Electronic Supplementary Material (ESI) for Dalton Transactions.

Tetraphenylporphyrin Electrocatalysts for the Hydrogen Evolution Reaction: Applicability of Molecular Volcano Plots to Experimental Operating Conditions

Supporting information

Felicia Zaar[a], *C. Moyses Araujo*[b,c], *Rikard Emanuelsson*[d], *Maria Strømme*[a], *Martin Sjödin*[a*]

[a]Department of Materials Science and Engineering, Division of Nanotechnology and Functional Materials, Uppsala University, Box 35, SE-751 03 Uppsala, Sweden
*martin.sjodin@angstrom.uu.se

[b]Materials Theory Division, Department of Physics and Astronomy, Ångström Laboratory, Uppsala University, Box 516, SE-751 20 Uppsala, Sweden

[c]Department of Engineering and Physics, Karlstad University, 651 88 Karlstad, Sweden.

[d]Department of Chemistry – BMC, Uppsala University, Box 576, SE-751 23 Uppsala, Sweden.

Contents

1 Electrochemical and spectroscopic characterization

1.1 Additional Experimental results

Figure S1 shows the SWVs of the porphyrins studied under catalytic conditions in this work. Figure S2 shows CVs of CoTPP with and without the L^0/L^{1-} transition. Figure S3, Figure S4 and Table S1 show the CVs of the porphyrins studied only experimentally in this work, the SWVs of the porphyrins studied only experimentally in this work, and a summary of the electrochemical results obtained, respectively[†]. Note that what is here reported as the M(III)/M(II) transition for Al(III)TPPCl, may represent a convolution of the M(III)/M(II) and L^{1+}/L^0 transitions. These peaks have previously been reported to appear within about 0.2 V of each other[1] and in both the CV and SWV reported here, the width of the peak in the relevant potential region may cover both transitions. However, it should also be noted that the L^{1+}/L^0 transition have been reported to occur at 0.4 vs. Fc/Fc^+ in DCM[2] which is close to the value reported here (0.36 V vs. Fc/Fc^+).

[†] Dimethylformamide (DMF, AnalaR NORMAPUR® ACS, Reag. Ph. Eur. analytical reagent, ≥99.8%) used for characterization of CoTPP was purchased from VWR chemicals.

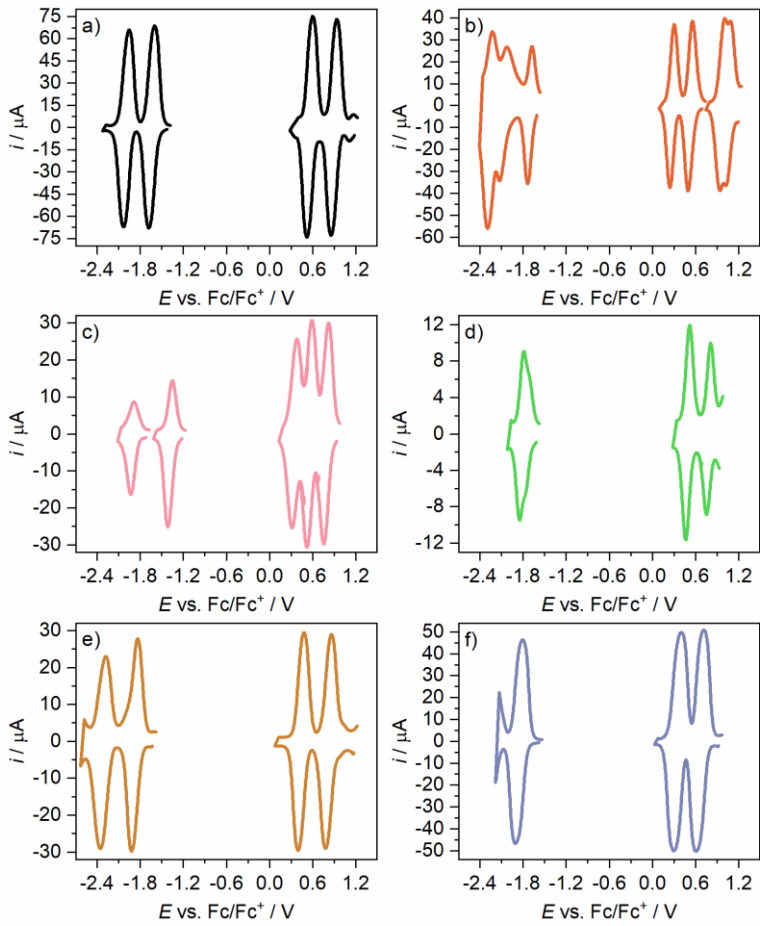


Figure S1. SWV of a) H_2TPP, b) FeTPP, c) CoTPP, d) NiTPP, e) CuTPP and f) ZnTPP.

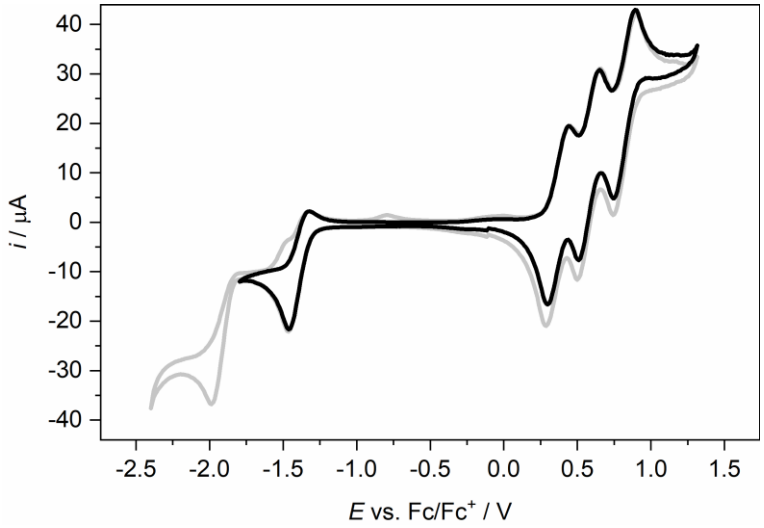


Figure S2. CV of CoTPP with and without the L^0/L^{1-} transition.

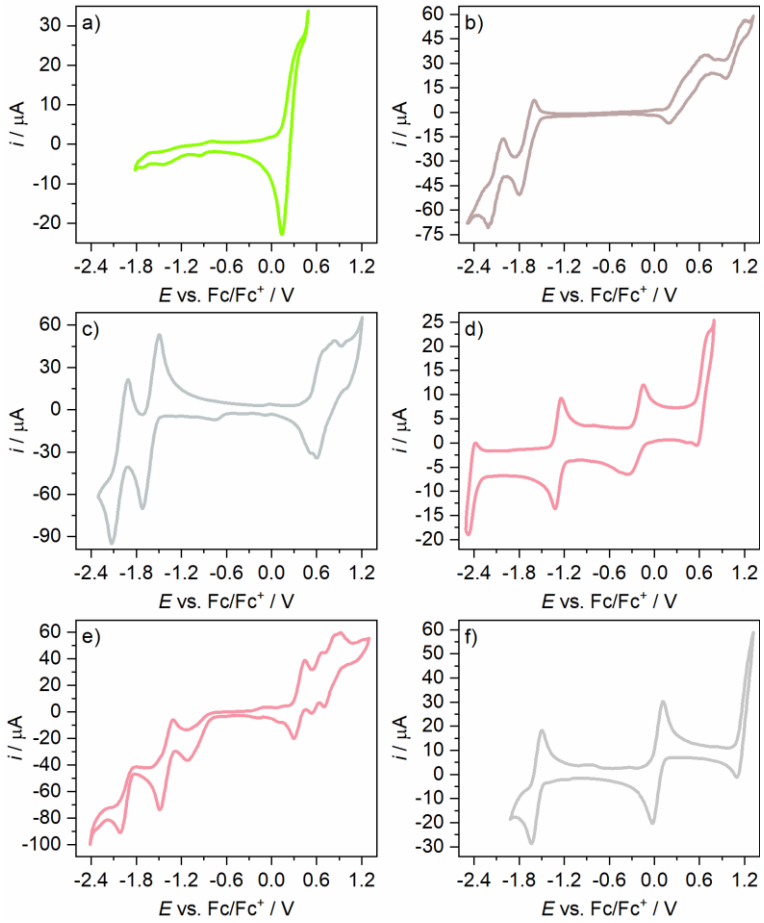


Figure S3. CV of a) MgTPP, b) Al(III)TPPCl, c) O=Ti(IV)TPP, d) CoTPP in DMF, e) Co(III)TPPCl and f) AgTPP.

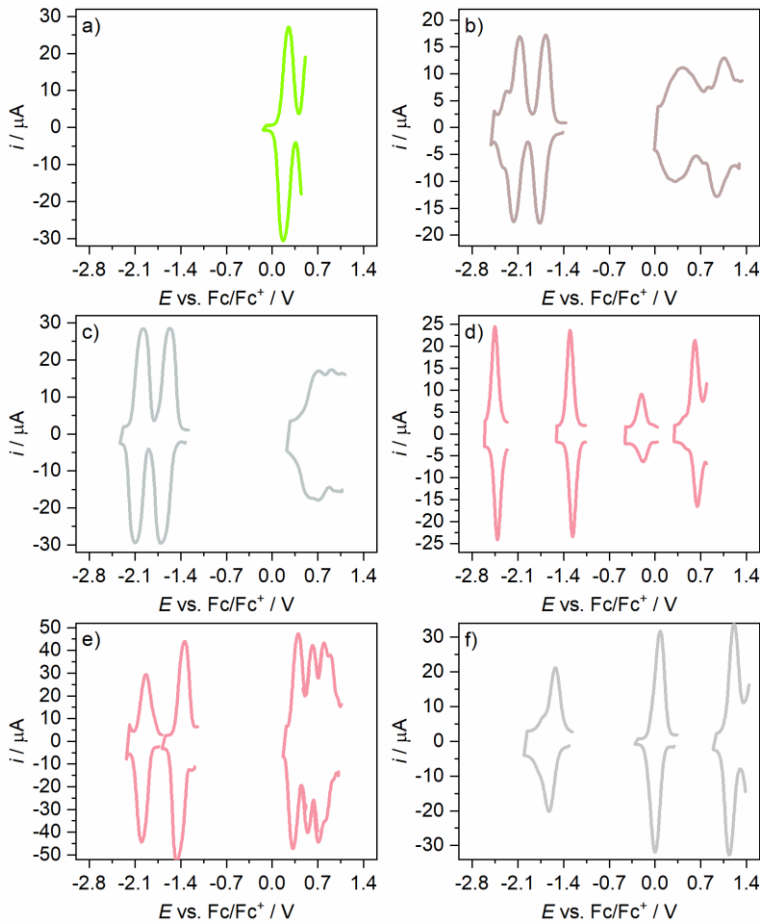


Figure S4. SWV of a) MgTPP, b) Al(III)TPPCl, c) O=Ti(IV)TPP, d) CoTPP in DMF, e) Co(III)TPPCl and f) AgTPP.

Table S1. Porphyrin redox chemistry obtained experimentally in this work (V vs. Fc/Fc^+, 0.1 M $TBAPF_6$/DCM. CV: 0.1 V/s. SWV: 15 Hz, 4 mV increment, 25 mV amplitude).

Porphyrin	Quantity	L^{1-}/L^{2-}	L^{0}/L^{1-}	M(II)/M(I)	M(III)/M(II)	L^{1+}/L^{0}	L^{2+}/L^{1+}
H_2TPP[a]	$E_{p,c}$	-2.08	-1.74			0.49	0.83
	$E_{p,a}$	-1.94	-1.59			0.62	0.99
	ΔE_p	0.14	0.15			0.13	0.14
	$E^{0'}$ *(CV)*	-2.01	-1.67			0.55	0.89
	$E^{0'}$ *(SWV)*	-1.99	-1.64			0.56	0.90
FeTPP	$E_{p,c}$			-1.75	0.24	0.5	0.95
	$E_{p,a}$			-1.62	0.37	0.63	1.20
	ΔE_p			0.13	0.13	0.13	0.25
	$E^{0'}$ *(CV)*			-1.68	0.32	0.58	1.08
	$E^{0'}$ *(SWV)*	-2.26	-2.07	-1.71	0.27	0.53	0.97
CoTPP	$E_{p,c}$		-1.98	-1.46	0.29	0.50	0.74
	$E_{p,a}$		~-1.46, -0.79	-1.32	0.45	0.66	0.90
	ΔE_p		N/A	0.14	0.16	0.16	0.16
	$E^{0'}$ *(CV)*		N/A	-1.39	0.37	0.58	0.82
	$E^{0'}$ *(SWV)*		-1.91	-1.39	0.34	0.55	0.79
NiTPP	$E_{p,c}$		-1.87			0.46	0.73

	$E_{p,a}$		-1.70			0.54	0.83
	ΔE_p		0.17			0.08	0.10
	$E^{0'}$ (CV)		-1.79			0.5	0.78
	$E^{0'}$ (SWV)		-1.82			0.49	0.78
	$E_{p,c}$		-1.95			0.37	0.75
	$E_{p,a}$		-1.80			0.51	0.89
CuTPP	ΔE_p		0.15			0.14	0.14
	$E^{0'}$ (CV)		-1.88			0.44	0.82
	$E^{0'}$ (SWV)	-2.32	-1.88			0.44	0.82
	$E_{p,c}$		-1.96			0.24	0.56
	$E_{p,a}$		-1.78			0.44	0.76
ZnTPP	ΔE_p		0.18			0.20	0.20
	$E^{0'}$ (CV)		-1.87			0.34	0.66
	$E^{0'}$ (SWV)		-1.85			0.36	0.66
	$E_{p,c}$					0.13	
	$E_{p,a}$					~0.39	
MgTPP	ΔE_p					0.26	
	$E^{0'}$ (CV)					0.26	
	$E^{0'}$ (SWV)					0.21	
	$E_{p,c}$	-2.20	-1.79		0.71		0.91
	$E_{p,a}$	-2.02	-1.59		0.19		1.21
Al(III)TPPCl[b]	ΔE_p	-0.18	0.20		0.52		0.30
	$E^{0'}$ (CV)	-2.11	-1.69		0.45		1.06
	$E^{0'}$ (SWV)	-2.12	-1.72		0.36		1.01
	$E_{p,c}$	-2.13	-1.71			~0.51	0.60
	$E_{p,a}$	-1.91	-1.49			~0.69	0.82
O=Ti(IV)TPP	ΔE_p	0.22	0.22			0.18	0.22
	$E^{0'}$ (CV)	-2.02	-1.60			0.60	0.71
	$E^{0'}$ (SWV)	-2.04	-1.64			0.71	0.74
	$E_{p,c}$		-2.47	-1.32	-0.33	0.56	
	$E_{p,a}$		-2.38	-1.25	-0.15	~0.73	
CoTPP in DMF	ΔE_p		0.11	0.07	0.18	0.17	
	$E^{0'}$ (CV)		-2.41	-1.28	-0.24	0.63	
	$E^{0'}$ (SWV)		-2.42	-1.27	-0.19	0.64	
	$E_{p,c}$		-2.01	-1.49	0.29	0.53	0.71
	$E_{p,a}$		~-1.83	-1.32	0.44	0.68	0.92
Co(III)TPPCl	ΔE_p		0.18	0.17	0.15	0.15	0.21
	$E^{0'}$ (CV)		-1.92	-1.4	0.37	0.59	0.82
	$E^{0'}$ (SWV)		-1.97	-1.4	0.36	0.58	0.75
	$E_{p,c}$		-1.64	-0.02			1.09
	$E_{p,a}$		-1.49	0.12			~1.27
AgTPP	ΔE_p		0.15	0.14			0.18
	$E^{0'}$ (CV)		-1.56	0.07			1.18
	$E^{0'}$ (SWV)		-1.64	-1.57	0.04	1.17	1.09

[a]CV data previously reported in ref. 3. [b]What is marked as the M(III)/M(II) transition for this compound may represent a convolution of the M(III)/M(II) and L^{1+}/L^{0} transitions.

1.2 Literature study of porphyrin redox chemistry

Figure S5, Figure S6 and Table S2 summarize experimentally obtained and previously reported half-wave potentials for tetraphenylporphyrins. In Figure S5, only results obtained in DCM are shown. **Fel! Hittar inte referenskälla.** S6 and **Fel! Hittar inte referenskälla.** S2 show results from multiple solvents. Figure S5 and Figure S6 show half-wave potentials vs. Fc/Fc^+, with all values originally measured against other reference potentials converted according to Table S3.

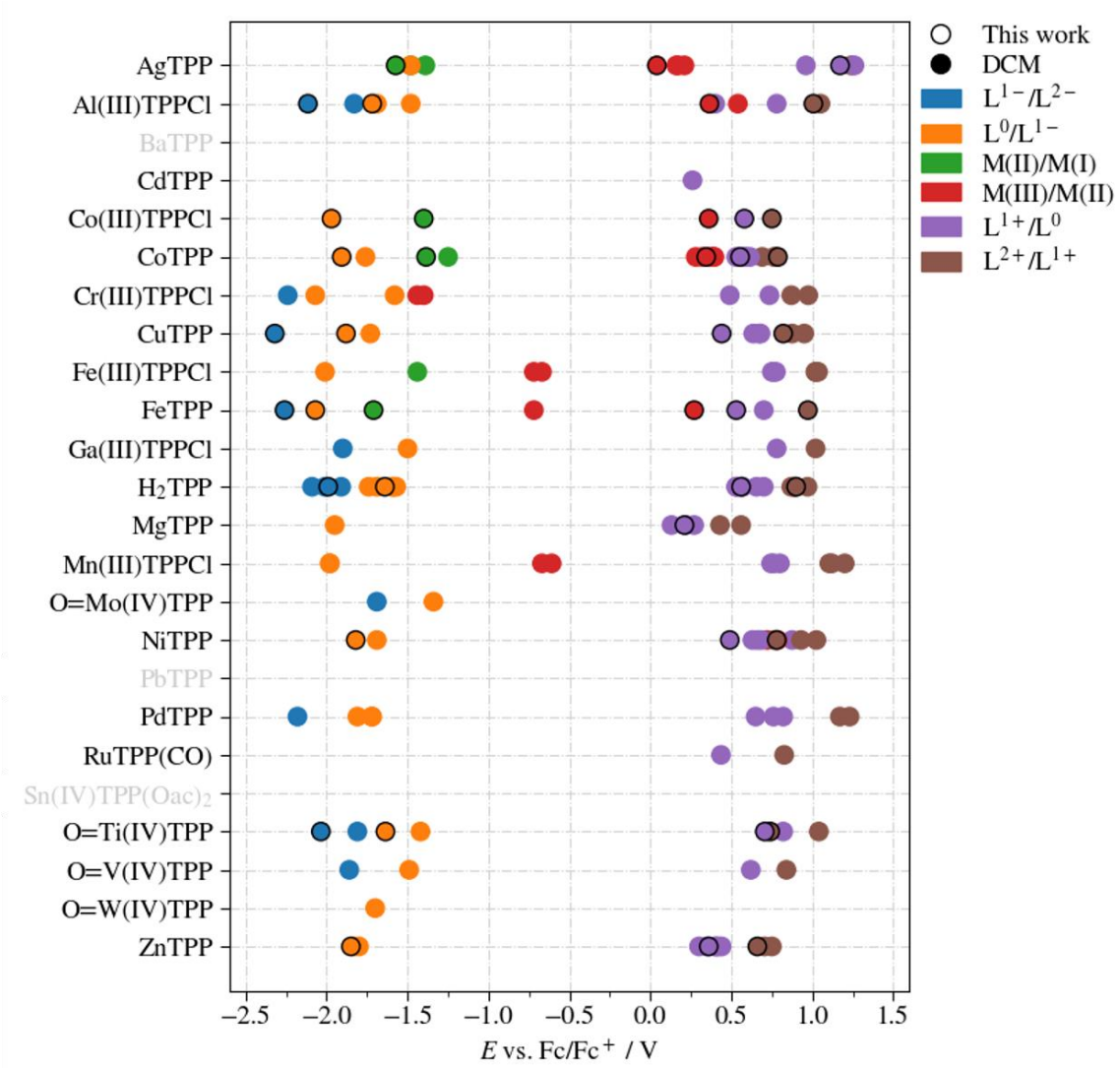


Figure S5. Half-wave potentials in DCM as measured in this work, and as previously reported. No values were found for BaTPP, PbTPP or $Sn(IV)TPP(OAc)_2$.

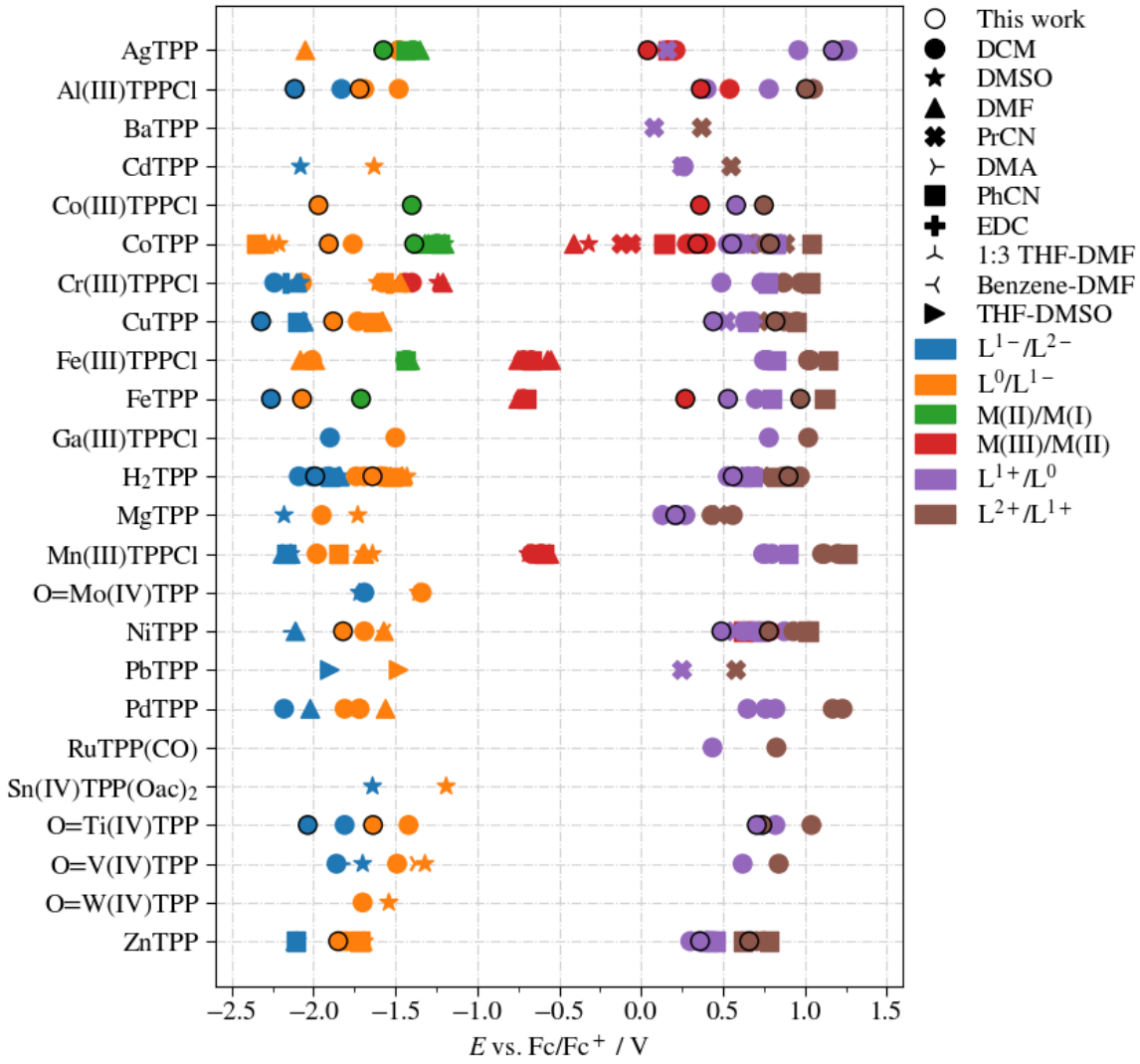


Figure S6. Half-wave potentials for tetraphenylporphyrins in different solvents as measured in this work, and as previously reported.

Table S2. Half-wave potentials of tetraphenylporphyrins measured in various solvents and against various reference electrodes.

