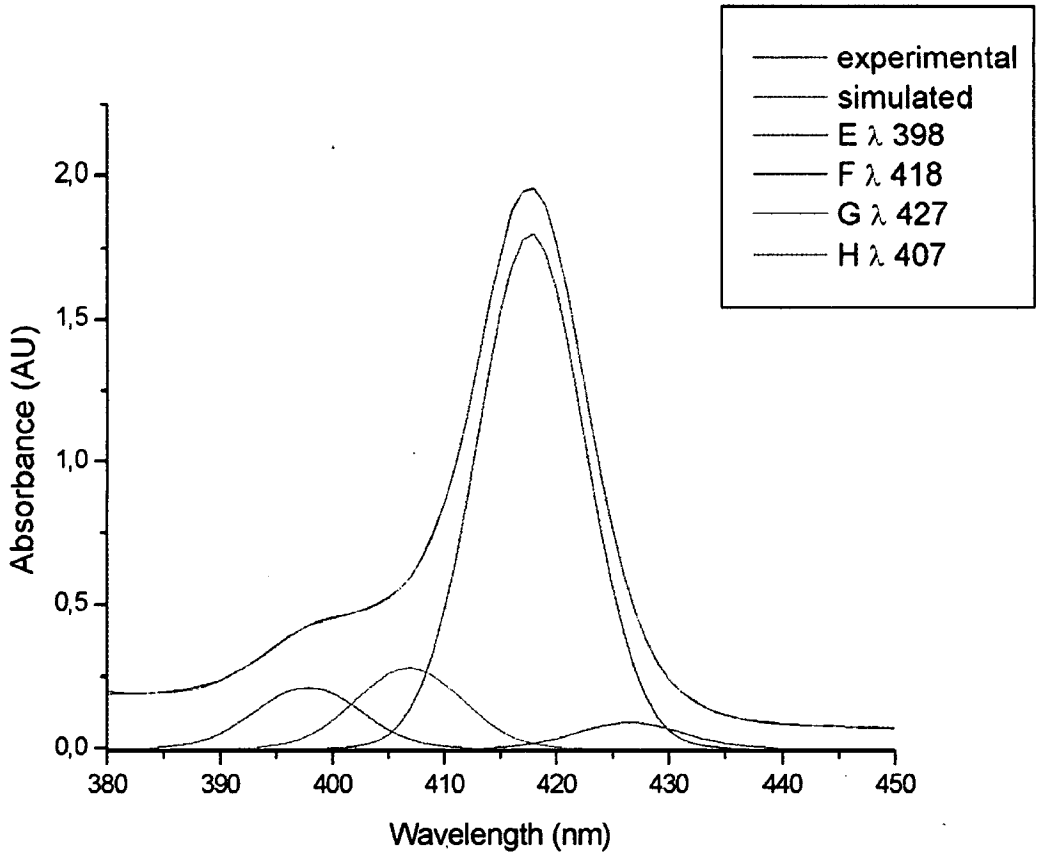

Figure S3. Deconvoluted UV/Vis absorption spectra of H_2TPP in the Soret region.