Porphyrin	L^{1-}/L^{2-}	L^{0}/L^{1-}	M(II)/M(I)	M(III)/M(II)	L^{1+}/L^{0}	L^{2+}/L^{1+}	Solvent	RE	Ref.
AgTPP			-1.01	0.59		1.62	DCM	SCE	4
AgTPP			-1.03	0.58			DMSO	SCE	4
AgTPP			-1.10				DCM	SCE	5
AgTPP		-1.67	-0.97				DMF	SCE	5
AgTPP		-1.10		0.55	1.64		DCM	SCE	6
AgTPP			-1.06	0.54	1.57		PhCN	PhCN	7
AgTPP				0.54	1.34		DCM	DCM	8
AgTPP					0.54		PrCN	PrCN	9
AgTPP			-1.57	0.04		1.17	DCM	Fc/Fc^{+}	This work
Al(III)TPPCl		-1.69			0.40		DCM	Fc/Fc^{+}	2
Al(III)TPPCl	-1.45	-1.10		0.92	1.16	1.43	DCM	SCE	1

Al(III)TPPCl	-2.12	-1.72		0.36		1.01	DCM	Fc/Fc^+	This work
BaTPP					0.46	0.75	PrCN	SCE	9
CdTPP					0.64		DCM	SCE	10
CdTPP	-1.70	-1.25					DMSO	SCE	11
CdTPP					0.63	0.93	PrCN	SCE	9
CoTPP		-1.38	-0.87	0.70	0.97	1.15	DCM	SCE	12
CoTPP				0.66	0.96		DCM	SCE	13
CoTPP				0.52	1.19	1.42	PhCN	SCE	14
CoTPP		-1.92	-0.82				DMF	SCE	15
CoTPP		-1.87	-0.82				DMSO	SCE	11
CoTPP		-1.83	-0.85	0.06			DMSO	SCE	16
CoTPP			-0.84	0.32			DMA	SCE	16
CoTPP			-0.89	0.26			PrCN	SCE	16
CoTPP			-0.87	-0.03			DMF	SCE	16
CoTPP				0.75	0.91	1.07	DCM	SCE	16
CoTPP				0.32	1.06	1.26	PrCN	SCE	9
CoTPP			-0.94				DMF	SCE	13
CoTPP				0.81	1.03	1.18	DCM	AgCl	17
CoTPP		-1.97	-0.85	0.52	1.20		PhCN	SCE	17
CoTPP		-2.4	-1.27	-0.19	0.64		DMF	Fc/Fc^+	This work
CoTPP		-1.91	-1.31	0.34	0.55	0.79	DCM	Fc/Fc^+	This work
H-CoTPP[a]		-1.80					DCM	Fc/Fc^+	This work
H-CoTPP[b]		-1.80					DCM	Fc/Fc^+	This work
Co(III)TPPCl		-1.97	-1.4	0.36	0.58	0.75	DCM	Fc/Fc^+	This work
Cr(III)TPPCl	-1.79	-1.16					EDC	SCE	18
Cr(III)TPPCl		-1.69		-1.06	0.87	1.25	DCM	SCE	19
Cr(III)TPPCl	-1.86	-1.20		-1.02			DCM	SCE	20
Cr(III)TPPCl	-1.70	-1.23		-0.86			DMSO	SCE	21
Cr(III)TPPCl					1.15	1.41	PhCN	SCE	21
Cr(III)TPPCl	-1.72	-1.09		-0.83			DMF	SCE	22
Cr(III)TPPCl					1.15	1.39	DCM	AgCl	17
CuTPP					1.05		DCM	SCE	13
CuTPP		-1.35			1.06	1.33	DCM	SCE	23
CuTPP	-1.68	-1.20					DMF	SCE	15
CuTPP	-1.68	-1.20					1:3 THF-DMF	SCE	11
CuTPP					0.90	1.16	PrCN	SCE	9
CuTPP	-1.68	-1.20					DMF	SCE	24
CuTPP	-1.72	-1.26			1.03	1.33	PhCN	SCE	7
CuTPP					1.05	1.29	DCM	AgCl	17
CuTPP	-2.32	-1.88			0.44	0.82	DCM	Fc/Fc^+	This work
H-CuTPP[a]		-1.79					DCM	Fc/Fc^+	This work
H-CuTPP[b]		-1.77					DCM	Fc/Fc^+	This work
FeTPP		-1.61	-1.03				DMF	SCE	25
FeTPP					1.08		DCM	SCE	13
FeTPP				-0.32	1.18	1.50	PhCN	SCE	14
FeTPP	-2.26	-2.07	-1.71	0.27	0.53	0.97	DCM	Fc/Fc^+	This work
H-FeTPP[a]		-1.61					DCM	Fc/Fc^+	This work
H-FeTPP[b]		-1.49					DCM	Fc/Fc^+	This work
Fe(III)TPPCl		-1.61	-1.03	-0.19			DMF	SCE	25

Fe(III)TPPCl				-0.34			DCM	SCE	13
Fe(III)TPPCl		-1.70	-1.04	-0.17			DMF	SCE	15
Fe(III)TPPCl					1.13	1.40	DCM	SCE	26
Fe(III)TPPCl				-0.37			DMF	SCE	13
Fe(III)TPPCl		-1.63	-1.06	-0.29	1.14	1.40	DCM	SCE	27
Fe(III)TPPCl			-1.06	-0.29	1.20	1.52	PhCN	SCE	28
Fe(III)TPPCl					1.19	1.45	DCM	AgCl	17
Ga(III)TPPCl	-1.52	-1.12			1.16	1.40	DCM	SCE	29
H_2TPP					0.95		DCM	SCE	13
H_2TPP		-1.21					DCM	SCE	5
H_2TPP	-1.52	-1.15					DMF	SCE	5
H_2TPP					1.00	1.20	PhCN	SCE	14
H_2TPP		-1.21			1.08	1.35	DCM	SCE	23
H_2TPP	-1.46	-1.08					DMF	SCE	15
H_2TPP	-1.47	-1.05					DMSO	SCE	11
H_2TPP					0.97	1.12	PrCN	SCE	9
H_2TPP					0.95	1.28	DCM	SSCE	30
H_2TPP	-1.46	-1.08					DMF	SCE	24
H_2TPP	-2.01	-1.69			0.53	0.87	DCM	Fc/Fc^+	31
H_2TPP	-1.53	-1.19					DCM	SCE	32
H_2TPP	-2.09	-1.74			0.53		DCM	Fc/Fc^+	33
H_2TPP					1.07	1.30	DCM	AgCl	17
H_2TPP	-1.52	-1.14			1.06	1.31	PhCN	SCE	28
H_2TPP	-1.99	-1.64			0.56	0.90	DCM	Fc/Fc^+	This work
H-H_2TPP[a]		-1.64					DCM	Fc/Fc^+	This work
H-H_2TPP[b]		-1.54					DCM	Fc/Fc^+	This work
MgTPP	-1.80	-1.35					DMSO	SCE	11
MgTPP					0.54	0.86	PrCN	SCE	9
MgTPP					0.13	0.43	DCM	Fc/Fc^+	2
MgTPP					0.60		DCM	SCE	34
MgTPP		-1.57			0.65	0.94	DCM	SCE	35
MgTPP					0.21		DCM	Fc/Fc^+	This work
Mn(III)TPPCl		-1.31		-0.31			DMSO	SCE	36
Mn(III)TPPCl		-1.60		-0.23	1.14	1.50	DCM	SCE	37
Mn(III)TPPCl	-1.76	-1.32		-0.22			DMF	SCE	15
Mn(III)TPPCl		-1.60		-0.29	1.18	1.58	DCM	SCE	38
Mn(III)TPPCl	-1.81	-1.31		-0.18			DMF	SCE	39
Mn(III)TPPCl	-1.76	-1.26		-0.24			DMSO	SCE	39
Mn(III)TPPCl					1.16	1.52	DCM	AgCl	17
Mn(III)TPPCl	-1.79	-1.47		-0.21	1.28	1.64	PhCN	SCE	28
O=Mo(IV)TPP	-1.31	-0.96					DCM	SCE	19
O=Mo(IV)TPP	-1.34	-0.98					DMSO	SCE	19
NiTPP				1.10	1.04		DCM	SCE	13
NiTPP				1.00	1.10	1.40	PhCN	SCE	14
NiTPP				1.20	1.29	1.44	DCM	AgCl	40
NiTPP	-1.75	-1.18					Benzene-DMF	SCE	11
NiTPP					0.95		PrCN	SCE	9
NiTPP	-1.73	-1.19					DMF	SCE	24
NiTPP		-1.31			1.01	1.31	DCM	SCE	41
NiTPP					1.10	1.18	DCM	AgCl	17
NiTPP		-1.82			0.49	0.78	DCM	Fc/Fc^+	This work

H-NiTPP[a]		-1.76			DCM	Fc/Fc^+	This work
H-NiTPP[b]		-1.76			DCM	Fc/Fc^+	This work
PbTPP	-1.52	-1.10			THF-DMSO	SCE	11
PbTPP			0.63	0.96	PrCN	SCE	9
PdTPP		-1.34	1.2	1.61	DCM	SCE	23
PdTPP	-1.64	-1.18			DMF	SCE	24
PdTPP	-1.80	-1.34	1.14	1.55	DCM	SCE	42
PdTPP		-1.81	0.65		DCM	Fc/Fc^+	43
RuTPP(CO)			0.82	1.21	DCM	SSCE	30
$Sn(IV)TPP(Oac)_2$	-1.26	-0.81			DMSO	SCE	11
O=Ti(IV)TPP	-1.43	-1.04	1.2	1.42	DCM	SCE	44
O=Ti(IV)TPP	-2.04	-1.64	0.71	0.74	DCM	Fc/Fc^+	This work
O=V(IV)TPP	-1.48	-1.11	1.00	1.22	DCM	SCE	19
O=V(IV)TPP	-1.32	-0.94			DMSO	SCE	19
O=V(IV)TPP	-1.45	-1.00			DMA	SCE	19
O=W(IV)TPP		-1.32			DCM	SCE	19
O=W(IV)TPP		-1.16			DMSO	SCE	19
ZnTPP			0.80		DCM	SCE	13
ZnTPP			0.79	1.00	PhCN	SCE	14
ZnTPP		-1.42	0.82	1.13	DCM	SCE	23
ZnTPP	-1.73	-1.32			DMF	SCE	45
ZnTPP			0.78		DCM	SCE	10
ZnTPP	-1.72	-1.31			DMSO	SCE	11
ZnTPP			0.71	1.03	PrCN	SCE	9
ZnTPP		-1.83	0.30		DCM	Fc/Fc^+	2
ZnTPP	-1.73	-1.34	0.83	1.16	PhCN	SCE	7
ZnTPP			0.73		DCM	SCE	34
ZnTPP			0.82	1.12	DCM	AgCl	17
ZnTPP		-1.85	0.36	0.66	DCM	Fc/Fc^+	This work
H-ZnTPP[a]		-1.80			DCM	Fc/Fc^+	This work
H-ZnTPP[b]		-1.77			DCM	Fc/Fc^+	This work

[a]Potential at the inflection point of the first cathodic wave involved in catalysis as measured by linear sweep voltammetry. [b]Average of inflection point potentials measured in the presence of between X and 22 equivalents of acid, where X is the number of equivalents where the cathodic peak potential stabilizes.

Table S3. Conversion between standard potentials of different reference electrodes used in this work.

↓ From/to →	SCE	SSCE	Ag/AgCl
SHE	0.244[46]	0.235[47]	0.209[48]
Fc/Fc^+	-0.48[a]	-0.484[b]	-0.515[b]

[a]Calculated from average difference between half-wave potentials of H_2TPP measured against DCM in this work, and half-wave potentials measured against SCE in other works. [b]Calculated from the difference between the standard potential of the given reference electrode and SCE vs. SHE.

1.3 UV/Vis absorbance

Figure S7 shows the UV/vis absorbance spectrum of MgTPP, Al(III)TPPCl, O=Ti(IV)TPP, CoTPP, Co(III)TPPCl and AgTPP. All spectra were collected in DCM except the one for CoTPP, which was recorded in DMF.

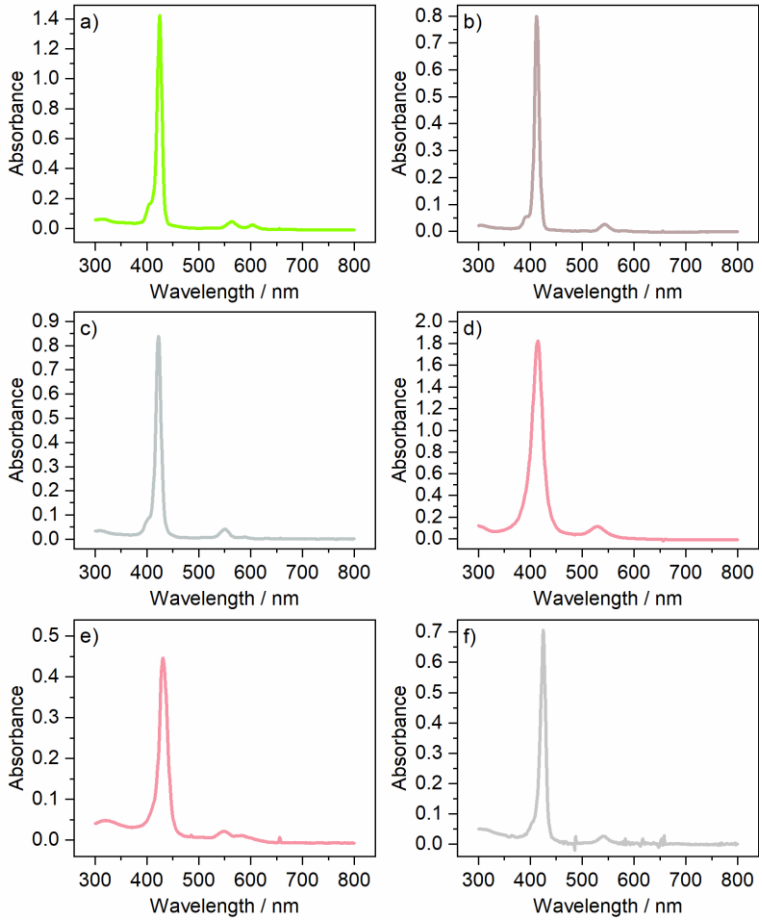
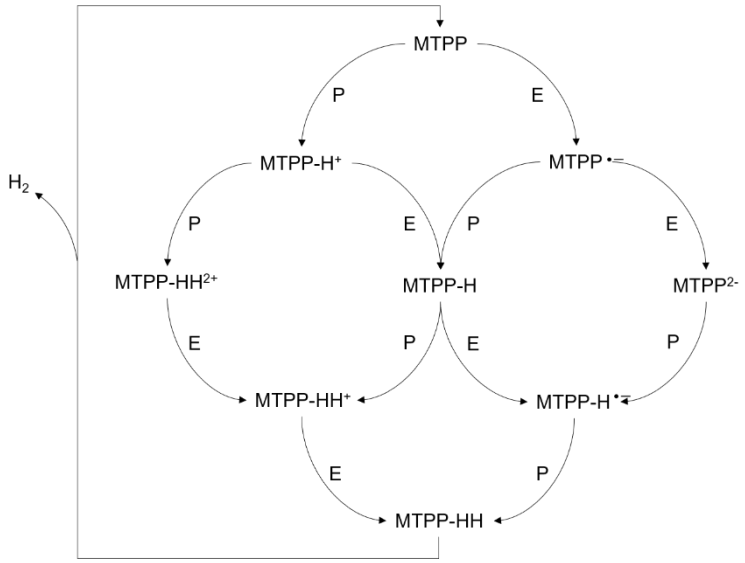


Figure S7. UV/vis of a) MgTPP, b) Al(III)TPPCl, c) O=Ti(IV)TPP, d) CoTPP in DMF, e) Co(III)TPPCl and f) AgTPP.

2 Compoutational study

2.1 Reaction scheme

Assuming that catalysis of the HER by tetraphenylporphyrins consists of two reductions and two protonations, the different possible reaction pathways can be described by Scheme S1.



Scheme S1. Possible reaction pathways for catalysis by MTPP porphyrins. Metal- and ligand centered reductions are not distinguished.

2.2 Population analysis

Mulliken spin densities were obtained for MTPP and H-MTPP, M = 2H, Co, Cu, Fe, Ni and Zn, from the single point energy calculations described in the main text. Figure S8-S11 show the Mulliken spin densities at isovalue 0.004 for the multiplicities (denoted mX, X=1,2 , ..., 6) resulting in the lowest electronic energy of each compound. H_2TPP, NiTPP and ZnTPP are left out, as the lowest electronic energies of these compounds were obtained for closed shell singlet states, and open-shell singlet states were not considered. Table S4 lists the Mulliken spin populations of each considered compound and Table S5 lists all HOMOs and LUMOs. For reference, Figure S12 and Figure S13 show the labelling of atoms in the optimized geometries, using H-H_2TPP and H-ZnTPP as examples. Figure S14 shows the change in CM5 charge on the ligand and on the metal between H-MTPP and MTPP. For M = Co, the total charge of the molecule was set to -1 as the reduction of Co(II) to Co(I) occurs before, but is not involved in, catalysis.

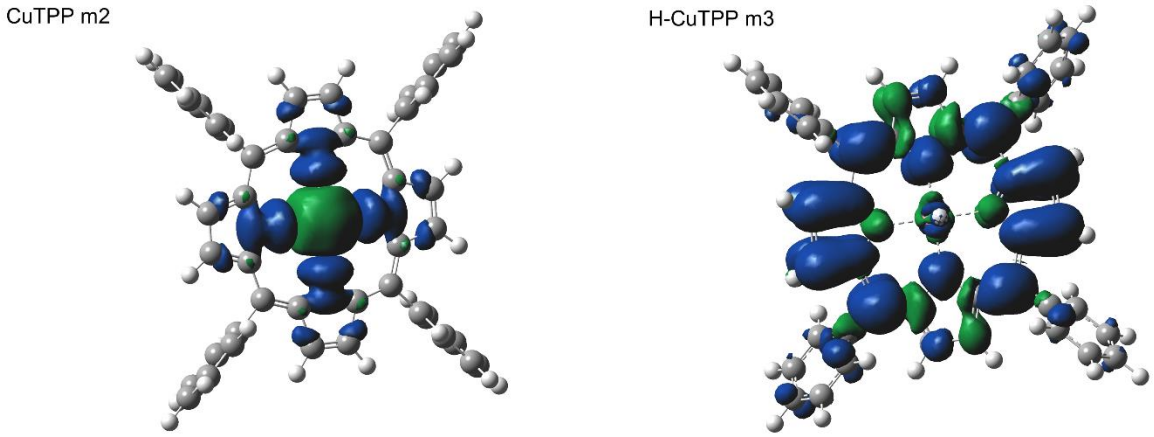


Figure S8. Spin density plots for CuTPP and H-CuTPP at isovalue 0.004.

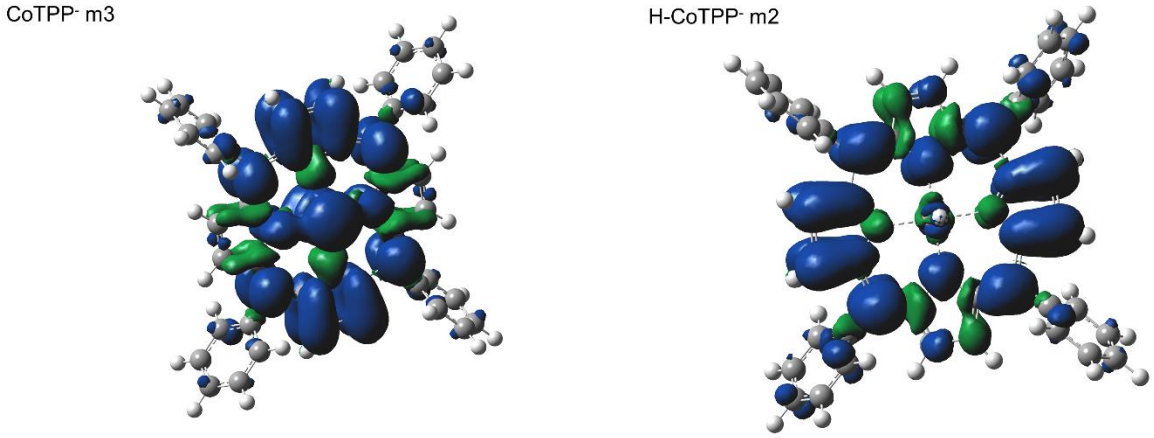


Figure S9. Spin density plots for $CoTPP^-$ and $H\text{-}CoTPP^-$ at isovalue 0.004.

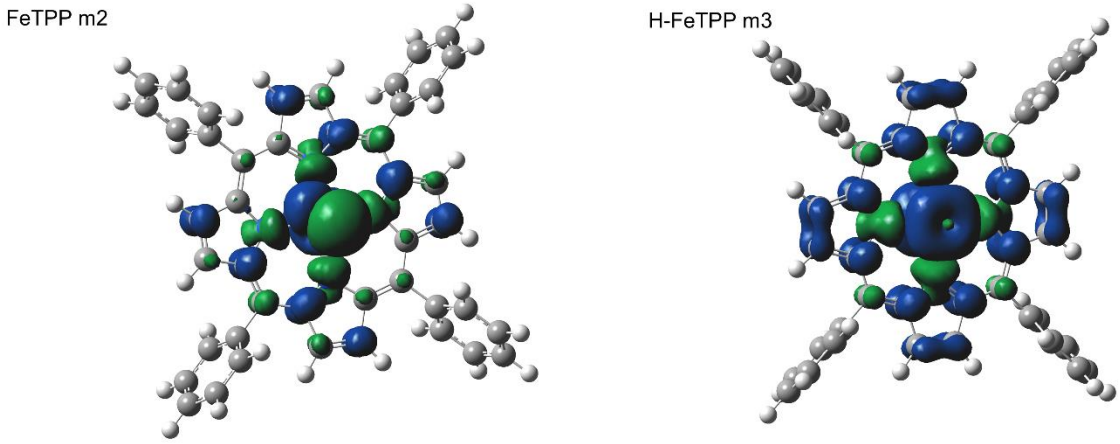


Figure S10. Spin density plots for FeTPP and H-FeTPP at isovalue 0.004.

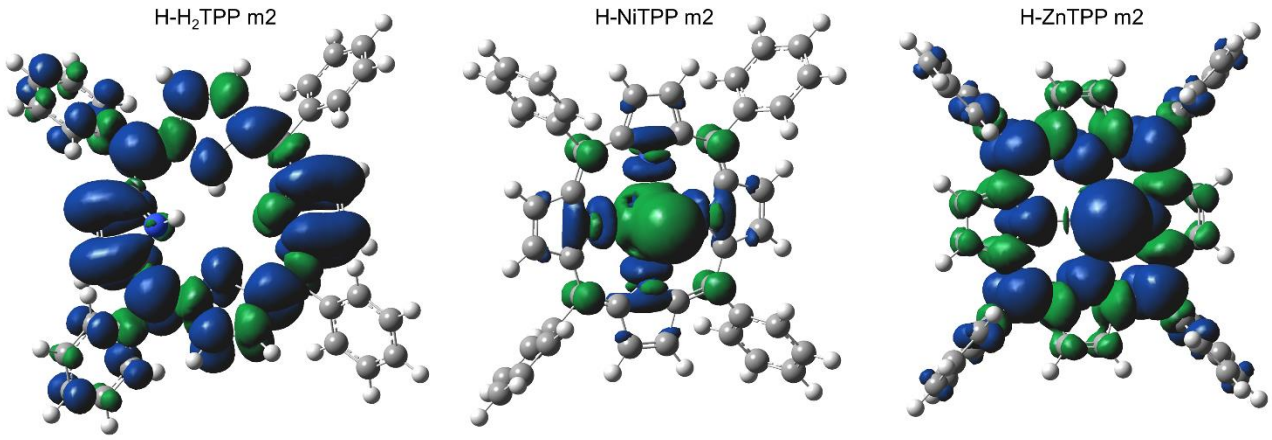


Figure S11. Spin density plots for H-H_2TPP, H-NiTPP and H-ZnTPP at isovalue 0.004.

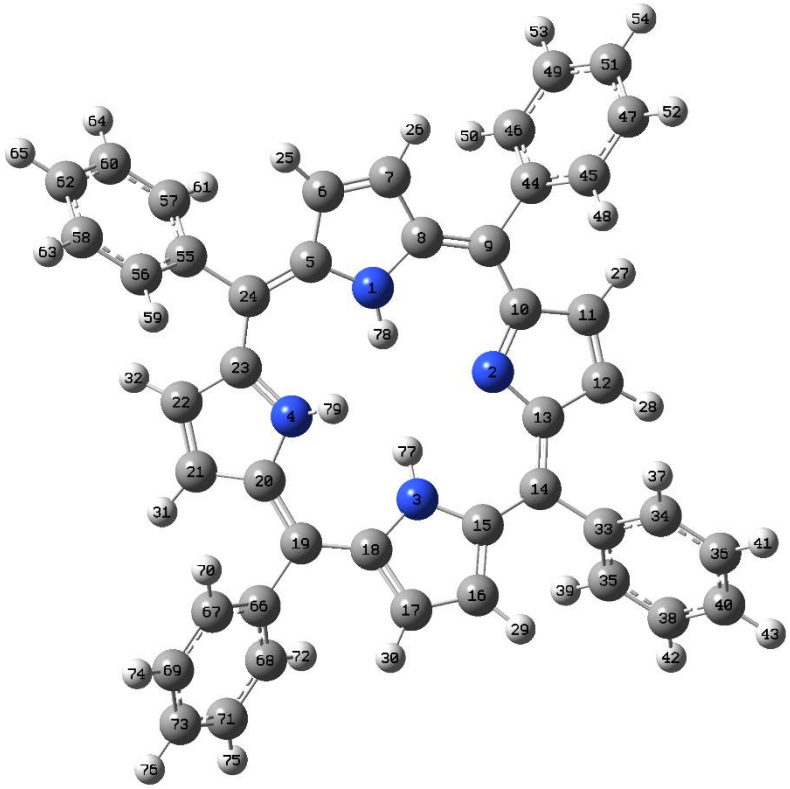


Figure S12. Atom numbering of H-H_2TPP.

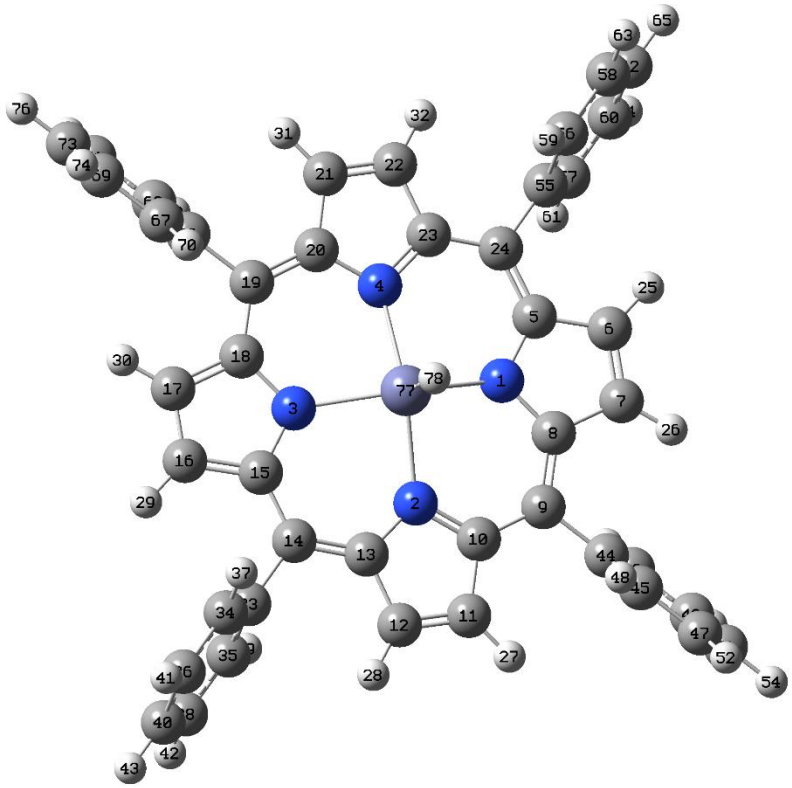


Figure S13. Atom numbering of H-ZnTPP.

Table S4. Mulliken spin densities for MTPP and H-MTPP. Values are obtained from the single point calculations described in the main text, for the multiplicities (mX) that the resulted in the electronic lowest energy.

Atom	H-H_2TPP m2	CoTPP$^-$ m3	H-CoTPP$^-$ m2	CuTPP m2	H-CuTPP m3	FeTPP m3	H-FeTPP m2	H-NiTPP m2	H-ZnTPP m2
1N	6.03E-02	-3.90E-02	1.01E-01	1.12E-01	1.68E-01	-6.71E-02	-4.50E-02	4.93E-02	1.15E-01
2N	-5.17E-02	7.59E-02	-1.28E-02	1.13E-01	1.60E-01	-6.71E-02	-4.03E-02	4.71E-02	1.13E-01
3N	6.03E-02	-3.90E-02	1.01E-01	1.12E-01	1.68E-01	-6.71E-02	-4.41E-02	4.93E-02	1.12E-01
4N	-5.88E-03	7.59E-02	-1.15E-02	1.13E-01	1.58E-01	-6.71E-02	-3.60E-02	4.73E-02	1.13E-01
5C	-4.20E-02	5.57E-02	2.34E-03	-2.79E-03	-1.74E-02	1.43E-02	1.33E-02	9.27E-03	-5.49E-02
6C	6.71E-02	6.68E-02	-1.64E-02	-5.48E-03	-1.64E-02	1.76E-02	9.60E-05	2.82E-03	-1.56E-02
7C	-4.61E-02	6.68E-02	1.68E-02	-5.48E-03	-1.29E-02	1.76E-02	2.53E-02	1.80E-03	-1.56E-02
8C	6.82E-02	5.57E-02	-2.74E-02	-2.79E-03	-1.81E-02	1.43E-02	3.31E-03	4.77E-03	-5.49E-02
9C	-2.63E-02	8.69E-02	1.31E-01	1.13E-02	4.51E-02	-1.49E-02	-1.11E-02	-1.45E-02	1.34E-01
10C	1.17E-01	-2.03E-02	4.36E-02	-3.14E-03	-1.73E-02	1.43E-02	-2.78E-04	1.06E-02	-3.74E-02
11C	4.92E-02	4.89E-03	7.61E-02	-5.84E-03	-1.57E-02	1.74E-02	2.38E-02	3.51E-03	-1.51E-02
12C	4.94E-02	4.89E-03	5.34E-02	-5.84E-03	-1.21E-02	1.74E-02	-1.58E-03	1.73E-03	-1.11E-02
13C	1.17E-01	-2.03E-02	6.97E-02	-3.14E-03	-1.45E-02	1.43E-02	1.38E-02	6.86E-03	-6.34E-02
14C	-2.59E-02	8.69E-02	6.46E-02	1.13E-02	4.65E-02	-1.49E-02	-2.09E-02	-1.55E-02	1.45E-01
15C	6.80E-02	5.57E-02	2.15E-03	-2.79E-03	-2.09E-02	1.43E-02	1.99E-02	8.37E-03	-4.62E-02
16C	-4.59E-02	6.68E-02	-1.79E-02	-5.48E-03	-1.29E-02	1.76E-02	1.84E-03	2.88E-03	-9.30E-03
17C	6.68E-02	6.68E-02	1.56E-02	-5.48E-03	-1.23E-02	1.76E-02	2.32E-02	1.28E-03	-9.30E-03
18C	-4.17E-02	5.57E-02	-3.22E-02	-2.79E-03	-1.17E-02	1.43E-02	-4.44E-03	5.22E-03	-4.62E-02
19C	1.66E-01	8.69E-02	1.30E-01	1.13E-02	4.22E-02	-1.49E-02	-9.74E-03	-1.66E-02	1.45E-01

20C	3.09E-02	-2.03E-02	4.81E-02	-3.14E-03	-2.01E-02	1.43E-02	-8.49E-03	1.00E-02	-6.34E-02
21C	7.54E-02	4.89E-03	7.45E-02	-5.84E-03	-1.51E-02	1.74E-02	2.09E-02	2.69E-03	-1.11E-02
22C	7.59E-02	4.88E-03	4.82E-02	-5.84E-03	-1.49E-02	1.74E-02	-3.16E-04	2.17E-03	-1.51E-02
23C	3.06E-02	-2.03E-02	7.55E-02	-3.14E-03	-1.04E-02	1.43E-02	1.87E-02	5.76E-03	-3.74E-02
24C	1.67E-01	8.69E-02	6.42E-02	1.13E-02	3.93E-02	-1.49E-02	-1.95E-02	-1.54E-02	1.34E-01
25H	-2.81E-03	-6.46E-03	1.68E-03	8.94E-04	1.04E-03	-7.33E-04	1.49E-04	7.29E-04	6.03E-04
26H	3.05E-03	-6.46E-03	4.17E-04	8.94E-04	9.99E-04	-7.33E-04	-7.33E-04	7.40E-04	6.03E-04
27H	-4.28E-03	1.13E-03	-6.98E-03	8.92E-04	9.28E-04	-7.40E-04	-7.79E-04	7.78E-04	4.84E-04
28H	-4.29E-03	1.13E-03	-5.80E-03	8.92E-04	9.65E-04	-7.40E-04	1.65E-04	7.21E-04	6.81E-04
29H	3.03E-03	-6.46E-03	1.75E-03	8.94E-04	1.15E-03	-7.33E-04	1.21E-04	7.51E-04	7.74E-04
30H	-2.79E-03	-6.46E-03	5.34E-04	8.94E-04	1.14E-03	-7.33E-04	-8.54E-04	7.27E-04	7.73E-04
31H	-5.38E-03	1.13E-03	-6.83E-03	8.92E-04	8.35E-04	-7.40E-04	-8.23E-04	7.40E-04	6.81E-04
32H	-5.40E-03	1.13E-03	-4.83E-03	8.92E-04	8.61E-04	-7.40E-04	1.54E-04	7.46E-04	4.83E-04
33C	1.14E-02	-1.95E-03	1.03E-02	-2.03E-03	1.24E-03	-6.58E-03	2.56E-03	-5.15E-04	5.51E-03
34C	-1.09E-02	-1.33E-02	1.59E-02	-1.85E-04	-1.73E-03	1.48E-03	-3.18E-04	2.62E-04	4.00E-05
35C	7.93E-04	1.88E-02	-1.69E-02	-5.30E-05	-1.20E-03	1.93E-03	3.74E-04	9.10E-05	3.95E-03
36C	1.06E-03	3.14E-03	-3.74E-03	2.90E-05	4.35E-04	1.33E-04	-1.17E-04	-6.90E-04	8.79E-04
37H	1.02E-03	2.29E-04	-9.60E-04	-8.00E-06	-4.10E-04	-3.30E-05	1.24E-04	2.05E-04	-1.22E-03
38C	7.04E-04	-5.10E-03	3.44E-03	4.60E-05	-3.49E-04	2.43E-04	1.81E-04	9.30E-05	-1.33E-03
39H	-3.26E-04	-3.32E-04	4.04E-04	-1.30E-05	-1.60E-04	-1.20E-05	-7.00E-06	6.50E-05	-9.10E-04
40C	1.79E-04	7.13E-03	5.57E-03	-5.70E-05	6.91E-04	6.10E-05	-2.41E-04	-4.36E-04	6.25E-03
41H	-6.40E-05	1.94E-04	-8.80E-05	2.00E-06	6.10E-05	-3.00E-05	-6.00E-06	-1.40E-05	3.18E-04
42H	-1.70E-04	-5.20E-05	1.25E-04	3.00E-06	5.60E-05	-3.70E-05	-3.00E-06	-2.40E-05	3.13E-04
43H	-4.10E-05	-3.28E-04	-3.29E-04	6.00E-06	-5.10E-05	8.00E-06	1.50E-05	2.20E-05	-3.74E-04
44C	1.15E-02	-1.95E-03	-1.17E-02	-2.03E-03	2.60E-03	-6.58E-03	-5.66E-03	-6.23E-04	1.10E-02
45C	-1.09E-02	1.88E-02	2.55E-02	-5.30E-05	-2.89E-03	1.93E-03	1.90E-03	3.26E-04	-2.53E-03
46C	7.46E-04	-1.33E-02	-1.12E-02	-1.85E-04	-1.69E-03	1.48E-03	2.05E-03	-1.84E-04	3.50E-03
47C	1.08E-03	-5.10E-03	-8.75E-03	4.60E-05	6.13E-04	2.43E-04	1.48E-04	-6.80E-04	1.43E-03
48H	1.03E-03	-3.32E-04	-5.49E-04	-1.30E-05	-5.62E-04	-1.20E-05	2.65E-04	2.08E-04	-1.49E-03
49C	7.26E-04	3.14E-03	7.63E-04	2.90E-05	-1.63E-04	1.33E-04	-7.00E-06	1.30E-04	-8.84E-04
50H	-3.23E-04	2.29E-04	1.89E-04	-8.00E-06	-1.37E-04	-3.30E-05	5.80E-05	8.10E-05	-8.65E-04
51C	1.52E-04	7.13E-03	1.14E-02	-5.70E-05	3.97E-04	6.10E-05	6.20E-05	-6.09E-04	6.10E-03
52H	-6.50E-05	-5.20E-05	1.43E-04	3.00E-06	5.60E-05	-3.70E-05	-2.30E-05	-1.50E-05	3.14E-04
53H	-1.72E-04	1.94E-04	2.09E-04	2.00E-06	5.30E-05	-3.00E-05	-3.50E-05	-2.80E-05	3.21E-04
54H	-3.90E-05	-3.28E-04	-6.68E-04	6.00E-06	-3.20E-05	8.00E-06	2.00E-06	3.20E-05	-3.72E-04
55C	-1.82E-02	-1.94E-03	3.70E-03	-2.03E-03	3.21E-03	-6.58E-03	2.48E-03	-4.02E-04	1.10E-02
56C	1.42E-02	1.88E-02	-1.54E-02	-5.30E-05	-2.67E-03	1.93E-03	-3.62E-04	2.35E-04	-2.53E-03
57C	2.41E-02	-1.33E-02	1.08E-02	-1.85E-04	-1.34E-03	1.48E-03	3.24E-04	-2.66E-04	3.50E-03
58C	-1.15E-02	-5.10E-03	4.28E-03	4.60E-05	5.77E-04	2.44E-04	-1.59E-04	-6.23E-04	1.44E-03
59H	-2.24E-04	-3.32E-04	-6.60E-05	-1.30E-05	-5.94E-04	-1.10E-05	1.38E-04	1.95E-04	-1.49E-03
60C	-1.34E-02	3.14E-03	-3.33E-03	2.90E-05	-3.16E-04	1.33E-04	1.38E-04	1.61E-04	-8.82E-04
61H	-1.93E-03	2.29E-04	1.00E-06	-8.00E-06	-1.49E-04	-3.30E-05	-1.60E-05	8.90E-05	-8.65E-04
62C	2.02E-02	7.13E-03	3.82E-03	-5.70E-05	6.02E-04	6.10E-05	-2.29E-04	-6.86E-04	6.10E-03
63H	5.47E-04	-5.20E-05	-3.20E-05	3.00E-06	6.70E-05	-3.70E-05	-5.00E-06	-1.90E-05	3.14E-04
64H	7.00E-04	1.94E-04	-1.81E-04	2.00E-06	5.80E-05	-3.00E-05	-1.00E-06	-2.80E-05	3.21E-04
65H	-1.38E-03	-3.28E-04	-5.70E-05	6.00E-06	-4.90E-05	8.00E-06	1.40E-05	3.60E-05	-3.72E-04
66C	-1.81E-02	-1.94E-03	-8.93E-03	-2.03E-03	2.38E-03	-6.58E-03	-7.25E-03	-5.00E-06	5.52E-03
67C	1.41E-02	-1.33E-02	2.30E-02	-1.85E-04	-2.34E-03	1.48E-03	1.44E-03	-1.10E-04	3.70E-05
68C	2.40E-02	1.88E-02	-9.98E-03	-5.30E-05	-1.11E-03	1.93E-03	2.59E-03	-2.80E-05	3.95E-03
69C	-1.14E-02	3.14E-03	-8.60E-03	2.90E-05	5.33E-04	1.33E-04	-7.20E-05	1.45E-04	8.80E-04
70H	-2.20E-04	2.29E-04	-7.86E-04	-8.00E-06	-5.36E-04	-3.30E-05	3.20E-05	8.10E-05	-1.22E-03
71C	-1.33E-02	-5.10E-03	5.01E-04	4.60E-05	-3.40E-04	2.44E-04	5.50E-04	-6.39E-04	-1.33E-03
72H	-1.92E-03	-3.32E-04	8.00E-05	-1.30E-05	-1.75E-04	-1.10E-05	1.78E-04	1.68E-04	-9.10E-04
73C	2.02E-02	7.13E-03	1.08E-02	-5.70E-05	7.23E-04	6.10E-05	1.13E-04	-6.21E-04	6.25E-03
74H	5.44E-04	1.94E-04	2.95E-04	2.00E-06	6.80E-05	-3.00E-05	-1.50E-05	-2.70E-05	3.18E-04
75H	6.96E-04	-5.20E-05	2.27E-04	3.00E-06	5.80E-05	-3.70E-05	-3.80E-05	-1.70E-05	3.13E-04

76H	-1.37E-03	-3.28E-04	-6.91E-04	6.00E-06	-5.50E-05	8.00E-06	2.00E-06	3.20E-05	-3.74E-04
77Zn	7.25E-04	1.14E+00	-1.06E-02	5.76E-01	7.02E-01	2.09E+00	1.20E+00	9.45E-01	1.42E-01
78H	7.24E-04	-	3.26E-03	-	7.10E-01	-	-1.23E-01	-1.57E-01	2.87E-01
79H	1.06E-04	-	-	-	-	-	-	-	-

Table S5. HOMO and LUMO of H-MTPP and MTPP, for the multiplicities (mX) resulting in the lowest electronic energy.

Compound	**HOMO**	**LUMO**
H_2TPP m1	-5.2801	-2.5815
H-H_2TPP m2	-3.8227	-2.6368
FeTPP m3	-5.3457	-2.4607
H-FeTPP m2	-5.4230	-2.4697
$CoTPP^-$ m3	-0.4912	0.5418
H-$CoTPP^-$ m2	-0.5113	0.5222
NiTPP m1	-5.3721	-2.4458
H-NiTPP m2	-5.4586	-2.7601
CuTPP m2	-5.3685	-2.4964
H-CuTPP m3	-5.2744	-2.5560
ZnTPP m1	-5.3269	-2.5119
H-ZnTPP m2	-5.3734	-2.6512

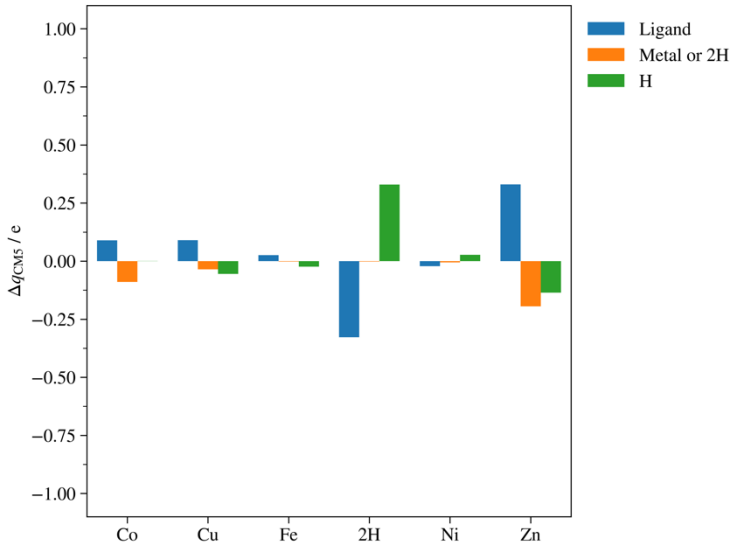


Figure S14. Change in CM5 charge on the ligand and on the metal between H-MTPP and MTPP. The charge on H in H-MTPP is also shown. For H-CoTPP and CoTPP, the total charge is set to -1.

Energies and energy correction**Fel! Hittar inte referenskälla.** Figure S15 shows half-wave potentials of the first oxidation (M(III)/M(II) or L^{1+}/L^{0}) as a function of the difference in free energy between $MTPP^{0}$ and $MTPP^{+}$. Table S6 shows the total charge (q), the multiplicity (M), the total energy ($\varepsilon_{\mathrm{opt}}$) and dispersion correction ($\varepsilon_{\mathrm{d,opt}}$) resulting from geometry optimization dispersion, the total energy ($\varepsilon_{\mathrm{freq}}$) and dispersion correction ($\varepsilon_{\mathrm{d,freq}}$) resulting from frequency calculations, the zero point correction, ($\varepsilon_{\mathrm{ZPE}}$), the correction to the internal energy ($\varepsilon_{\mathrm{int}}$), the correction to the enthalpy (H_{corr}), the correction to Gibbs free energy (G_{corr}), the entropy (S), and the total energy resulting from single point calculations ($\varepsilon_{\mathrm{sp}}$) for all compounds used in the computational study. The entropy was obtained from $S = (H_{\mathrm{corr}} - G_{\mathrm{corr}})/T$, where $T = 298.15$ K.

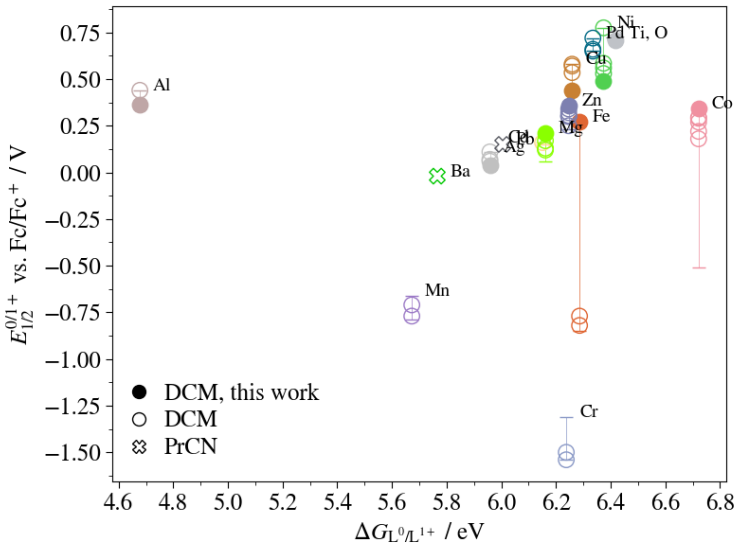


Figure S15. Half-wave potential of the first oxidation (M(III)/M(II) for Al, Ag, Co, Cr, and Fe, L^{1+}/L^{0} for all other compounds shown here) as a function of the difference in free energy between $MTPP^{0}$ and $MTPP^{+}$. Filled markers indicate values obtained experimentally in this study, open markers indicate values obtained from literature and the bars represent all literature values obtained in solvents other than DCM.

Table S6. Energies and energy corrections resulting from geometry optimizations, frequency calculations and single point calculations. For compounds marked NC (not-converged), one or more calculations did not converge after several attempts, and the results were left out.