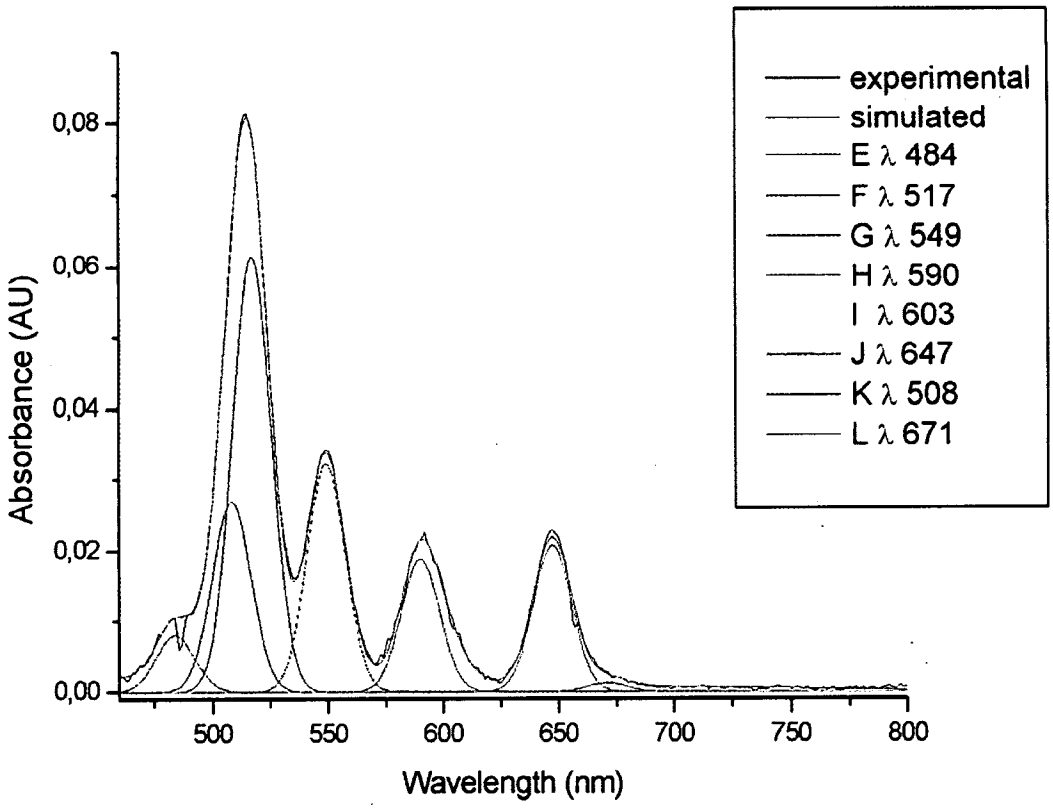

Figure S4. Deconvoluted UV/Vis absorption spectra of H_2TPP in the Q-band region.

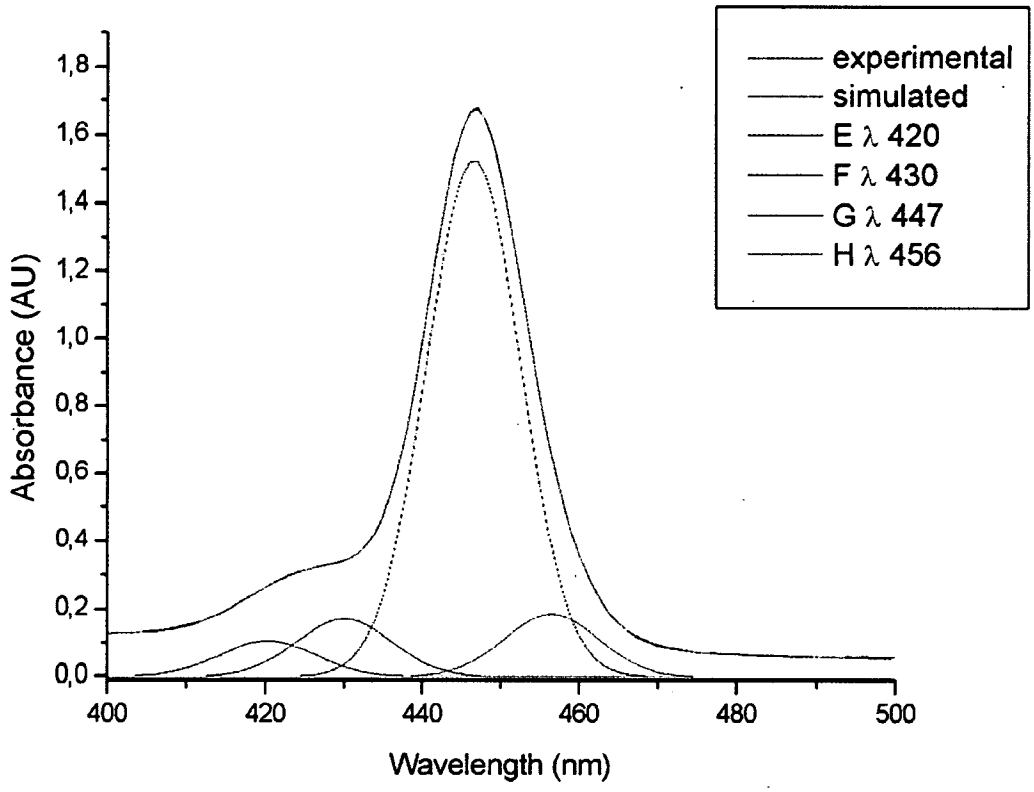

Figure S5. Deconvoluted UV/Vis absorption spectra of $[H_4TPP](F)_2$ in the Soret region