Name	q	M	ε_{opt}	$\varepsilon_{d,opt}$	ε_{freq}	$\varepsilon_{d,freq}$	ε_{ZPE}	ε_{int}	H_{corr}	G_{corr}	S	ε_{sp}
AgTPP	-1	1	-2 059.70571	-0.09826	-2 059.70574	-0.09824	0.59105	0.62878	0.62972	0.51911	3.710E-04	-2 060.12945
AgTPP	-1	3	-2 059.70288	-0.09791	-2 059.70289	-0.09792	0.59127	0.62888	0.62982	0.51831	3.740E-04	-2 060.12771
AgTPP	-1	5	-2 059.64945	-0.09793	-2 059.64945	-0.09793	0.58938	0.62726	0.62820	0.51565	3.775E-04	-2 060.07365
AgTPP	0	2	-2 059.64574	-0.09769	-2 059.64574	-0.09769	0.59522	0.63256	0.63350	0.52251	3.723E-04	-2 060.06610
AgTPP	0	4	-2 059.58820	-0.09794	-2 059.58820	-0.09794	0.59197	0.62960	0.63055	0.51873	3.750E-04	-2 060.01108
AgTPP	0	6	-2 059.51846	-0.09781	-2 059.51846	-0.09781	0.59007	0.62810	0.62904	0.51561	3.805E-04	-2 059.94125
AgTPP	1	1	-2 059.43136	-0.09864	-2 059.43136	-0.09864	0.59765	0.63426	0.63520	0.52804	3.594E-04	-2 059.85195
AgTPP	1	3	-2 059.41718	-0.09816	-2 059.41718	-0.09816	0.59544	0.63258	0.63353	0.52355	3.689E-04	-2 059.83821
AgTPP	1	5	-2 059.34770	-0.09802	-2 059.34770	-0.09802	0.59190	0.62971	0.63065	0.51819	3.772E-04	-2 059.76901
AlTPP	0	2	-2 155.19247	-0.09286	-2 155.19247	-0.09286	0.59760	0.63398	0.63493	0.52606	3.651E-04	-2 155.60153
AlTPP	1	1	-2 155.02256	-0.09236	-2 155.02256	-0.09236	0.60003	0.63559	0.63653	0.52756	3.655E-04	-2 155.43042
BaTPP	0	1	-1 938.20749	-0.09411	-1 938.20748	-0.09411	0.59272	0.63064	0.63159	0.51907	3.774E-04	-1 938.62098
BaTPP	0	3	-1 938.15652	-0.09469	-1 938.15652	-0.09469	0.59045	0.62840	0.62935	0.51667	3.779E-04	-1 938.56899
BaTPP	0	5	-1 938.08828	-0.09474	-1 938.08828	-0.09474	0.58827	0.62654	0.62748	0.51362	3.819E-04	-1 938.50064
BaTPP	1	2	-1 937.99435	-0.09478	-1 937.99705	-0.09516	0.59387	0.63139	0.63233	0.52158	3.715E-04	-1 938.40554
BaTPP	1	4	-1 937.93077	-0.09500	-1 937.93077	-0.09500	0.59089	0.62901	0.62996	0.51673	3.797E-04	-1 938.34202
BaTPP	1	6	-1 937.83567	-0.09514	-1 937.83567	-0.09514	0.58677	0.62545	0.62639	0.51153	3.852E-04	-1 938.24633
CdTPP	0	1	-2 080.44116	-0.09747	-2 080.44116	-0.09747	0.59406	0.63167	0.63261	0.52131	3.733E-04	-2 080.86744
CdTPP	0	3	-2 080.39081	-0.09811	-2 080.39081	-0.09811	0.59233	0.62982	0.63077	0.51995	3.717E-04	-2 080.81654
CdTPP	0	5	-2 080.32190	-0.09805	-2 080.32190	-0.09805	0.58989	0.62778	0.62872	0.51633	3.770E-04	-2 080.74752
CdTPP	1	2	-2 080.21414	-0.09794	-2 080.21420	-0.09794	0.59418	0.63176	0.63270	0.52088	3.751E-04	-2 080.63822
CdTPP	1	4	-2 080.15156	-0.09812	-2 080.15156	-0.09812	0.59216	0.62984	0.63078	0.51908	3.747E-04	-2 080.57577
CdTPP	1	6	-2 080.05247	-0.09799	-2 080.05668	-0.09808	0.58804	0.62639	0.62733	0.51373	3.810E-04	-2 080.47654
CoTPP	-1	1	-2 058.62158	-0.09502	-2 058.63653	-0.09511	0.59431	0.63144	0.63239	0.52193	3.705E-04	-3 295.99441
CoTPP	-1	3	-2 058.63485	-0.09513	-2 058.63485	-0.09513	0.59373	0.63091	0.63186	0.51984	3.757E-04	-3 296.00229
CoTPP	-1	5	-2 058.63210	-0.09513	-2 058.63210	-0.09513	0.59219	0.62965	0.63059	0.51900	3.743E-04	-3 295.99301
CoTPP	0	2	-2 058.58386	-0.09488	-2 058.58386	-0.09488	0.59782	0.63472	0.63567	0.52356	3.760E-04	-3 295.94981
CoTPP	0	4	-2 058.51969	-0.09515	-2 058.51969	-0.09515	0.59387	0.63108	0.63202	0.52045	3.742E-04	-3 295.88476
CoTPP	0	6	-2 058.51860	-0.09521	-2 058.51860	-0.09521	0.59288	0.63041	0.63136	0.51905	3.767E-04	-3 295.87739
CoTPP NC	1	1										
CoTPP	1	3	-2 058.34056	-0.09478	-2 058.34056	-0.09478	0.59834	0.63468	0.63563	0.52718	3.637E-04	-3 295.70337
CoTPP	1	5	-2 058.28500	-0.09481	-2 058.28500	-0.09481	0.59520	0.63203	0.63298	0.52367	3.666E-04	-3 295.66977
CrTPP NC	0	1										
CrTPP	0	3	-1 999.73096	-0.09388	-1 999.73096	-0.09388	0.59674	0.63363	0.63457	0.52395	3.710E-04	-2 957.61580
CrTPP	0	5	-1 999.77254	-0.09387	-1 999.77254	-0.09387	0.59673	0.63359	0.63453	0.52365	3.719E-04	-2 957.65831
CrTPP	1	2	-1 999.50194	-0.09436	-1 999.50194	-0.09436	0.59654	0.63330	0.63424	0.52525	3.656E-04	-2 957.36785
CrTPP	1	4	-1 999.54377	-0.09435	-1 999.54377	-0.09435	0.59646	0.63324	0.63418	0.52458	3.676E-04	-2 957.42700
CrTPP	1	6	-1 999.54306	-0.09436	-1 999.54306	-0.09436	0.59668	0.63342	0.63437	0.52464	3.680E-04	-2 957.42632
CuTPP	0	2	-2 110.05438	-0.09658	-2 110.05438	-0.09658	0.59671	0.63389	0.63484	0.52337	3.739E-04	-3 553.66374
CuTPP	0	4	-2 109.99348	-0.09686	-2 109.99348	-0.09686	0.59326	0.63074	0.63169	0.51954	3.762E-04	-3 553.60236
CuTPP	0	6	-2 109.92429	-0.09676	-2 109.92429	-0.09676	0.59163	0.62951	0.63046	0.51638	3.826E-04	-3 553.53303
CuTPP	1	1	-2 109.81133	-0.09770	-2 109.82612	-0.09746	0.59720	0.63400	0.63495	0.52665	3.632E-04	-3 553.42054
CuTPP	1	3	-2 109.82460	-0.09707	-2 109.82460	-0.09707	0.59661	0.63364	0.63459	0.52410	3.706E-04	-3 553.43153
CuTPP	1	5	-2 109.75586	-0.09693	-2 109.75586	-0.09693	0.59364	0.63127	0.63221	0.51926	3.788E-04	-3 553.36305
FeTPP	-1	2	-2 036.72129	-0.09607	-2 036.72129	-0.09607	0.59417	0.63123	0.63217	0.52166	3.707E-04	-3 176.93760
FeTPP	-1	4	-2 036.71562	-0.09612	-2 036.71562	-0.09612	0.59356	0.63072	0.63166	0.52036	3.733E-04	-3 176.93522
FeTPP	-1	6	-2 036.71434	-0.09606	-2 036.71434	-0.09606	0.59175	0.62929	0.63023	0.51834	3.753E-04	-3 176.91406
FeTPP	0	1	-2 036.60881	-0.09602	-2 036.64389	-0.09603	0.59774	0.63447	0.63541	0.52619	3.663E-04	-3 176.82720
FeTPP	0	3	-2 036.66313	-0.09585	-2 036.66312	-0.09585	0.59753	0.63444	0.63538	0.52382	3.742E-04	-3 176.88120
FeTPP	0	5	-2 036.65309	-0.09588	-2 036.65879	-0.09588	0.59565	0.63292	0.63387	0.52217	3.746E-04	-3 176.81085
FeTPP	1	2	-2 036.43295	-0.09634	-2 036.43295	-0.09634	0.59738	0.63415	0.63510	0.52516	3.687E-04	-3 176.64844
FeTPP	1	4	-2 036.43089	-0.09589	-2 036.43089	-0.09589	0.59790	0.63409	0.63503	0.52429	3.714E-04	-3 176.65101
FeTPP	1	6	-2 036.43033	-0.09635	-2 036.43033	-0.09635	0.59570	0.63291	0.63385	0.52286	3.723E-04	-3 176.64159
H_2TPP	0	1	-1 913.82681	-0.09151	-1 913.82681	-0.09151	0.61839	0.65490	0.65584	0.54674	3.659E-04	-1 914.21574
H_2TPP	1	2	-1 913.59938	-0.09197	-1 913.59938	-0.09197	0.61867	0.65503	0.65597	0.54716	3.650E-04	-1 913.98595
MgTPP	0	1	-2 112.86290	-0.09348	-2 112.86290	-0.09348	0.59673	0.63343	0.63437	0.52583	3.641E-04	-2 113.26693
MgTPP	1	2	-2 112.63642	-0.09398	-2 112.63642	-0.09398	0.59683	0.63341	0.63436	0.52628	3.625E-04	-2 113.03813
MnTPP	0	2	-2 017.06677	-0.09558	-2 017.06677	-0.09558	0.59715	0.63400	0.63495	0.52455	3.703E-04	-3 064.13066
MnTPP	0	4	-2 017.09233	-0.09558	-2 017.09233	-0.09558	0.59708	0.63395	0.63489	0.52387	3.724E-04	-3 064.15888
MnTPP	0	6	-2 017.10390	-0.09553	-2 017.10390	-0.09553	0.59497	0.63234	0.63328	0.52139	3.753E-04	-3 064.16408
MnTPP	1	1	-2 016.79507	-0.09564	-2 016.83534	-0.09565	0.59765	0.63380	0.63474	0.52702	3.613E-04	-3 063.86374
MnTPP	1	3	-2 016.86372	-0.09606	-2 016.86372	-0.09606	0.59701	0.63376	0.63470	0.52519	3.673E-04	-3 063.92290
MnTPP	1	5	-2 016.89993	-0.09566	-2 016.89993	-0.09566	0.59783	0.63397	0.63492	0.52602	3.653E-04	-3 063.96624

NiTPP	0	1	-2 083.68021	-0.09629	-2 083.68021	-0.09629	0.59811	0.63488	0.63582	0.52596	3.685E-04	-3 421.50232
NiTPP	0	3	-2 083.67257	-0.09640	-2 083.67257	-0.09640	0.59660	0.63372	0.63467	0.52335	3.734E-04	-3 421.48578
NiTPP	0	5	-2 083.61198	-0.09666	-2 083.61198	-0.09666	0.59324	0.63064	0.63158	0.51981	3.749E-04	-3 421.42472
NiTPP	1	2	-2 083.43964	-0.09575	-2 083.44019	-0.09601	0.59829	0.63468	0.63562	0.52779	3.617E-04	-3 421.25855
NiTPP	1	4	-2 083.44365	-0.09688	-2 083.44365	-0.09688	0.59657	0.63354	0.63448	0.52424	3.698E-04	-3 421.25446
NiTPP	1	6	-2 083.37487	-0.09674	-2 083.37487	-0.09674	0.59353	0.63110	0.63205	0.51942	3.777E-04	-3 421.18591
PbTPP	0	1	-1 916.10900	-0.09523	-1 916.10900	-0.09523	0.59401	0.63189	0.63284	0.52036	3.773E-04	-2 106.01488
PbTPP	0	3	-1 916.05911	-0.09531	-1 916.05911	-0.09531	0.59135	0.62945	0.63039	0.51681	3.810E-04	-2 105.96446
PbTPP	0	5	-1 915.99141	-0.09524	-1 915.99141	-0.09524	0.58935	0.62784	0.62878	0.51350	3.867E-04	-2 105.89664
PbTPP	1	2	-1 915.88856	-0.09566	-1 915.88856	-0.09566	0.59436	0.63208	0.63303	0.52103	3.757E-04	-2 105.79201
PbTPP	1	4	-1 915.82196	-0.09554	-1 915.82196	-0.09554	0.59128	0.62960	0.63054	0.51608	3.839E-04	-2 105.72562
PbTPP	1	6	-1 915.72849	-0.09553	-1 915.72849	-0.09553	0.58789	0.62673	0.62767	0.51141	3.899E-04	-2 105.63119
PdTPP	0	1	-2 040.64438	-0.09747	-2 040.64439	-0.09746	0.59772	0.63455	0.63549	0.52555	3.687E-04	-2 041.06686
PdTPP	0	3	-2 040.57988	-0.09777	-2 040.57988	-0.09777	0.59367	0.63091	0.63185	0.52069	3.728E-04	-2 041.00176
PdTPP	0	5	-2 040.50833	-0.09769	-2 040.50833	-0.09769	0.59183	0.62951	0.63045	0.51721	3.798E-04	-2 040.93008
PdTPP	1	2	-2 040.41130	-0.09799	-2 040.41130	-0.09799	0.59729	0.63401	0.63495	0.52581	3.661E-04	-2 040.83136
PdTPP	1	4	-2 040.33999	-0.09787	-2 040.33999	-0.09787	0.59390	0.63128	0.63222	0.52034	3.752E-04	-2 040.76031
PdTPP	1	6	-2 040.25065	-0.09784	-2 040.25065	-0.09784	0.59018	0.62820	0.62914	0.51441	3.848E-04	-2 040.67086
O=Ti(IV)TPP	0	1	-2 046.39667	-0.09842	-2 046.39667	-0.09842	0.60002	0.63820	0.63914	0.52649	3.779E-04	-2 837.95494
O=Ti(IV)TPP	0	3	-2 046.33174	-0.09851	-2 046.33174	-0.09851	0.59769	0.63593	0.63688	0.52476	3.760E-04	-2 837.88910
O=Ti(IV)TPP	0	5	-2 046.26486	-0.09842	-2 046.26486	-0.09842	0.59498	0.63363	0.63458	0.52091	3.812E-04	-2 837.82207
O=Ti(IV)TPP	1	2	-2 046.16114	-0.09905	-2 046.16114	-0.09905	0.60001	0.63800	0.63895	0.52740	3.741E-04	-2 837.71709
O=Ti(IV)TPP	1	4	-2 046.09419	-0.09915	-2 046.09419	-0.09915	0.59736	0.63577	0.63671	0.52353	3.796E-04	-2 837.65019
O=Ti(IV)TPP	1	6	-2 045.99968	-0.09882	-2 045.99968	-0.09882	0.59342	0.63241	0.63335	0.51885	3.840E-04	-2 837.55499
O=V(IV)TPP	0	2	-2 059.73414	-0.09868	-2 059.73414	-0.09868	0.60096	0.63889	0.63984	0.52758	3.765E-04	-2 932.47328
O=V(IV)TPP	0	4	-2 059.66824	-0.09864	-2 059.66824	-0.09864	0.59842	0.63647	0.63741	0.52557	3.751E-04	-2 932.40640
O=V(IV)TPP	0	6	-2 059.60196	-0.09858	-2 059.60196	-0.09858	0.59581	0.63424	0.63518	0.52194	3.798E-04	-2 932.33996
O=V(IV)TPP	1	1	-2 059.48045	-0.09928	-2 059.49865	-0.09915	0.60061	0.63849	0.63943	0.52834	3.726E-04	-2 932.22492
O=V(IV)TPP	1	3	-2 059.49860	-0.09915	-2 059.49860	-0.09915	0.60062	0.63848	0.63943	0.52763	3.750E-04	-2 932.23541
O=V(IV)TPP	1	5	-2 059.42967	-0.09868	-2 059.42967	-0.09868	0.59813	0.63633	0.63727	0.52484	3.771E-04	-2 932.16619
ZnTPP	0	1	-2 139.85144	-0.09632	-2 139.85144	-0.09632	0.59580	0.63318	0.63412	0.52330	3.717E-04	-3 692.54494
ZnTPP	0	3	-2 139.79116	-0.09659	-2 139.79116	-0.09659	0.59238	0.63013	0.63108	0.51896	3.761E-04	-3 692.48438
ZnTPP	0	5	-2 139.72230	-0.09649	-2 139.72230	-0.09649	0.59070	0.62885	0.62980	0.51586	3.821E-04	-3 692.41542
ZnTPP	1	2	-2 139.62203	-0.09681	-2 139.62203	-0.09681	0.59573	0.63301	0.63396	0.52374	3.697E-04	-3 692.31331
ZnTPP	1	4	-2 139.55363	-0.09666	-2 139.55363	-0.09666	0.59274	0.63062	0.63157	0.51876	3.784E-04	-3 692.24521
ZnTPP	1	6	-2 139.45616	-0.09653	-2 139.45616	-0.09653	0.58909	0.62759	0.62853	0.51359	3.855E-04	-3 692.14730
H-AgTPP	-1	2	-2 060.24464	-0.10143	-2 060.24464	-0.10143	0.59705	0.63571	0.63665	0.52317	3.8061E-04	-2 060.66977
H-AgTPP	-1	4	-2 060.21421	-0.10010	-2 060.21421	-0.10010	0.59455	0.63317	0.63411	0.52054	3.8092E-04	-2 060.63944
H-AgTPP	-1	6	-2 060.15799	-0.10025	-2 060.15799	-0.10025	0.59207	0.63101	0.63195	0.51735	3.8438E-04	-2 060.58262
H-AgTPP	0	1	-2 060.23631	-0.10276	-2 060.23631	-0.10276	0.60658	0.64454	0.64549	0.53437	3.7267E-04	-2 060.66032
H-AgTPP	0	3	-2 060.15457	-0.09999	-2 060.15457	-0.09999	0.59816	0.63652	0.63747	0.52441	3.7921E-04	-2 060.57837
H-AgTPP	0	5	-2 060.09518	-0.10032	-2 060.09518	-0.10032	0.59450	0.63325	0.63420	0.52025	3.8218E-04	-2 060.51862
H-AgTPP	1	2	-2 059.93479	-0.10150	-2 059.93479	-0.10150	0.59961	0.63754	0.63849	0.52831	3.6954E-04	-2 060.35574
H-AgTPP	1	4	-2 059.92270	-0.10071	-2 059.92270	-0.10071	0.59783	0.63615	0.63709	0.52478	3.7670E-04	-2 060.34435
H-AgTPP	1	6	-2 059.84890	-0.09990	-2 059.84890	-0.09990	0.59507	0.63382	0.63476	0.52098	3.8164E-04	-2 060.27046
H-AlTPP	0	1	-2 155.79716	-0.09483	-2 155.79716	-0.09483	0.60541	0.64237	0.64332	0.53275	3.7085E-04	-2 156.20592
H-BaTPP	0	2	-1 938.71315	-0.09512	-1 938.71315	-0.09512	0.59386	0.63350	0.63445	0.51778	3.9132E-04	-1 939.12629
H-BaTPP	0	4	-1 938.65872	-0.09871	-1 938.65872	-0.09871	0.59213	0.63183	0.63278	0.51646	3.9012E-04	-1 939.07143
H-BaTPP	0	6	-1 938.58885	-0.09930	-1 938.58885	-0.09930	0.58934	0.62958	0.63053	0.51198	3.9762E-04	-1 939.00181
H-CdTPP	0	2	-2 080.97451	-0.10047	-2 080.97451	-0.10047	0.59819	0.63686	0.63780	0.52411	3.8133E-04	-2 081.40159
H-CdTPP	0	4	-2 080.90522	-0.10044	-2 080.90522	-0.10044	0.59581	0.63483	0.63577	0.52096	3.8508E-04	-2 081.33218
H-CdTPP	0	6	-2 080.82433	-0.10141	-2 080.82433	-0.10141	0.59030	0.62877	0.62971	0.51590	3.8174E-04	-2 081.25062
H-CoTPP	-1	2	-2 059.19784	-0.09802	-2 059.19785	-0.09802	0.60166	0.63904	0.63999	0.52844	3.7413E-04	-3 296.56790
H-CoTPP	-1	4	-2 059.18698	-0.09741	-2 059.18698	-0.09741	0.59783	0.63627	0.63722	0.52365	3.8092E-04	-3 296.54862
H-CoTPP	-1	6	-2 059.15619	-0.09767	-2 059.15619	-0.09767	0.59684	0.63497	0.63591	0.52279	3.7942E-04	-3 296.51974
H-CoTPP	0	1	-2 059.14650	-0.09790	-2 059.14649	-0.09790	0.60617	0.64315	0.64410	0.53273	3.7352E-04	-3 296.51514
H-CoTPP	0	3	-2 059.11335	-0.09774	-2 059.11335	-0.09774	0.60117	0.63933	0.64027	0.52692	3.8018E-04	-3 296.47721
H-CoTPP	0	5	-2 059.09847	-0.09752	-2 059.09847	-0.09752	0.60064	0.63853	0.63947	0.52636	3.7939E-04	-3 296.46037
H-CoTPP	1	2	-2 058.91409	-0.09817	-2 058.91409	-0.09817	0.60555	0.64246	0.64341	0.53383	3.6751E-04	-3 296.28016
H-CoTPP	1	4	-2 058.88427	-0.09840	-2 058.88427	-0.09841	0.60165	0.63934	0.64028	0.52940	3.7192E-04	-3 296.19551
H-CoTPP	1	6	-2 058.86570	-0.09835	-2 058.86570	-0.09835	0.60074	0.63831	0.63926	0.52823	3.7241E-04	-3 296.22495
H-CrTPP	0	2	-2 000.30062	-0.09656	-2 000.30062	-0.09656	0.60317	0.64067	0.64161	0.52988	3.7476E-04	-2 958.18863
H-CrTPP	0	4	-2 000.33865	-0.09653	-2 000.33865	-0.09653	0.60359	0.64088	0.64182	0.53010	3.7470E-04	-2 958.22535
H-CrTPP	0	6	-2 000.27357	-0.09533	-2 000.27357	-0.09533	0.59706	0.63458	0.63552	0.52314	3.7694E-04	-2 958.15983
H-CuTPP	0	1	-2 110.54481	-0.09974	-2 110.55977	-0.10023	0.59981	0.63791	0.63885	0.52722	3.7442E-04	-3 554.15488
H-CuTPP	0	3	-2 110.56414	-0.09975	-2 110.56414	-0.09975	0.59993	0.63801	0.63895	0.52563	3.8009E-04	-3 554.17388
H-CuTPP	0	5	-2 110.50010	-0.10016	-2 110.50010	-0.10016	0.59617	0.63461	0.63555	0.52162	3.8212E-04	-3 554.10955
H-FeTPP	-1	1	-2 037.27142	-0.09894	-2 037.27142	-0.09894	0.60267	0.63972	0.64067	0.53120	3.6716E-04	-3 177.49649
H-FeTPP	-1	3	-2 037.26671	-0.09886	-2 037.26671	-0.09886	0.59903	0.63686	0.63780	0.52513	3.7792E-04	-3 177.48958
H-FeTPP	-1	5	-2 037.25115	-0.09882	-2 037.25116	-0.09881	0.59840	0.63629	0.63723	0.52393	3.8001E-04	-3 177.47269

H-FeTPP	0	2	-2 037.21428	-0.09860	-2 037.21428	-0.09860	0.60420	0.64161	0.64255	0.53023	3.7672E-04	-3 177.43572
H-FeTPP	0	4	-2 037.19377	-0.09851	-2 037.19406	-0.09849	0.60203	0.63972	0.64066	0.52742	3.7982E-04	-3 177.41417
H-FeTPP	0	6	-2 037.20100	-0.09827	-2 037.20100	-0.09826	0.60154	0.63931	0.64025	0.52722	3.7912E-04	-3 177.41697
H-FeTPP	1	1	-2 036.94215	-0.09944	-2 036.98309	-0.09949	0.60447	0.64150	0.64244	0.53375	3.6457E-04	-3 177.19534
H-FeTPP	1	3	-2 036.99075	-0.09930	-2 036.99075	-0.09930	0.60496	0.64212	0.64306	0.53216	3.7195E-04	-3 177.21144
H-FeTPP	1	5	-2 036.97703	-0.09880	-2 036.97703	-0.09880	0.60206	0.63970	0.64065	0.52885	3.7499E-04	-3 177.17054
H-H_2TPP	0	2	-1 914.41101	-0.09436	-1 914.41101	-0.09436	0.62920	0.66613	0.66707	0.55770	3.6685E-04	-1 914.80029
H-MgTPP	0	2	-2 113.36678	-0.09674	-2 113.36678	-0.09674	0.59816	0.63662	0.63756	0.52442	3.7946E-04	-2 113.77110
H-MnTPP	0	1	-2 017.59432	-0.09858	-2 017.63089	-0.09849	0.60323	0.64095	0.64189	0.53100	3.7192E-04	-3 064.66452
H-MnTPP	0	3	-2 017.65149	-0.09849	-2 017.65149	-0.09849	0.60418	0.64139	0.64234	0.53150	3.7177E-04	-3 064.71997
H-MnTPP	0	5	-2 017.65075	-0.09809	-2 017.65075	-0.09809	0.60081	0.63886	0.63981	0.52635	3.8054E-04	-3 064.71572
H-NiTPP	0	2	-2 084.22124	-0.09798	-2 084.22125	-0.09797	0.60262	0.64033	0.64127	0.52918	3.7598E-04	-3 422.03989
H-NiTPP	0	4	-2 084.18246	-0.09947	-2 084.18246	-0.09947	0.60171	0.63987	0.64082	0.52710	3.8139E-04	-3 421.99460
H-NiTPP	0	6	-2 084.11327	-0.09947	-2 084.11327	-0.09947	0.59960	0.63781	0.63875	0.52623	3.7740E-04	-3 421.92786
H-NiTPP	1	1	-2 083.99221	-0.09851	-2 083.99221	-0.09851	0.60578	0.64281	0.64376	0.53512	3.6439E-04	-3 421.81381
H-NiTPP	1	3	-2 083.99089	-0.09872	-2 083.99089	-0.09872	0.60271	0.64013	0.64108	0.53088	3.6962E-04	-3 421.80656
H-NiTPP	1	5	-2 083.94992	-0.10045	-2 083.94992	-0.10045	0.60088	0.63861	0.63956	0.52831	3.7313E-04	-3 421.76265
H-PbTPP	0	2	-1 916.57969	-0.09519	-1 916.57969	-0.09519	0.60001	0.63804	0.63898	0.52657	3.7701E-04	-2 106.47791
H-PbTPP	0	4	-1 916.51688	-0.09502	-1 916.51688	-0.09502	0.59814	0.63653	0.63747	0.52324	3.8312E-04	-2 106.41401
H-PbTPP	0	6	-1 916.47043	-0.09915	-1 916.47044	-0.09915	0.59003	0.63059	0.63154	0.51160	4.0226E-04	-2 106.37449
H-PdTPP	0	2	-2 041.15873	-0.10037	-2 041.15873	-0.10037	0.60143	0.63904	0.63999	0.52802	3.7553E-04	-2 041.58109
H-PdTPP	0	4	-2 041.08935	-0.10025	-2 041.08935	-0.10025	0.59896	0.63655	0.63749	0.52689	3.7094E-04	-2 041.51064
H-PdTPP	0	6	-2 041.02369	-0.10048	-2 041.02369	-0.10048	0.59586	0.63428	0.63523	0.52031	3.8543E-04	-2 041.44531
H-[O=Ti(IV)TPP]	0	2	-2 046.89844	-0.10270	-2 046.89842	-0.10270	0.60069	0.64110	0.64204	0.52301	3.9923E-04	-2 838.45711
H-[O=Ti(IV)TPP]	0	4	-2 046.83106	-0.10306	-2 046.83106	-0.10306	0.59858	0.63885	0.63979	0.52224	3.9425E-04	-2 838.38908
H-[O=Ti(IV)TPP]	0	6	-2 046.73700	-0.10280	-2 046.73700	-0.10280	0.59617	0.63668	0.63763	0.51952	3.9615E-04	-2 838.29493
H-[O=V(IV)TPP]	0	1	-2 060.21090	-0.10175	-2 060.23681	-0.10302	0.60279	0.64206	0.64301	0.52920	3.8171E-04	-2 932.95214
H-[O=V(IV)TPP]	0	3	-2 060.23630	-0.10303	-2 060.23630	-0.10303	0.60248	0.64196	0.64290	0.52762	3.8664E-04	-2 932.97560
H-[O=V(IV)TPP]	0	5	-2 060.16899	-0.10340	-2 060.16899	-0.10340	0.59940	0.63855	0.63950	0.52521	3.8334E-04	-2 932.90759
H-ZnTPP	0	2	-2 140.36519	-0.09883	-2 140.36519	-0.09883	0.59973	0.63794	0.63889	0.52627	3.7773E-04	-3 693.05788
H-ZnTPP	0	4	-2 140.29271	-0.10109	-2 140.29271	-0.10109	0.59354	0.63318	0.63413	0.51748	3.9124E-04	-3 692.98655
H-ZnTPP	0	6	-2 140.22011	-0.09950	-2 140.22011	-0.09950	0.59228	0.63178	0.63273	0.51693	3.8839E-04	-3 692.91313
H_2	0	1	-1.17897	0.00000	-1.17897	0.00000	0.01012	0.01248	0.01343	-0.00137	4.9619E-05	-1.17957

3 Catalysis

3.1 CVs before and after catalysis

Figure S16 shows CVs in 0.1 M $TBAPF_6$/DCM before and after catalysis for H_2TPP, FeTPP, CoTPP, NiTPP, CuTPP and ZnTPP. The small reductive wave around -1.4 V vs. Fc/Fc^+ visible for some porphyrins is caused by trace amounts of oxygen, and the small reversible peak at 0 V vs. Fc/Fc^+ is the ferrocene reaction.

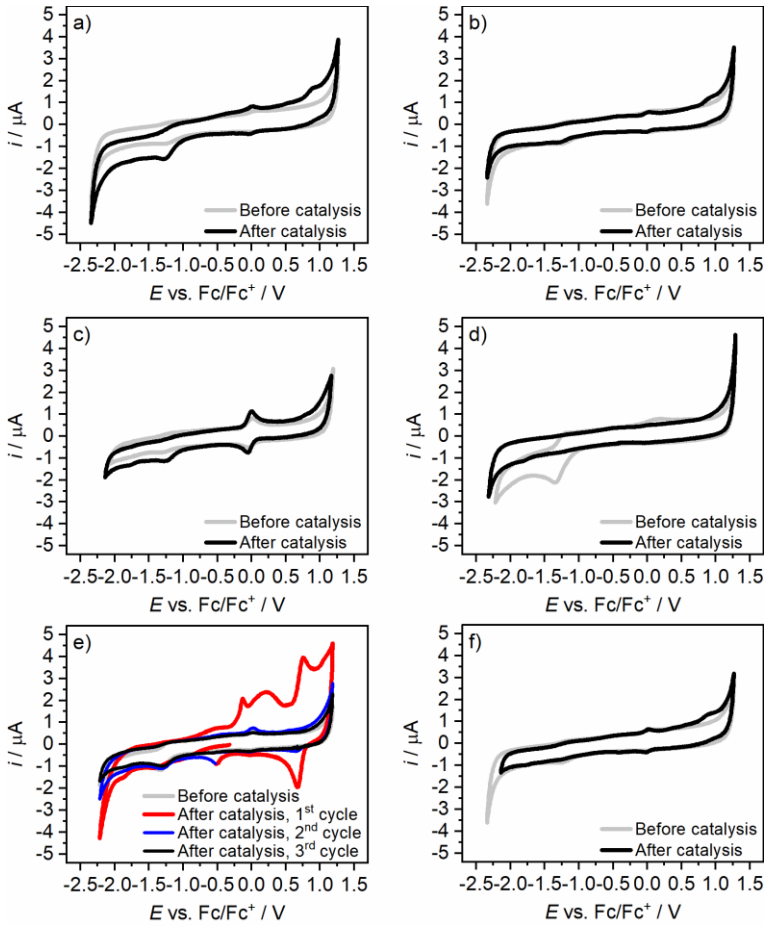


Figure S16. CV before and after catalysis for a) H_2TPP, b) FeTPP, c) CoTPP, d) NiTPP, e) CuTPP and f) ZnTPP.

3.2 UV/vis absorbance of BzOH

Figure S17 shows the UV/vis absorbance spectrum of BzOH in DCM, normalized by the maximum absorbance.

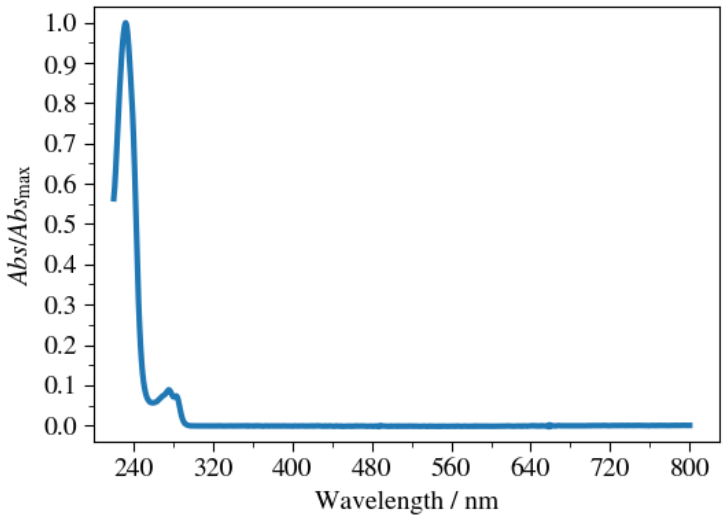


Figure S17. UV/vis absorbance spectrum of BzOH in DCM.

3.3 EPEP kinetics

For the EPEP mechanism, a rate equation can be obtained from the following:

$$MTPP + e^- \underset{k_{1b}}{\overset{k_{1f}}{\rightleftharpoons}} MTPP^-$$

$$MTPP^- + H^+ \underset{k_{2b}}{\overset{k_{2f}}{\rightleftharpoons}} H\text{-}MTPP$$

$$H\text{-}MTPP + e^- \underset{k_{3b}}{\overset{k_{3f}}{\rightleftharpoons}} H\text{-}MTPP^-$$

$$H\text{-}MTPP^- + H^+ \xrightarrow{k_{cat}} MTPP + H_2$$

$$\frac{d[\mathrm{MTPP^-}]}{dt} = k_{1\mathrm{f}}[\mathrm{MTPP}] - k_{1\mathrm{b}}[\mathrm{MTPP^-}] - k_{2\mathrm{f}}[\mathrm{MTPP^-}][\mathrm{H^+}] \quad (1)$$

$$\frac{d[\text{H-MTPP}]}{dt} = k_{2\mathrm{f}}[\mathrm{MTPP^-}][\mathrm{H^+}] + k_{3\mathrm{b}}[\text{H-MTPP}^-] - k_{2\mathrm{b}}[\text{H-MTPP}] - k_{3\mathrm{f}}[\text{H-MTPP}] \quad (2)$$

$$\frac{d[\text{H-MTPP}^-]}{dt} = k_{3\mathrm{f}}[\text{H-MTPP}] - k_{3\mathrm{b}}[\text{H-MTPP}^-] - k_{\mathrm{cat}}[\text{H-MTPP}^-][\mathrm{H^+}] \quad (3)$$

Assuming steady state, such that all the above derivatives are 0, gives

$$\begin{aligned}\frac{d[\mathrm{H_2}]}{dt} &= k_{\mathrm{cat}}[\text{H-MTPP}^-][\mathrm{H^+}] \\ &= \frac{k_{1\mathrm{f}}k_{2\mathrm{f}}k_{3\mathrm{f}}k_{\mathrm{cat}}[\mathrm{H^+}]^2[\mathrm{MTPP}]}{k_{1\mathrm{b}}k_{2\mathrm{b}}k_{3\mathrm{b}} + k_{1\mathrm{b}}k_{2\mathrm{b}}k_{\mathrm{cat}}[\mathrm{H^+}] + k_{1\mathrm{b}}k_{3\mathrm{b}}k_{\mathrm{cat}}[\mathrm{H^+}] + k_{2\mathrm{f}}k_{3\mathrm{f}}k_{\mathrm{cat}}[\mathrm{H^+}]^2}\end{aligned} \quad (4)$$

3.4 Reaction rates and reaction orders at reference potentials

Figure S18-S23 show the reaction rates and reaction order fits at $E = -2$ V and $E = -2.15$ V vs. Fc/Fc^+. Only these two potentials were used in the fit, as the concentration of active catalyst at the electrode surface C_{cat} can be approximated as the bulk concentration of the catalytic compound C^*_{cat} at high driving forces. Then, the reaction rates and linear reaction order fits can be used to obtain an approximate value of the global catalytic rate constant through

$$\text{Rate} \propto \mathrm{k_{cat}} C_{\mathrm{cat}}[\mathrm{H^+}] \approx k_{\mathrm{cat}} C^*_{\mathrm{cat}}[\mathrm{H^+}] \propto slope \cdot [\mathrm{H^+}] \quad (5)$$

Figure S24 shows LSVs of H_2TPP, FeTPP, CoTPP, NiTPP, CuTPP and ZnTPP at varying concentrations in the presence of approximately 44 mM BzOH, and Figure S25 shows linear fits of the peak current as a function porphyrin concentration. Figure 26 and Figure 27 show the relation between the reaction rates and the binding energies, and between the corresponding rate constants and the binding energies, respectively. Figure 28 shows the relation between the reaction rates and the half-wave potential of the first reduction reaction involved in catalysis.

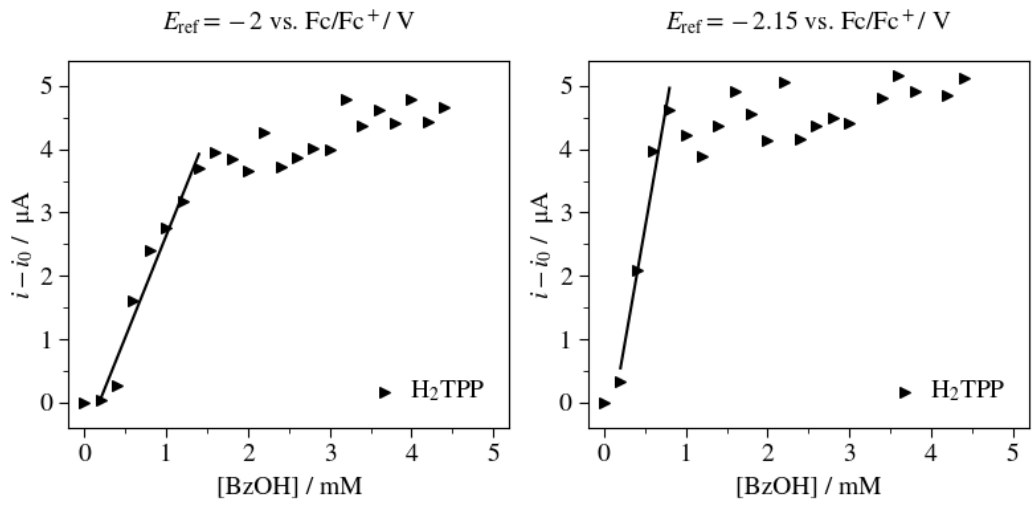


Figure S18. Reaction order fits for H_2TPP at $E_{ref} = -2$ and -2.15 V vs. Fc/Fc$^+$.

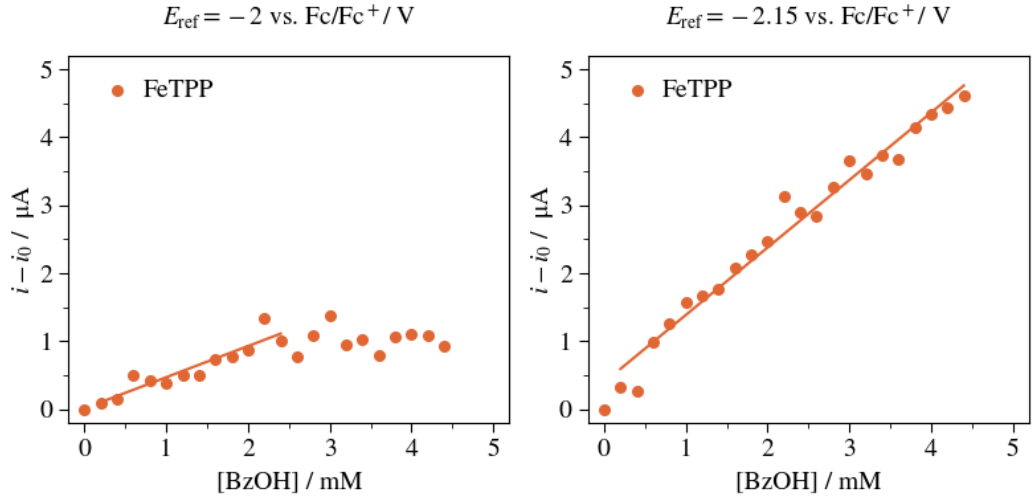


Figure S19. Reaction order fits for FeTPP at $E_{ref} = -2$ and -2.15 V vs. Fc/Fc$^+$.

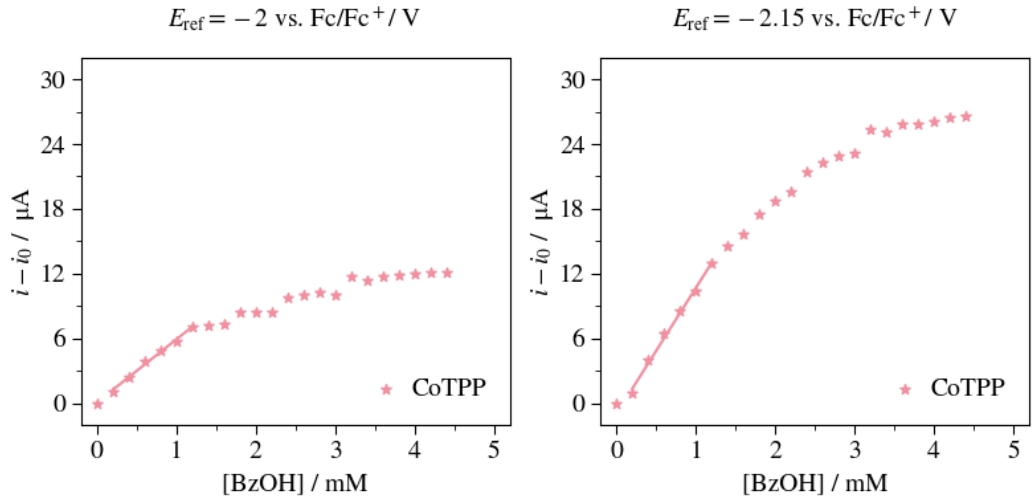


Figure S20. Reaction order fits for CoTPP at $E_{ref} = -2$ and -2.15 V vs. Fc/Fc+.

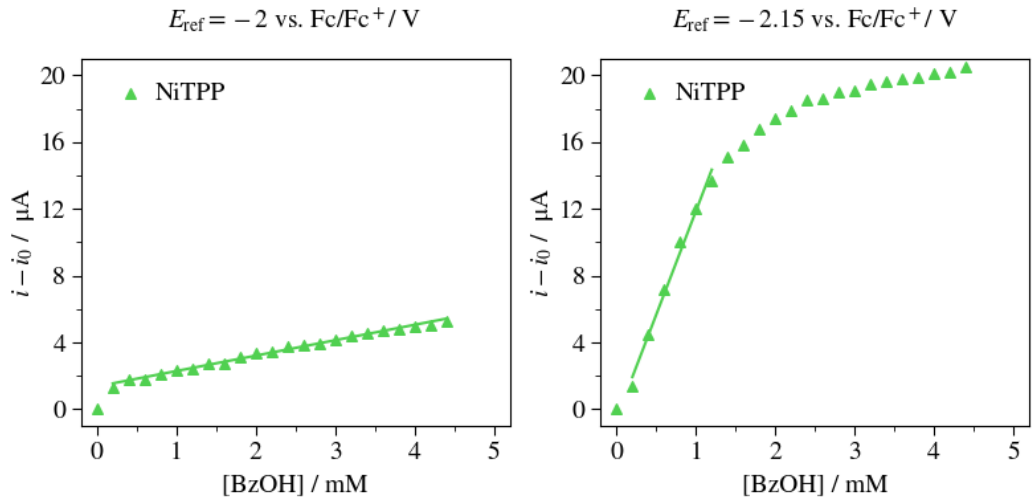


Figure S21. Reaction order fits for NiTPP at $E_{\mathrm{ref}} = -2$ and -2.15 V vs. Fc/Fc$^+$.

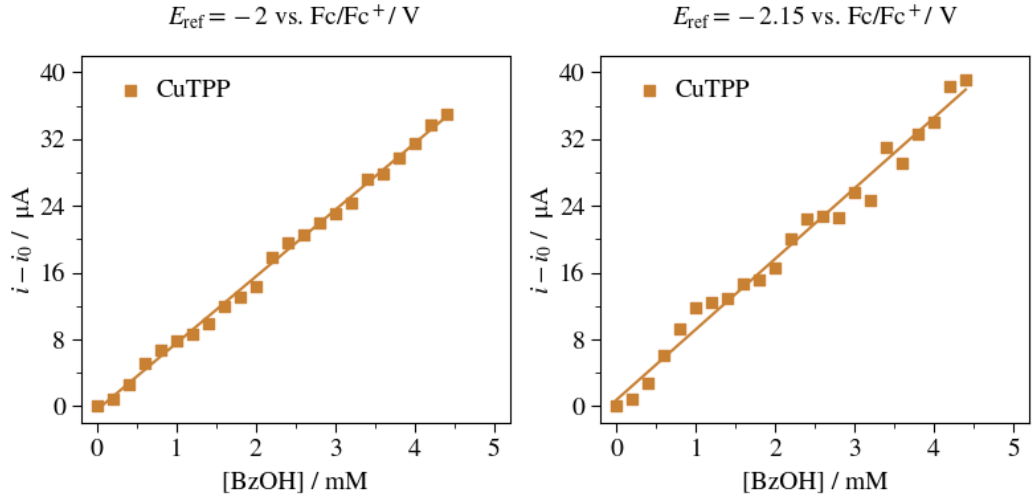


Figure S22. Reaction order fits for CuTPP at $E_{\mathrm{ref}} = -2$ and -2.15 V vs. Fc/Fc$^+$.

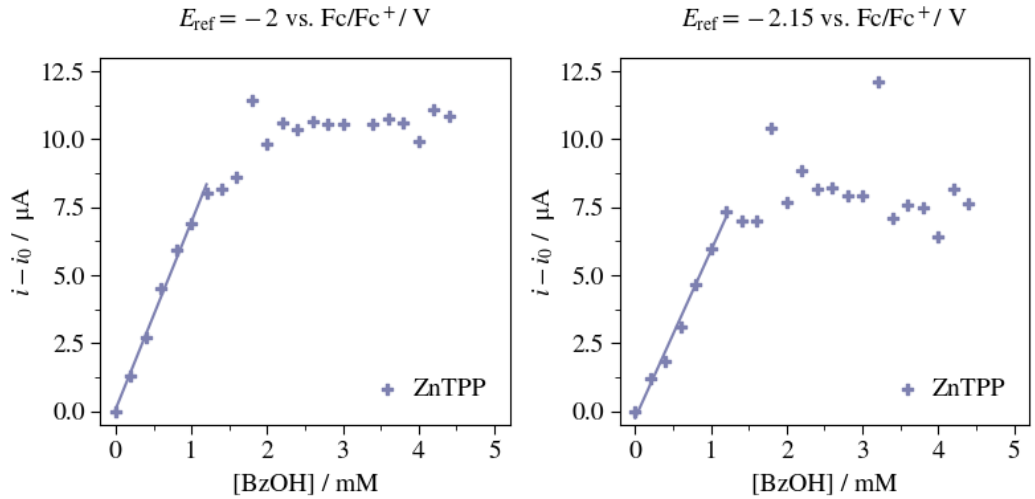


Figure S23. Reaction order fits for ZnTPP at $E_{\mathrm{ref}} = -2$ and -2.15 V vs. Fc/Fc+.

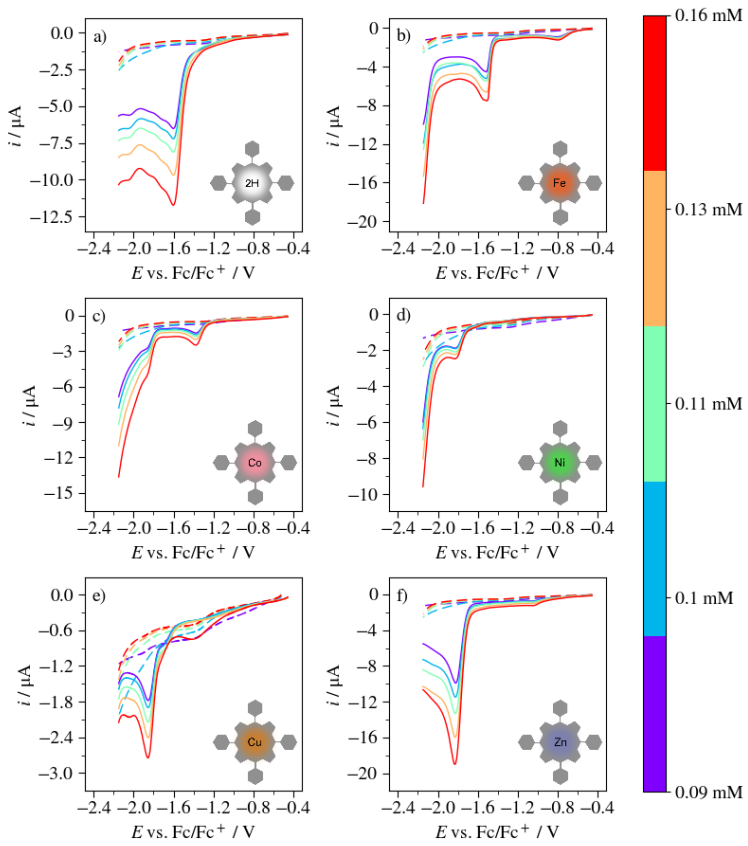


Figure S24. LSVs of H_2TPP, FeTPP, CoTPP, NiTPP, CuTPP and ZnTPP in the presence of approximately 44 mM BzOH. (0.1 M $TBAPF_6$/DCM, 0.1 V/s). The colorbar indicates [MTPP].