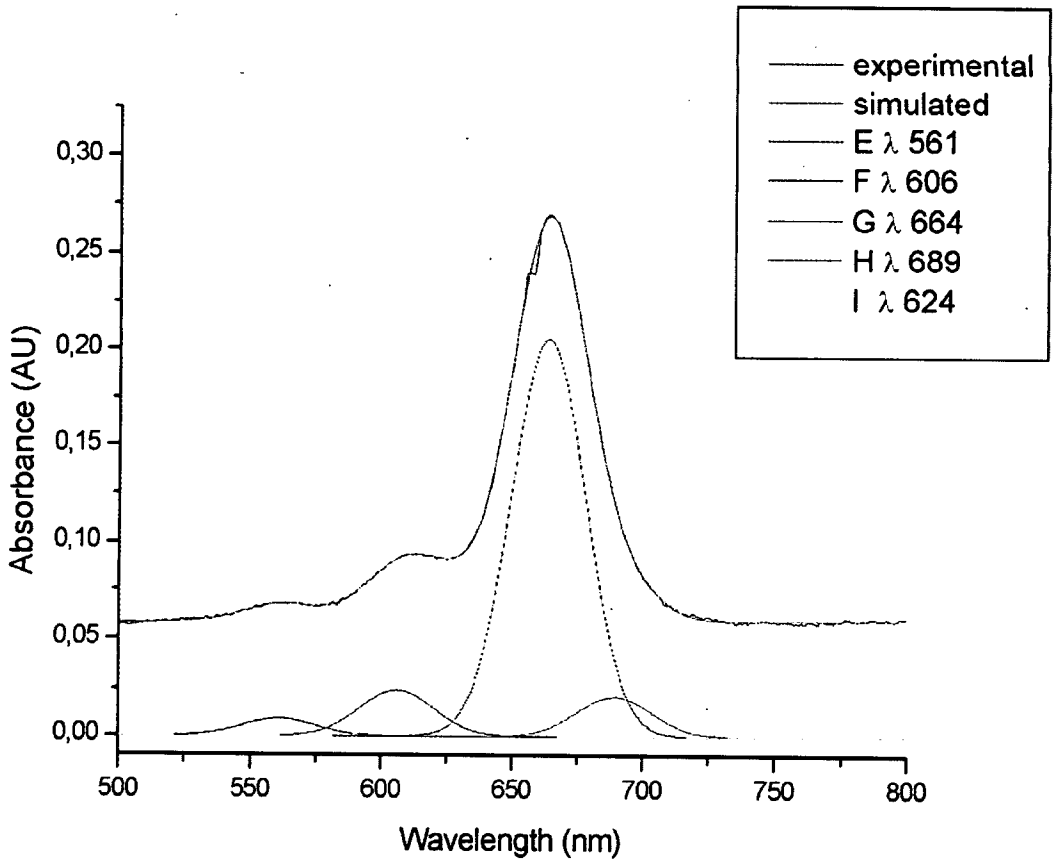

Figure S6. Deconvoluted UV/Vis absorption spectra of $[H_4TPP](F)_2$ in the Q-band region