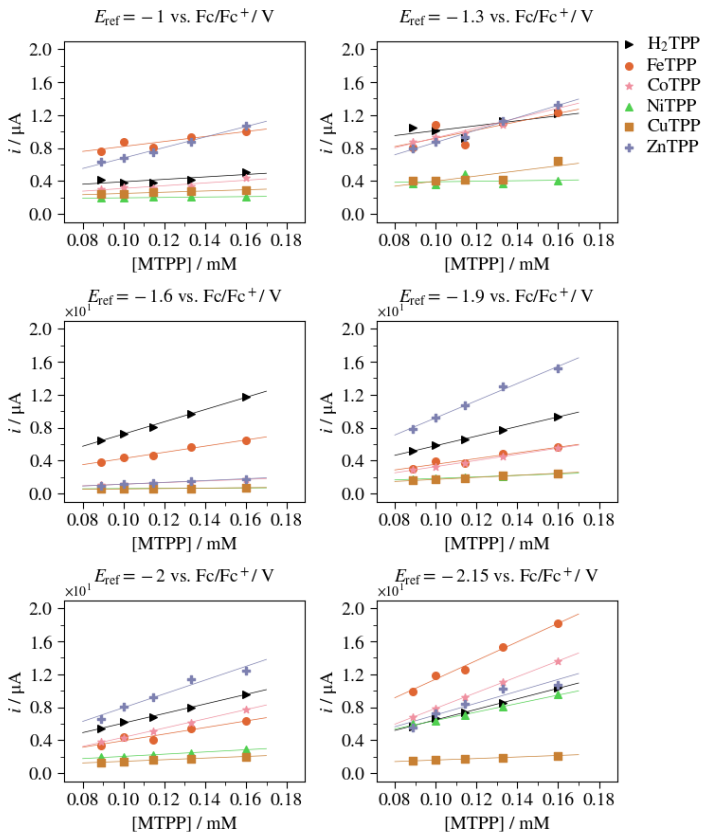


Figure S25. Current as a function of porphyrin concentration at various E_{ref}, including linear fits showing a first order reaction.

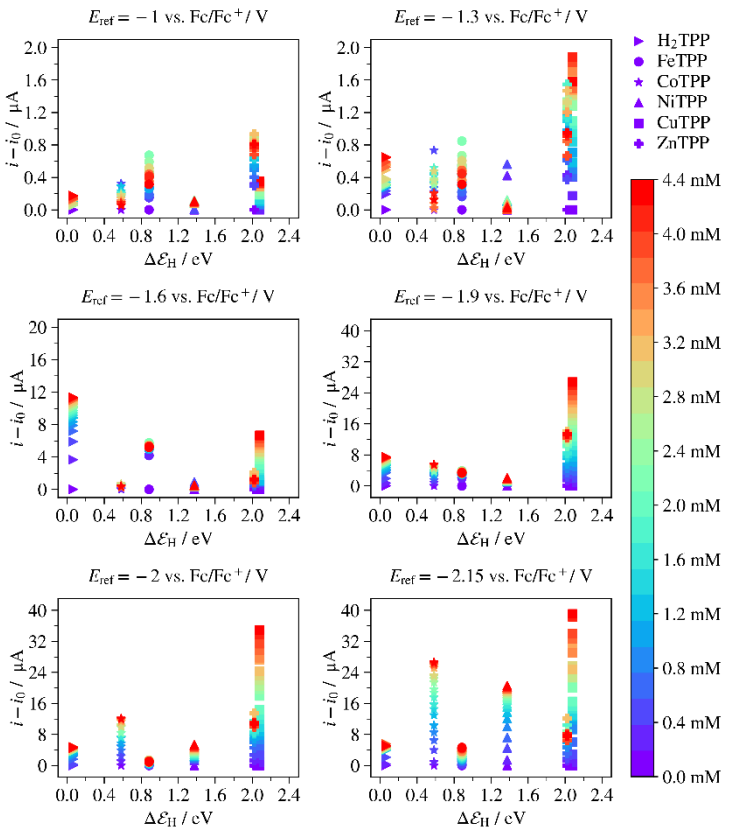


Figure S26. Reaction rates at various E_{ref} as a function of binding energy. The colorbar indicates [BzOH].

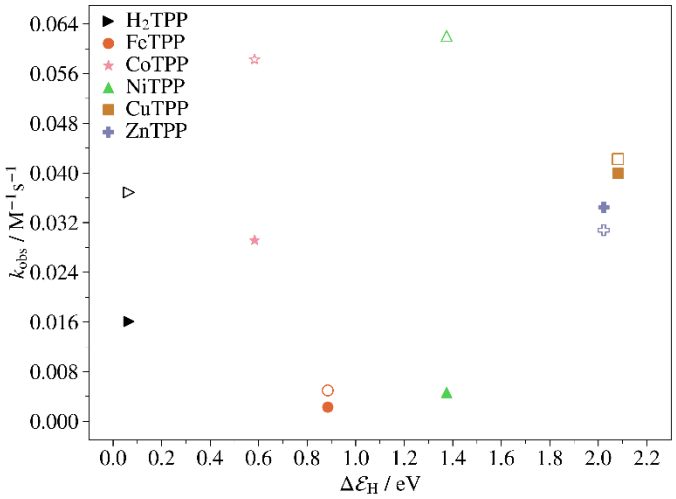


Figure S27. Rate constant k_{obs} calculated from the linear portion of the reaction rates marked in Figure S18-S23. Filled markers represent values obtained using $E_{ref} = -2$ vs. Fc/Fc$^+$ and empty markers represent values obtained using $E_{ref} = -2.15$ V vs. Fc/Fc$^+$.

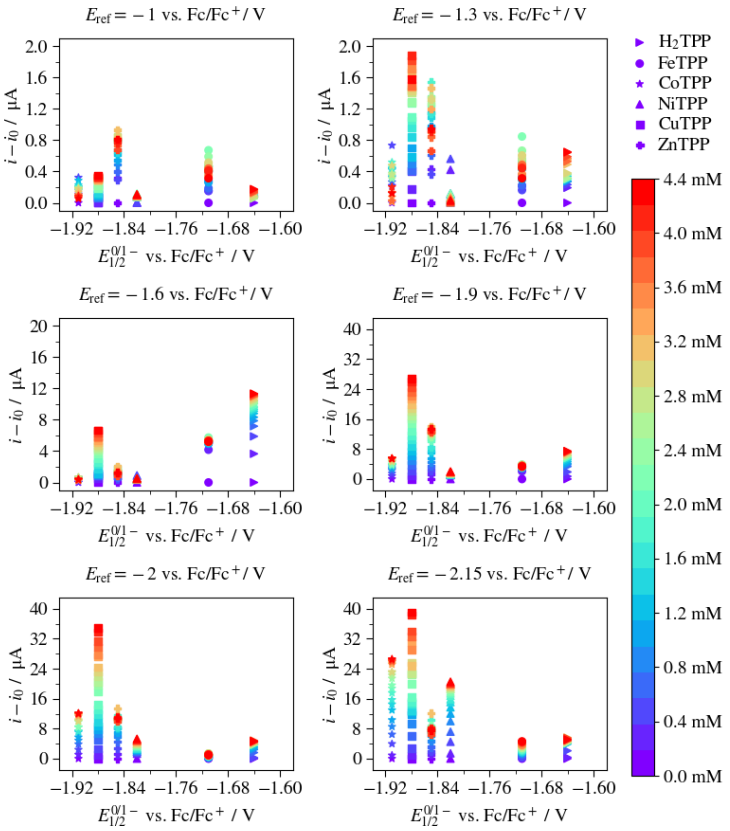


Figure 28. Reactions rates obtained at various E_{ref}. vs. the half-wave potential of the first reduction reaction involved in catalysis (L^0/L^{1-} for all porphyrins except FeTPP, for which M(II)/M(I) was used). The colorbar indicates [BzOH].

3.5 Reaction rates from the Tafel equation

Figure S29-S34 illustrate the process of obtaining reaction rates through linear fits of the Tafel equations for H_2TPP, FeTPP, CoTPP, NiTPP, CuTPP, ZnTPP. Figure S35 shows a summary of these rate equations, and Table S7 shows the charge transfer coefficients α obtained from the linear fits. Figure 36 and Figure 37 show the relation between the reaction rates and the binding energies, and between the corresponding rate constants and the binding energies, respectively.

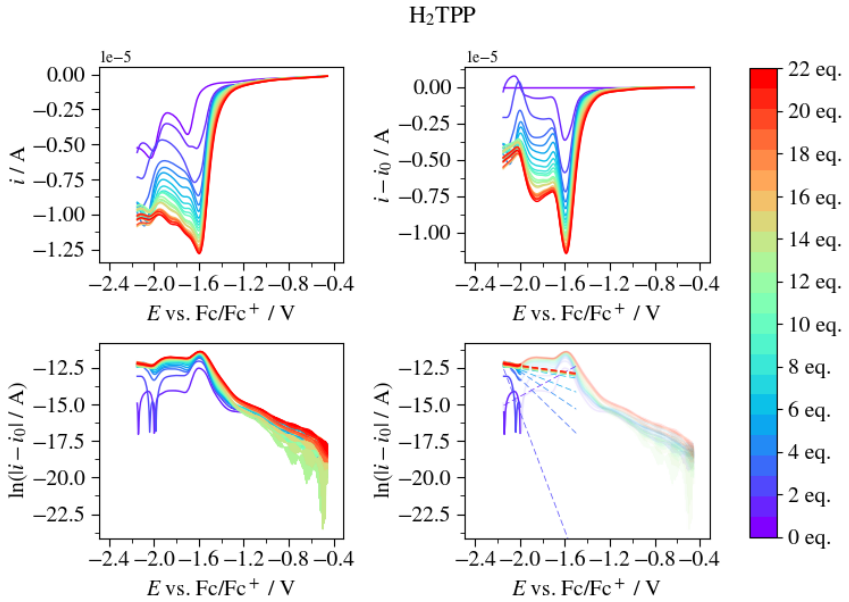


Figure S29. LSV, LSV subtracted by pure porphyrin response, logarithm of current difference, and logarithm of current difference with Tafel equation linear fit for H_2TPP. The colorbar indicates the amount of BzOH.

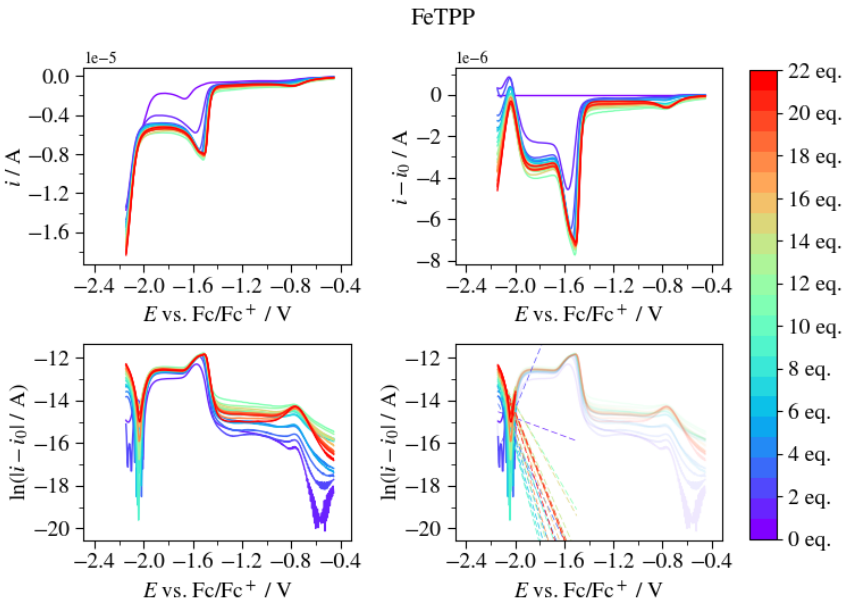


Figure S30. LSV, LSV subtracted by non-catalytic porphyrin response, logarithm of current difference, and logarithm of current difference with Tafel equation linear fit for FeTPP. The colorbar indicates the amount of BzOH.

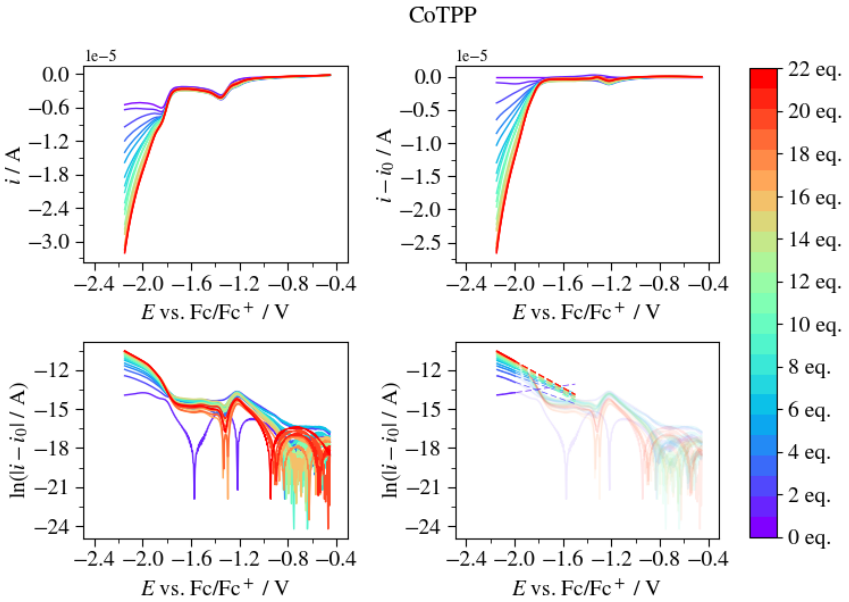


Figure S31. LSV, LSV subtracted by non-catalytic porphyrin response, logarithm of current difference, and logarithm of current difference with Tafel equation linear fit for CoTPP. The colorbar indicates the amount of BzOH.

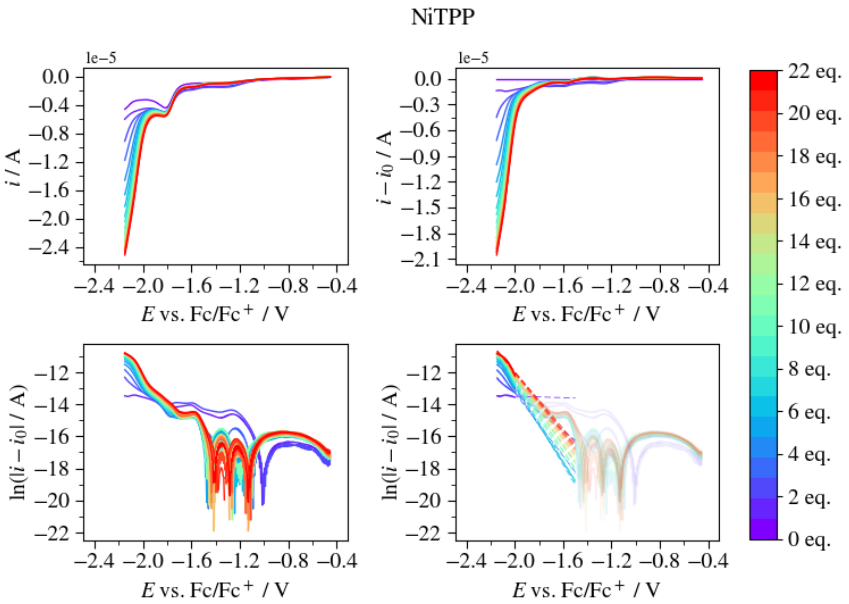


Figure S32. LSV, LSV subtracted by non-catalytic porphyrin response, logarithm of current difference, and logarithm of current difference with Tafel equation linear fit for NiTPP. The colorbar indicates the amount of BzOH.

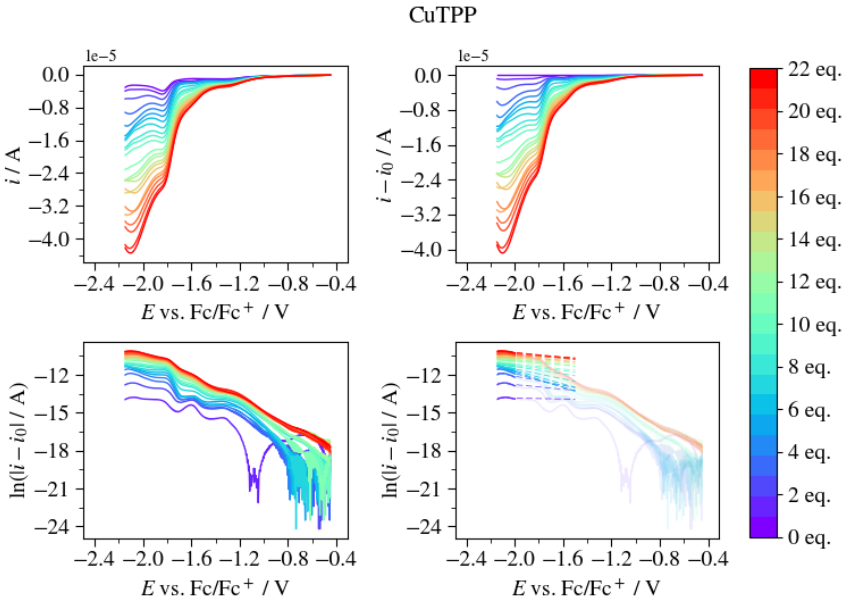


Figure S33. LSV, LSV subtracted by non-catalytic porphyrin response, logarithm of current difference, and logarithm of current difference with Tafel equation linear fit for CuTPP. The colorbar indicates the amount of BzOH.

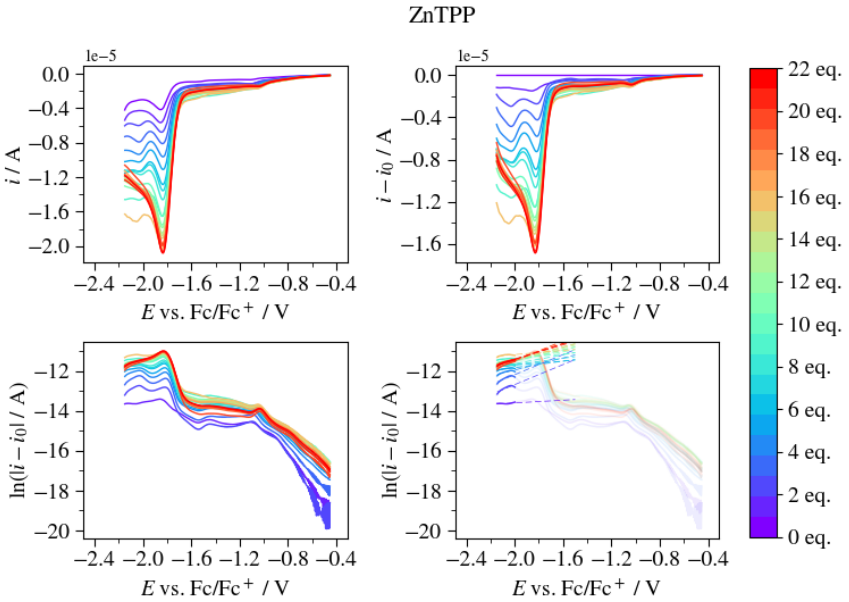


Figure S34. LSV, LSV subtracted by non-catalytic porphyrin response, logarithm of current difference, and logarithm of current difference with Tafel equation linear fit for ZnTPP. The colorbar indicates the amount of BzOH.

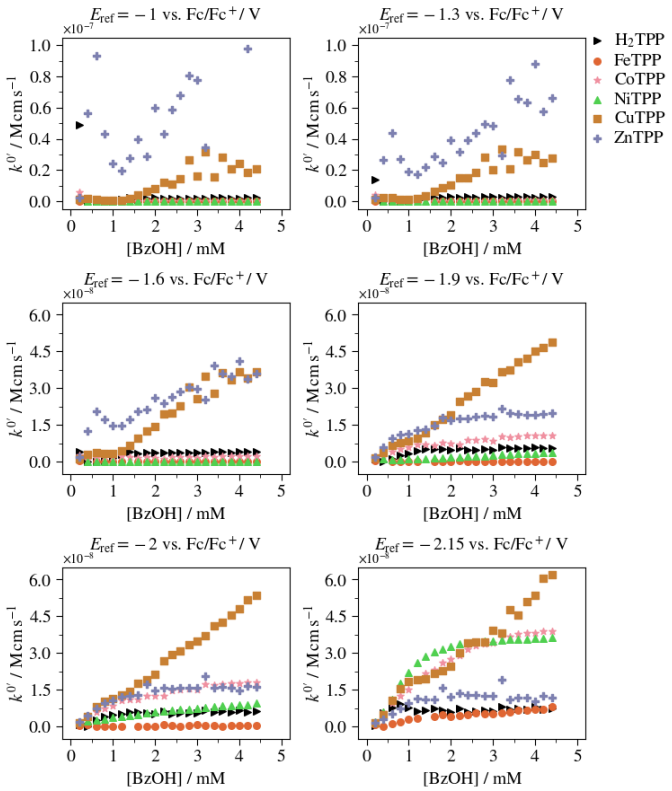


Figure S35. Reaction rates calculated from linear fits of the Tafel equation between -2 and -2.15 V vs. Fc/Fc$^+$ using various E_{ref}.

Table S7. Charge transfer coefficient α calculated from linear fits of the Tafel equation.

Eq.	[BzOH]	H$_2$TPP	FeTPP	CoTPP	NiTPP	CuTPP	ZnTPP
1	**0.20**	0.1067	0.0368	0.0338	0.0059	0.0043	0.0087
2	**0.40**	0.5214	0.3793	0.0869	0.1520	0.0235	0.0648
3	**0.60**	0.1912	0.3715	0.0835	0.2546	0.0466	0.0648
4	**0.80**	0.1322	0.4283	0.0922	0.2936	0.0717	0.0388
5	**1.00**	0.0786	0.5151	0.0979	0.3063	0.0797	0.0210
6	**1.20**	0.0346	0.5847	0.1011	0.3190	0.0686	0.0125
7	**1.40**	0.0242		0.1162	0.3137	0.0506	0.0207
8	**1.60**	0.0351	0.6420	0.1285	0.3149	0.0379	0.0289
9	**1.80**	0.0278	0.6754	0.1247	0.3002	0.0278	0.0136
10	**2.00**	0.0226	0.4894	0.1351	0.2914	0.0250	0.0357
11	**2.20**	0.0318	0.2852	0.1428	0.2890	0.0205	0.0255
12	**2.40**	0.0236	0.4017	0.1314	0.2778	0.0249	0.0340
13	**2.60**	0.0260	0.5807	0.1340	0.2757	0.0191	0.0371
14	**2.80**	0.0259	0.3777	0.1344	0.2723	0.0058	0.0417
15	**3.00**	0.0248	0.3013	0.1413	0.2621	0.0198	0.0410
16	**3.20**	0.0344	0.4521	0.1301	0.2561	0.0040	0.0133
17	**3.40**	0.0247	0.4202	0.1339	0.2494	0.0253	0.0586
18	**3.60**	0.0277	0.5594	0.1328	0.2448	0.0105	0.0517
19	**3.80**	0.0276	0.4202	0.1315	0.2431	0.0200	0.0511
20	**4.00**	0.0328	0.4136	0.1317	0.2383	0.0176	0.0653
21	**4.20**	0.0250	0.4236	0.1314	0.2361	0.0266	0.0458
22	**4.40**	0.0256	0.4999	0.1320	0.2297	0.0242	0.0518

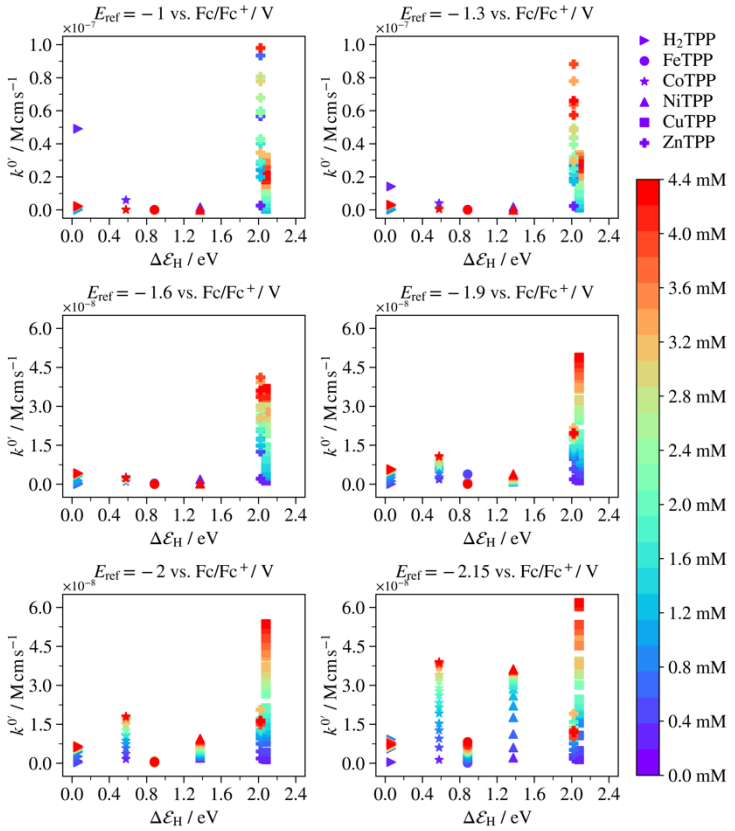


Figure S36. Reaction rates obtained from linear fits of the Tafel equation at various E_{ref}, as a function of binding energy. The colorbar indicates [BzOH].

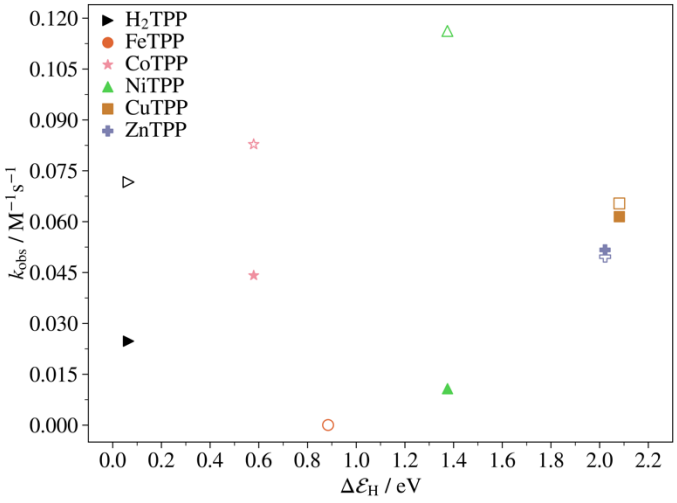


Figure S37. Rate constant k_{obs} calculated from the linear portion of the reaction rates obtained using the Tafel equation. Filled markers represent values obtained using $E_{\mathrm{ref}} = -2$ vs. Fc/Fc$^+$ and empty markers represent values obtained using $E_{\mathrm{ref}} = -2.15$ V vs. Fc/Fc$^+$.

3.6 Reaction rates and reaction orders from current plateau analysis

Figure S38-S40 show observed rate constants (which may be more accurately described as reaction rates, as they are obtained from the increase in catalytic current with acid concentration) obtained from current plateau analysis. The plots include linear or second order fits that should reflect the reaction orders according to the current plateau model.

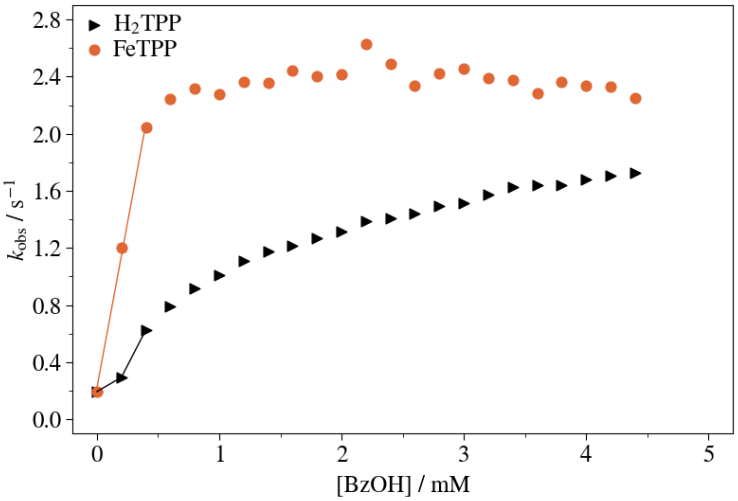


Figure S38. Observed rate constants and reaction order fits obtained from current plateau analysis for H_2TPP and FeTPP.

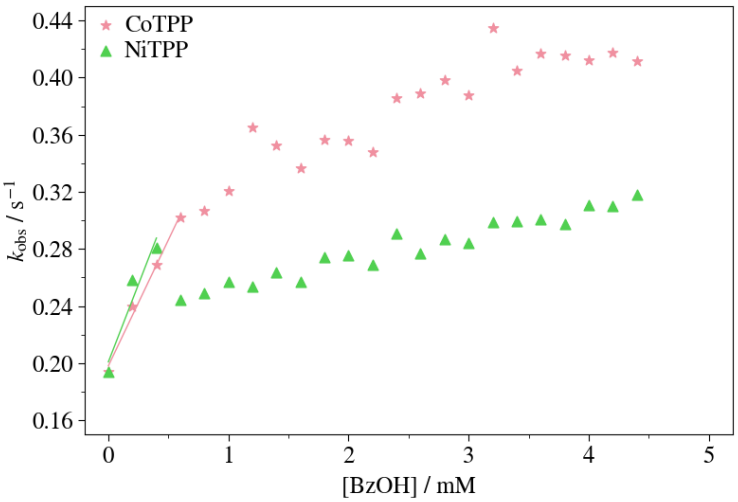


Figure S39. Observed rate constants and reaction order fits obtained from current plateau analysis for CoTPP and NiTPP.

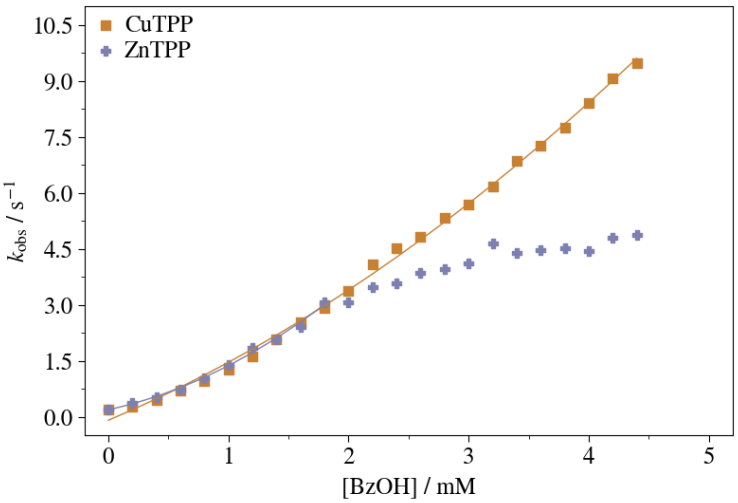


Figure S40. Observed rate constants and reaction order fits obtained from current plateau analysis for CuTPP and ZnTPP.

3.7 Reaction rates from FOWA analysis

Table S8-S10 show the cathodic peak potentials $E_{p,c}$, the inflection point potentials E_{infl}, and the potential at $i = i_{cat}/2$ where i_{cat} is the peak current of the catalytic wave, respectively. These values were used as approximations of $E_{cat/2}$, in addition to the half-wave potential of the first porphyrin reduction involved in catalysis (L^0/L^{1-} for all porphyrins except FeTPP, for which the half-wave potential of the M(II)/M(I) transition was used).

Table S8. Cathodic peak potentials of the catalytic wave in the presence of increasing amounts of benzoic acid. Bold numbers mark the amount of acid at which the peak potential stabilizes after a notable change with acid concentration. The average is taken from the bold number until the last value. The last line shows the difference between the first value (0 equivalents) and the average (> 0 equivalents).

Equivalents	H_2TPP	FeTPP	CoTPP	NiTPP	CuTPP	ZnTPP
0	-1.7003	-1.6652	-1.8464	-1.8162	-1.8380	-1.8568
1	-1.6197	-1.5794	**-1.8519**	**-1.8162**	**-1.8380**	**-1.8565**
2	-1.6395	-1.5541	-1.8565	-1.8162	-1.8432	-1.8467
3	-1.6041	-1.5388		-1.8263	-1.8432	-1.8364
4	**-1.5992**	-1.5294		-1.8263	-1.8380	-1.8364
5	-1.5992	**-1.5236**		-1.8205	-1.8380	-1.8315
6	-1.5992	-1.5236		-1.8263	-1.8329	-1.8373
7	-1.5992	-1.5190		-1.8205	-1.8380	-1.8370
8	-1.5992	-1.5190		-1.8263	-1.8432	-1.8370
9	-1.6041	-1.5190		-1.8263	-1.8432	-1.8415
10	-1.5992	-1.5190		-1.8205	-1.8380	-1.8412
11	-1.6041	-1.5135		-1.8205		-1.8415
12	-1.5992	-1.5135		-1.8205		-1.8367
13	-1.5992	-1.5135		-1.8205		-1.8412
14	-1.5992	-1.5135		-1.8263		-1.8415
15	-1.5992	-1.5135		-1.8263		-1.8419
16	-1.5992	-1.5135		-1.8263		-1.8415
17	-1.5992	-1.5086		-1.8263		-1.8364
18	-1.5992	-1.5086		-1.8306		-1.8370
19	-1.5992	-1.5086		-1.8263		-1.8364
20	-1.5992	-1.5086		-1.8263		-1.8364
21	-1.5940	-1.5086		-1.8263		-1.8364
22	-1.5992	-1.5086		-1.8306		-1.8367
Average:	-1.6024	-1.5142	-1.8542	-1.8242	-1.8396	-1.8393
Difference:	0.0978	0.1510	-0.0078	-0.0080	-0.0016	0.0175

Table S9. Inflection point potentials of the catalytic wave in the presence of increasing amounts of benzoic acid. Bold numbers mark the amount of acid at which the peak potential stabilizes after a notable change with acid concentration. The average is taken from the bold number until the last value. The last line shows the difference between the first value (0 equivalents) and the average (> 0 equivalents).

Equivalents	H_2TPP	FeTPP	CoTPP	NiTPP	CuTPP	ZnTPP
0	-1.6447	-1.6139	-1.7958	-1.7555	-1.7874	-1.7964
1	-1.5235	-1.5138	**-1.7912**	**-1.7604**	**-1.7822**	**-1.8010**
2	-1.5336	-1.4933	-1.7955	-1.7558	-1.7825	-1.7759
3	-1.5391	-1.4936	-1.7958	-1.7552	-1.7718	-1.7704
4	**-1.5434**	-1.4881	-1.8010	-1.7555	-1.7672	-1.7656
5	-1.5437	**-1.4885**	-1.8016	-1.7607	-1.7624	-1.7707
6	-1.5388	-1.4881	-1.8003	-1.7555	-1.7630	-1.7710
7	-1.5437	-1.4827	-1.8010	-1.7561	-1.7627	-1.7710
8	-1.5440	-1.4885	-1.8016	-1.7610	-1.7672	-1.7704
9	-1.5391	-1.4833	-1.7958	-1.7607	-1.7624	-1.7707
10	-1.5388	-1.4833	-1.8061	-1.7604	-1.7675	-1.7750
11	-1.5385	-1.4830	-1.8016	-1.7555	-1.7624	-1.7759
12	-1.5339	-1.4833	-1.8065	-1.7506	-1.7672	-1.7759
13	-1.5336	-1.4827	-1.7967	-1.7610	-1.7627	-1.7698
14	-1.5333	-1.4836	-1.8013	-1.7552	-1.7620	-1.7762
15	-1.5336	-1.4833	-1.8013	-1.7549	-1.7624	-1.7710
16	-1.5339	-1.4781	-1.8016	-1.7558	-1.7675	-1.7759
17	-1.5339	-1.4836	-1.8013	-1.7558	-1.7675	-1.7710
18	-1.5339	-1.4781	-1.8061	-1.7604	-1.7675	-1.7659
19	-1.5336	-1.4784	-1.8061	-1.7558	-1.7566	-1.7707
20	-1.5239	-1.4787	-1.8058	-1.7555	-1.7620	-1.7704
21	-1.5287	-1.4784	-1.8013	-1.7555	-1.7669	-1.7656
22	-1.5239	-1.4784	-1.8010	-1.7610	-1.7672	-1.7659
Average:	-1.5356	-1.4824	-1.8009	-1.7572	-1.7664	-1.7726
Difference:	0.1091	0.1315	-0.0051	-0.0017	0.0210	0.0238

Table S10. Potentials at $i = i_{\mathrm{cat}}/2$ of catalytic wave in the presence of increasing amounts of benzoic acid. Bold numbers mark the amount of acid at which the peak potential stabilizes after a notable change with acid concentration. The average is taken from the bold number until the last value. The last line shows the difference between the first value (0 equivalents) and the average (> 0 equivalents).

Equivalents	H_2TPP	FeTPP	CoTPP	NiTPP	CuTPP	ZnTPP
0	-1.6298	-1.5638	-1.7659	-1.7353	-1.7572	-1.7707
1	-1.5190	-1.5031	**-1.7662**	**-1.7198**	**-1.7572**	**-1.7656**
2	-1.5232	-1.4933	-1.7607	-1.7158	-1.7523	-1.7607
3	-1.5235	-1.4885	-1.7711	-1.7302	-1.7520	-1.7555
4	**-1.5239**	-1.4827	-1.7711	-1.7308	-1.7523	-1.7552
5	-1.5232	**-1.4833**	-1.7711	-1.7308	-1.7523	-1.7555
6	-1.5235	-1.4781	-1.7711	-1.7305	-1.7523	-1.7558
7	-1.5239	-1.4781	-1.7707	-1.7302	-1.7474	-1.7561
8	-1.5235	-1.4781	-1.7707	-1.7305	-1.7419	-1.7558
9	-1.5232	-1.4781	-1.7759	-1.7308	-1.7419	-1.7555
10	-1.5187	-1.4784	-1.7762	-1.7308	-1.7422	-1.7561
11	-1.5187	-1.4735	-1.7704	-1.7305	-1.7367	-1.7604
12	-1.5184	-1.4732	-1.7756	-1.7302	-1.7324	-1.7610
13	-1.5190	-1.4735	-1.7762	-1.7311	-1.7321	-1.7610
14	-1.5141	-1.4732	-1.7756	-1.7305	-1.7270	-1.7561
15	-1.5132	-1.4729	-1.7759	-1.7311	-1.7266	-1.7558
16	-1.5080	-1.4732	-1.7805	-1.7305	-1.7266	-1.7610
17	-1.5086	-1.4735	-1.7808	-1.7302	-1.7270	-1.7552
18	-1.5043	-1.4729	-1.7805	-1.7305	-1.7270	-1.7558
19	-1.5034	-1.4729	-1.7805	-1.7299	-1.7221	-1.7561
20	-1.4982	-1.4680	-1.7808	-1.7305	-1.7215	-1.7555
21	-1.4982	-1.4680	-1.7808	-1.7302	-1.7221	-1.7558
22	-1.4933	-1.4683	-1.7808	-1.7302	-1.7215	-1.7555
Average:	-1.5135	-1.4743	-1.7747	-1.7293	-1.7370	-1.7573
Difference:	0.1162	0.0896	-0.0088	0.0060	0.0202	0.0134

3.7.1 FOWA using $E_{cat/2} \approx E_{1/2}^{0/1-}$

Figure S41 shows the FOWA plots of H_2TPP, FeTPP, CoTPP, NiTPP, CuTPP and ZnTPP using $\mathrm{E}_{\mathrm{cat}/2} \approx \mathrm{E}_{1/2}^{0/1-}$. Figure S42 shows linear fits at each concentration in the interval $x = [0.002, 0.05]$, and Figure S43 shows the corresponding observed rate constants. Figure S44 and Figure S45 show linear fits and observed rate constants, respectively, obtained from the interval $x = [0.1, 0.2]$. Figure S46 and

Figure S47 show the observed rate constants obtained from the two intervals as functions of the binding energy of H.

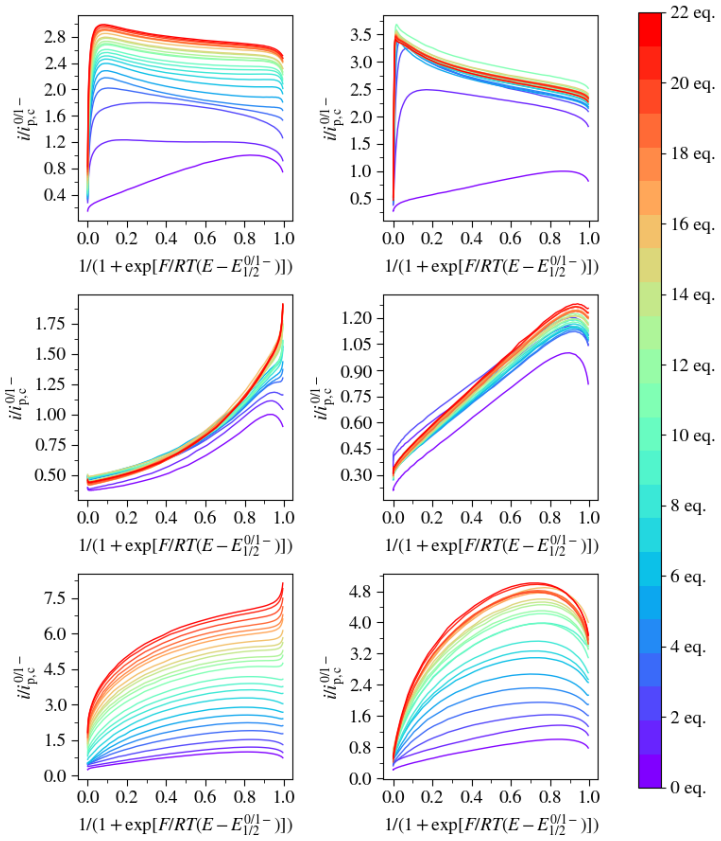


Figure S41. FOWA plot using $E_{cat/2} \approx E_{1/2}^{0/1-}$ (the L^0/L^{1-} transition was used for all porphyrins except FeTPP, for which the M(II)/M(I) transition was used). From upper left to lower right: H_2TPP, FeTPP, CoTPP, NiTPP, CuTPP, ZnTPP.

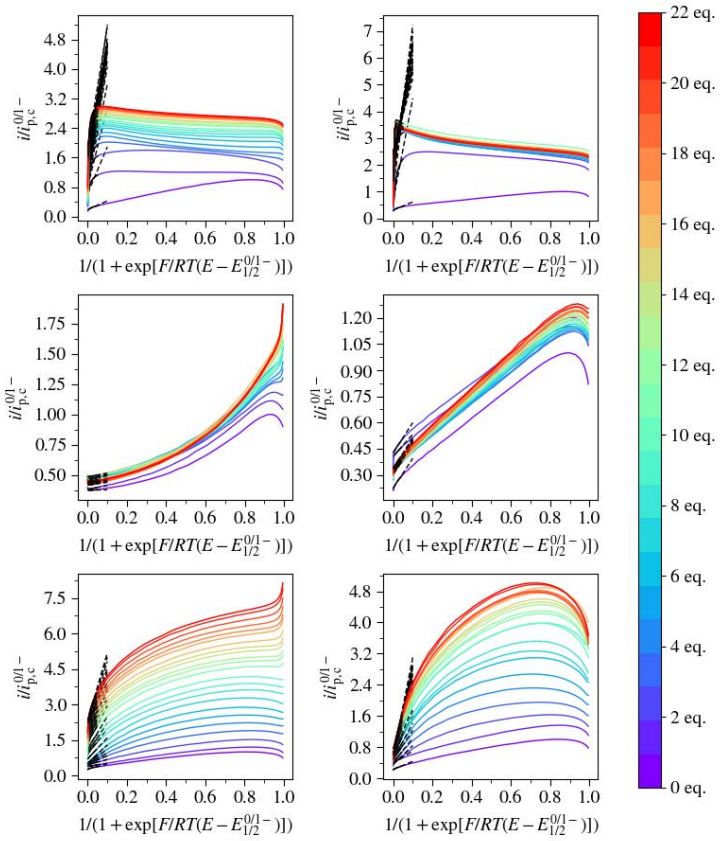


Figure S42. Linear fit of the FOWA plot in Figure S41 between $x = 0.002$ and $x = 0.05$. From upper left to lower right: H_2TPP, FeTPP, CoTPP, NiTPP, CuTPP, ZnTPP

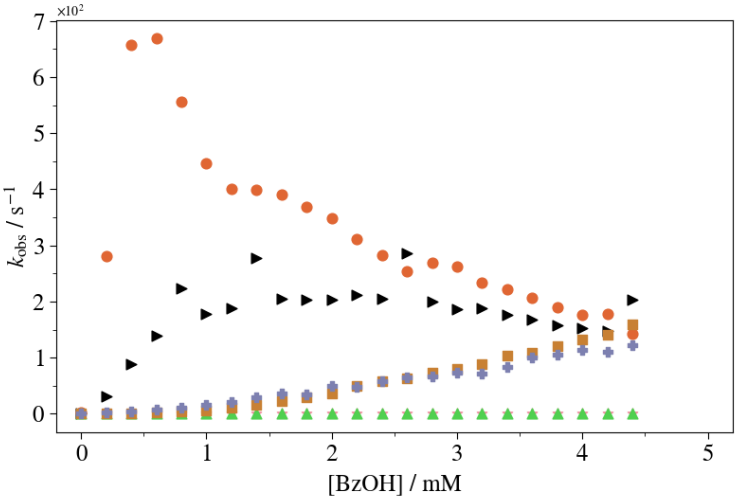


Figure S43. k_{obs} obtained from the fit in Figure S42.

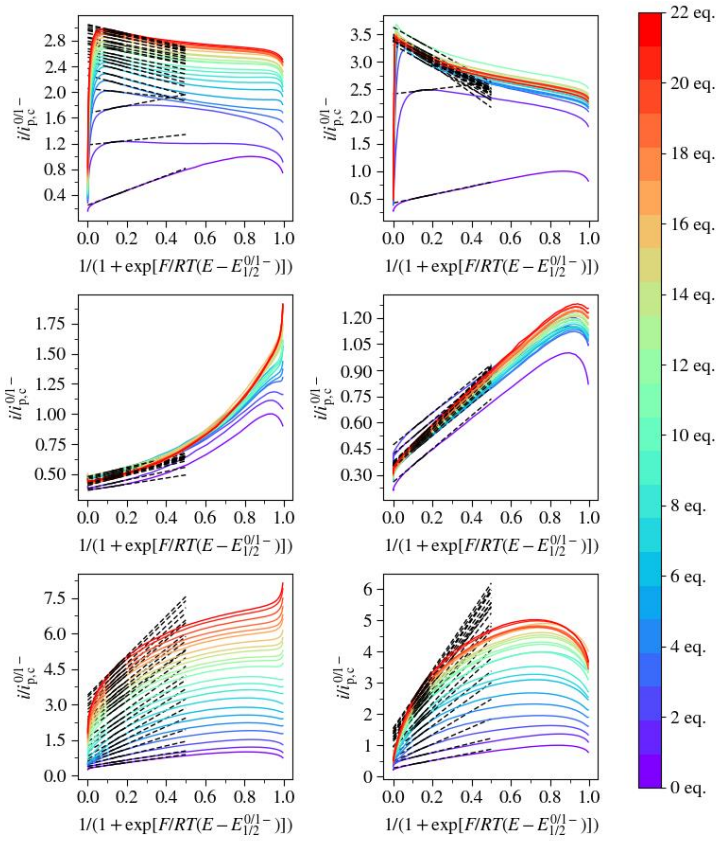


Figure S44. Linear fit of the FOWA plot in Figure S41 between $x = 0.1$ and $x = 0.2$. From upper left to lower right: H_2TPP, FeTPP, CoTPP, NiTPP, CuTPP, ZnTPP.

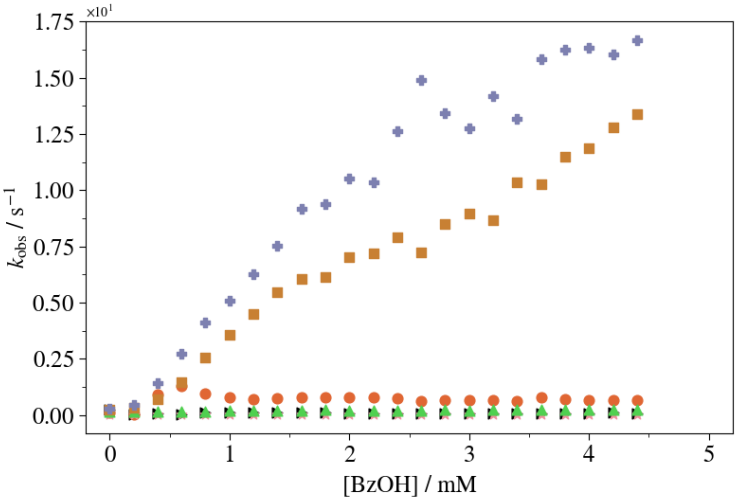


Figure S45. k_{obs} obtained from the fit in Figure S44.

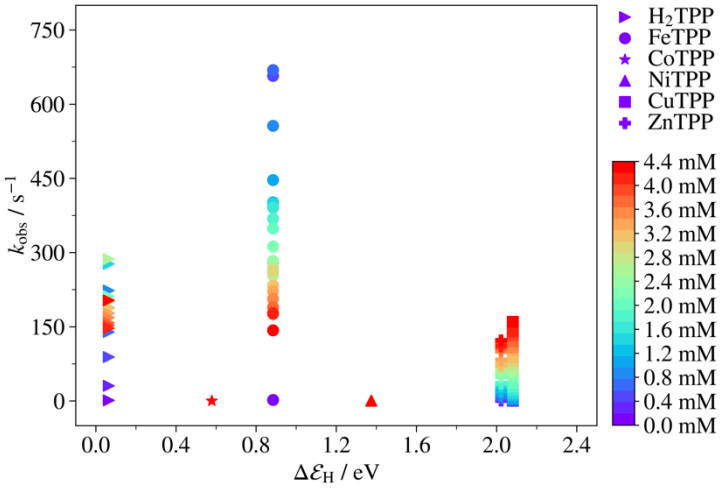


Figure S46. k_{obs} obtained from the interval $x = [0.002, 0.05]$ using $E_{\mathrm{cat/2}} \approx E_{1/2}^{0/1-}$.