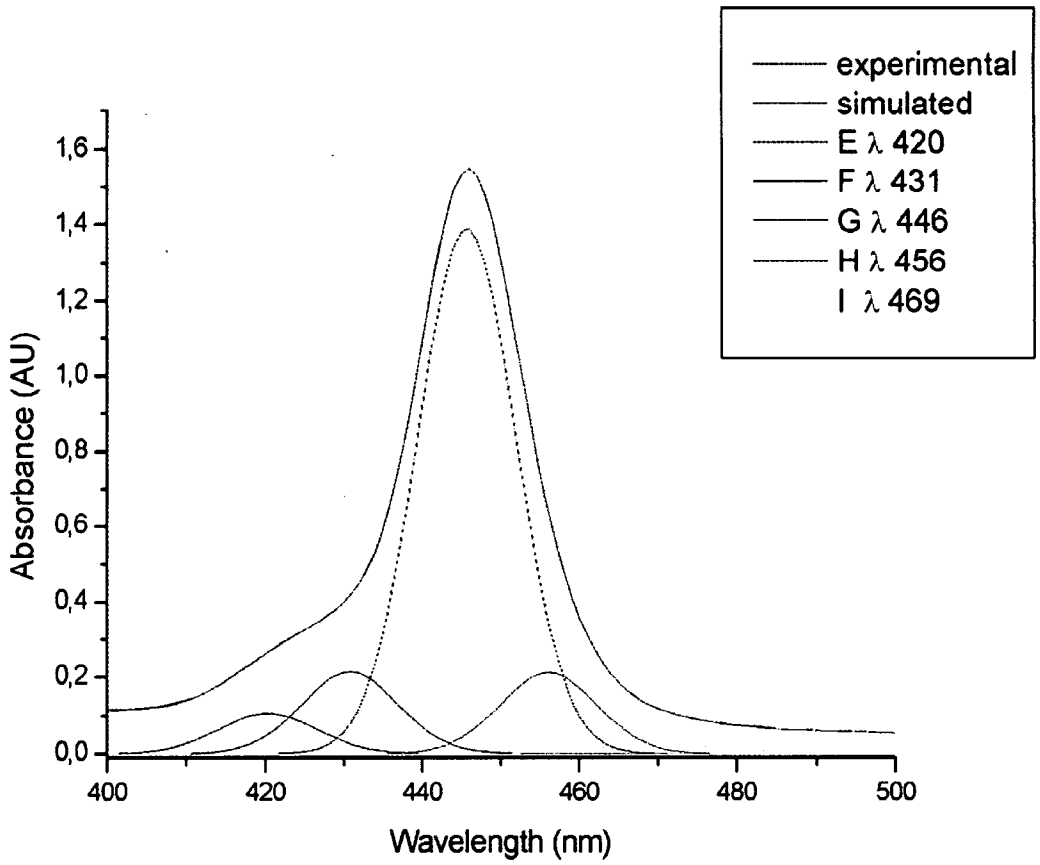

Figure S7. Deconvoluted UV/Vis absorption spectra of $[H_4TPP](Cl)_2$ in the Soret region.

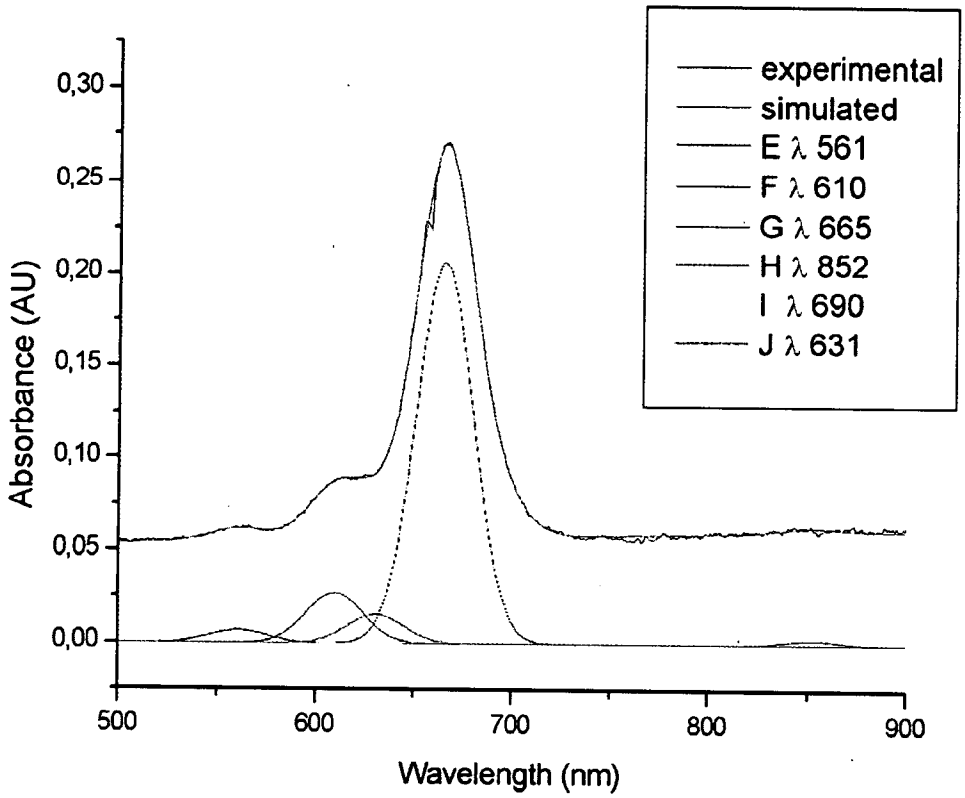

Figure S8. Deconvoluted UV/Vis absorption spectra of $[H_4TPP](Cl)_2$ in the Q-band region.