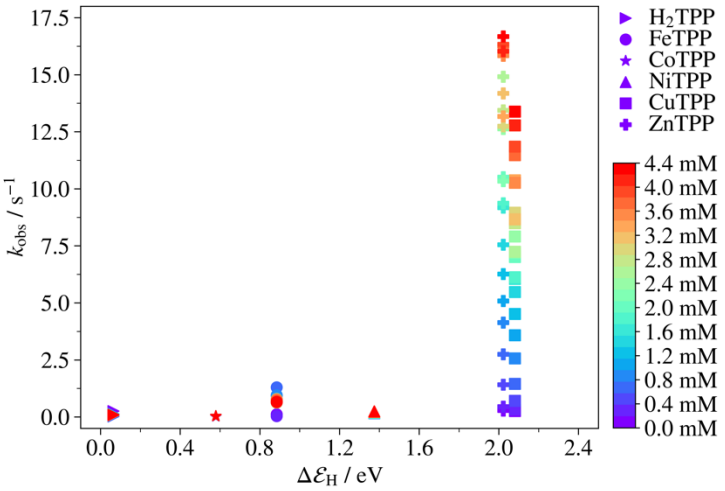


Figure S47. k_{obs} obtained from the interval $x = [0.1, 0.2]$ using $E_{\mathrm{cat/2}} \approx E_{1/2}^{0/1-}$.

3.7.2 FOWA using $E_{cat/2} \approx E_{infl}$

Figure S48 shows the FOWA plots of H_2TPP, FeTPP, CoTPP, NiTPP, CuTPP and ZnTPP using $E_{\mathrm{cat/2}} \approx E_{\mathrm{infl}}$. Figure S49 shows linear fits at each concentration in the interval $x = [0.002, 0.05]$, and Figure S50 the corresponding observed rate constants. Figure S51 and Figure S52 show linear fits and observed rate constants, respectively, obtained from the interval $x = [0.1, 0.2]$. Figure S53 and Figure S54 show linear fits and observed rate constants, respectively, from the interval $x =$

$[E_{\mathrm{infl}} + 0.1, E_{\mathrm{infl}} + 0.2]$. Figure S55-S57 show the observed rate constants obtained from the three intervals as functions of the binding energy of H.

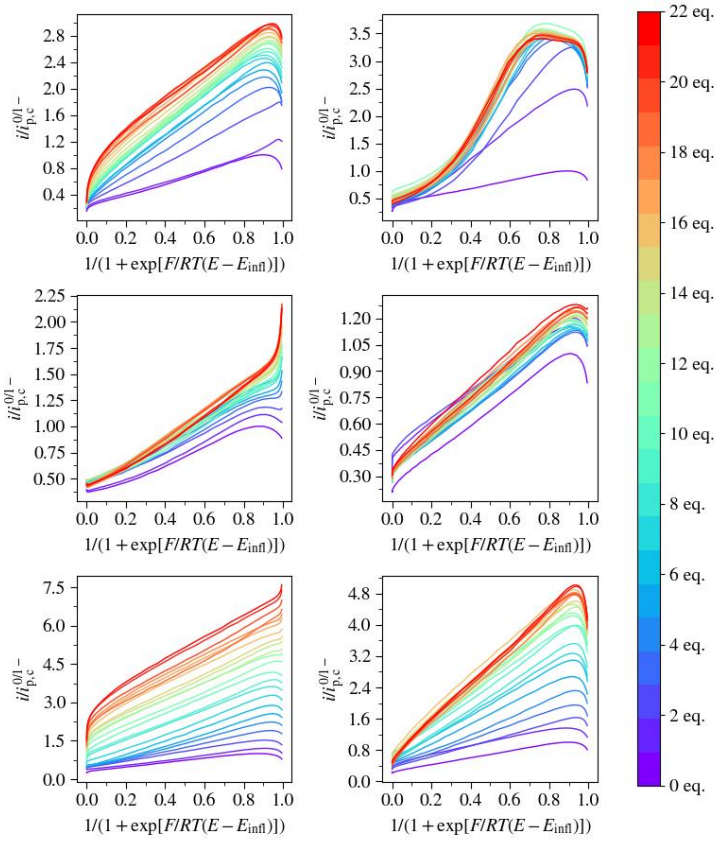


Figure S48. FOWA plot using $E_{\mathrm{cat/2}} \approx E_{\mathrm{infl}}$ (the L^0/L^{1-} transition was used for all porphyrins except FeTPP, for which the M(II)/M(I) transition was used). From upper left to lower right: H_2TPP, FeTPP, CoTPP, NiTPP, CuTPP, ZnTPP.

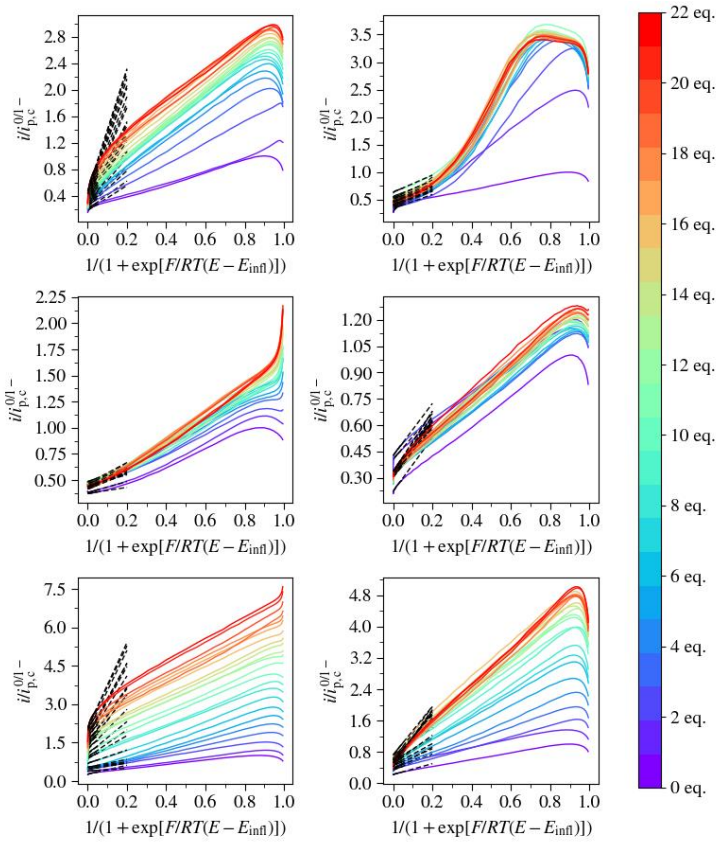


Figure S49. Linear fit of the FOWA plot in Figure S48 between $x = 0.002$ and $x = 0.05$. From upper left to lower right: H_2TPP, FeTPP, CoTPP, NiTPP, CuTPP, ZnTPP.

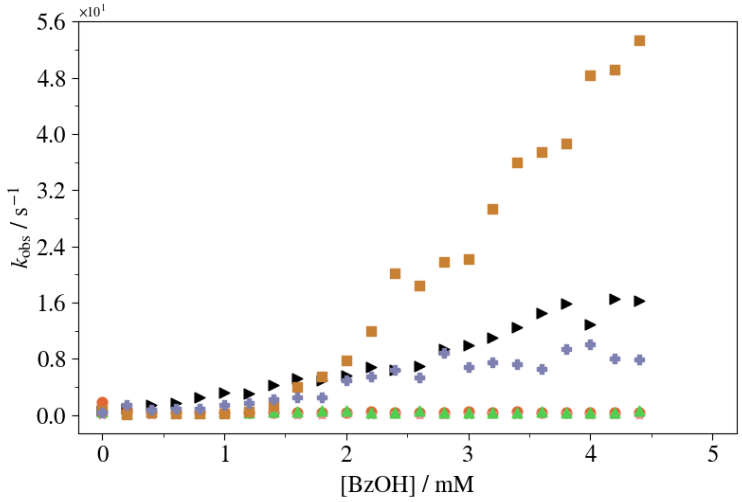


Figure S50. k_{obs} obtained from the fit in Figure S49.

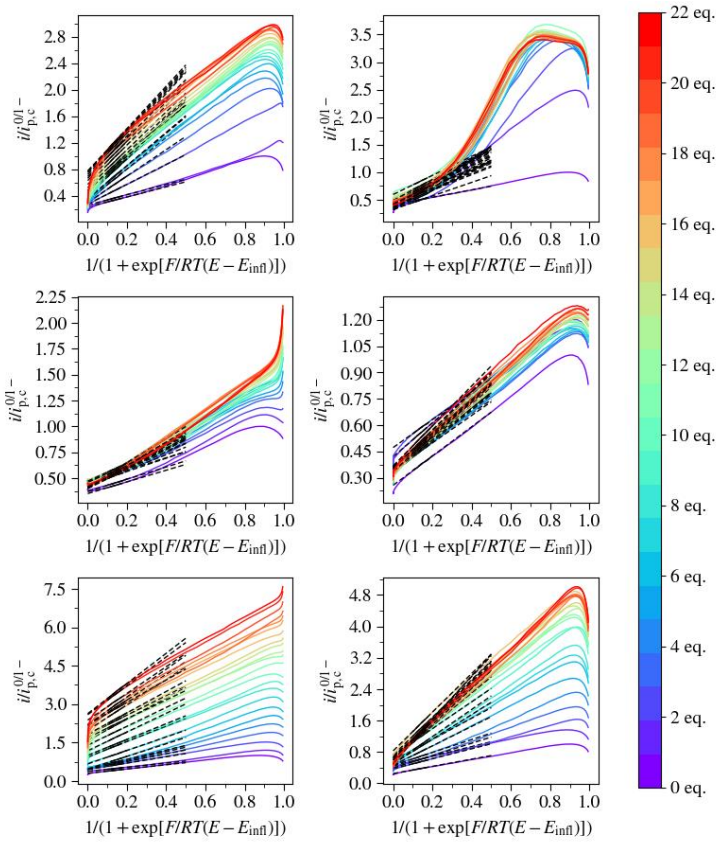


Figure S51. Linear fit of the FOWA plot in Figure S48 between $x = 0.1$ and $x = 0.2$. From upper left to lower right: H_2TPP, FeTPP, CoTPP, NiTPP, CuTPP, ZnTPP.

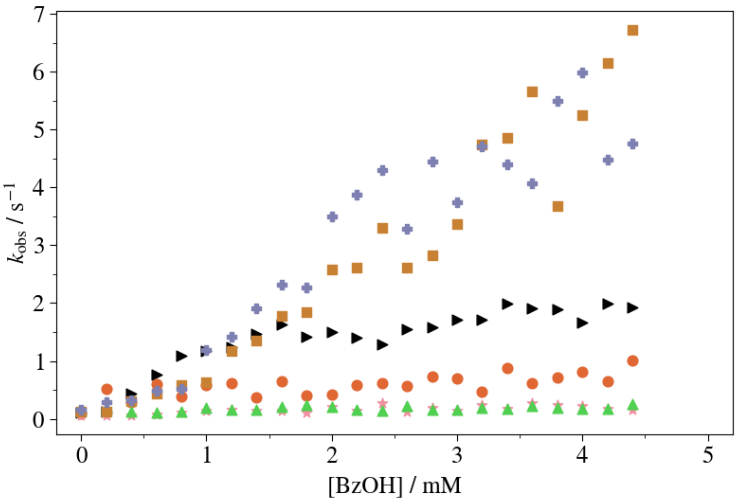


Figure S52. k_{obs} obtained from the fit in Figure S51.

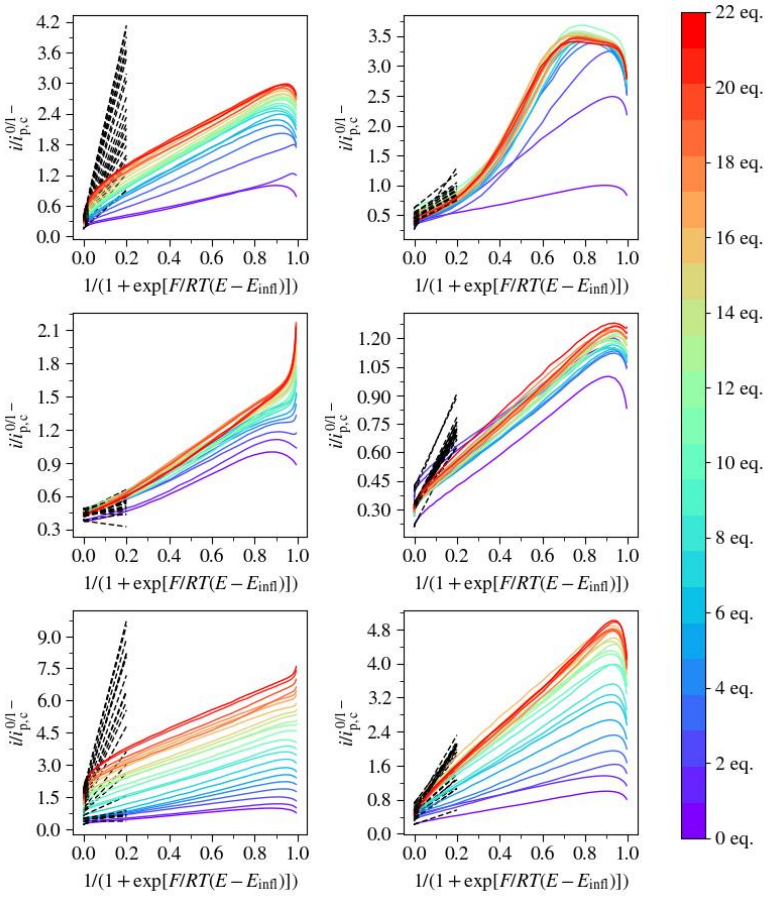


Figure S53. Linear fit of the FOWA plot in Figure S48 between $x = E_{\mathrm{infl}} + 0.1$ and $x = E_{\mathrm{infl}} + 0.2$. From upper left to lower right: H_2TPP, FeTPP, CoTPP, NiTPP, CuTPP, ZnTPP.

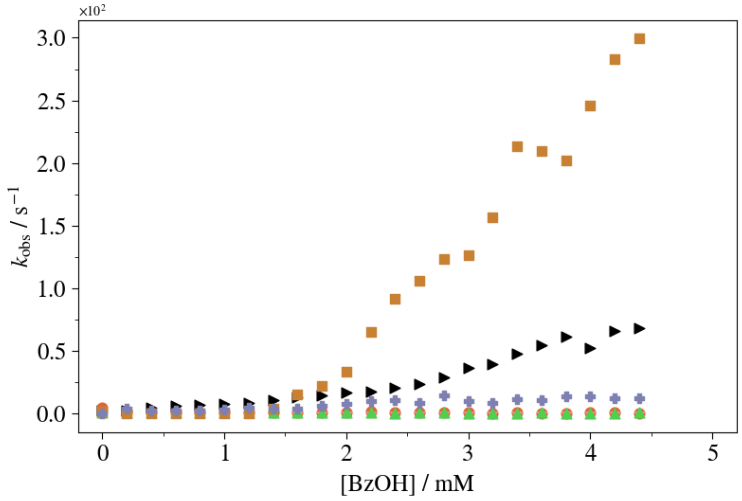


Figure S54. k_{obs} obtained from the fit in Figure S53.

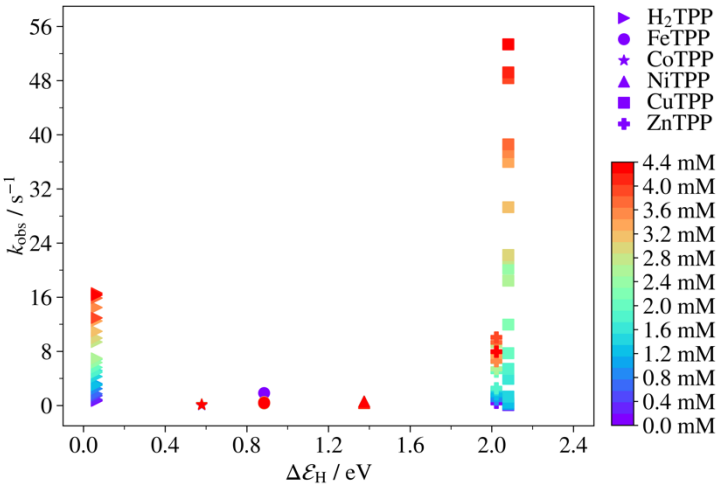


Figure S55. k_{obs} obtained from the interval $x = [0.002, 0.05]$ using $E_{\mathrm{cat/2}} \approx E_{\mathrm{infl}}$.

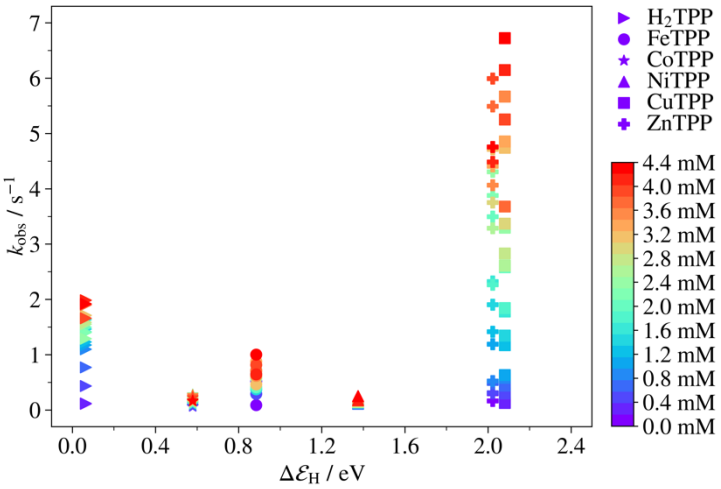


Figure S56. k_{obs} obtained from the interval $x = [0.1, 0.2]$ using $E_{\mathrm{cat/2}} \approx E_{\mathrm{infl}}$.

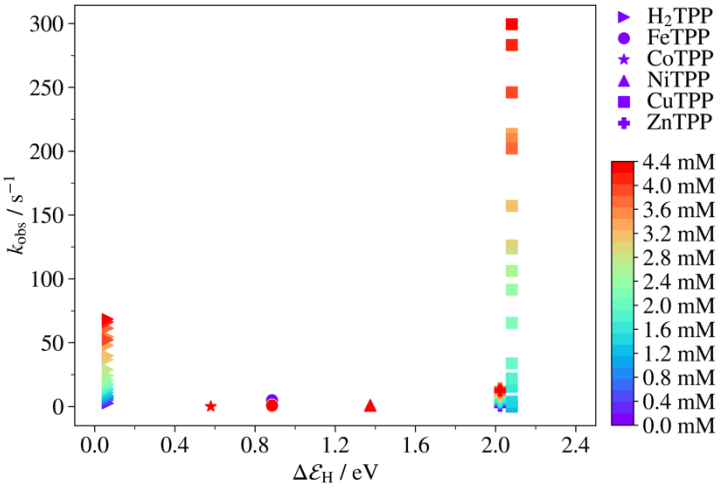


Figure S57. k_{obs} obtained from the interval $x = [E_{\mathrm{infl}} + 0.1, E_{\mathrm{infl}} + 0.2]$ using $E_{\mathrm{cat/2}} \approx E_{\mathrm{infl}}$.

3.7.3 FOWA using $E_{cat/2} \approx E_{i_{cat/2}}$

Figure S58 shows the FOWA plots of H_2TPP, FeTPP, CoTPP, NiTPP, CuTPP and ZnTPP using $E_{\mathrm{cat/2}} \approx \mathrm{E}_{i_{\mathrm{cat/2}}}$. Figure S59 shows linear fits at each concentration in the interval $x = [0.002, 0.05]$, and Figure S60 the corresponding observed rate constants. Figure S61 and Figure S62 show linear fits and observed rate constants, respectively, obtained from the interval $x = [0.1, 0.2]$. Figure S63 and Figure S64 show linear fits and observed rate constants, respectively, obtained from the interval $x = [\mathrm{E}_{i_{\mathrm{cat/2}}} + 0.1, \mathrm{E}_{i_{\mathrm{cat/2}}} + 0.2]$. Figure S65-S67 show the observed rate constants obtained from the three intervals as functions of the binding energy of H.

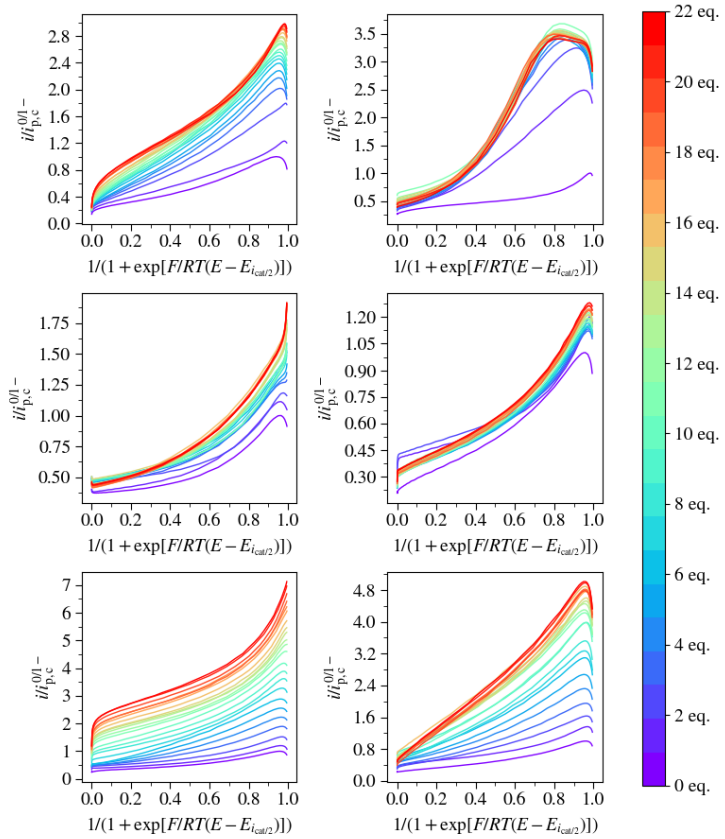


Figure S58. FOWA plot using $E_{\mathrm{cat/2}} \approx E_{\mathrm{infl}}$ (the L^0/L^{1-} transition was used for all porphyrins except FeTPP, for which the M(II)/M(I) transition was used). From upper left to lower right: H_2TPP, FeTPP, CoTPP, NiTPP, CuTPP, ZnTPP.

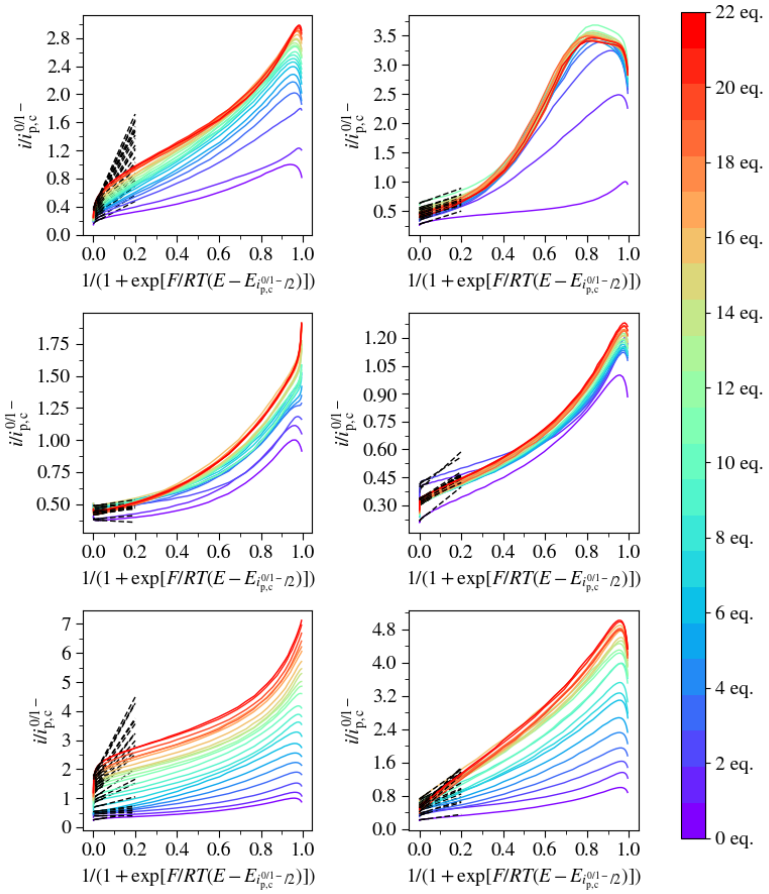


Figure S59. Linear fit of the FOWA plot in Figure S58 between $x = 0.002$ and $x = 0.05$. From upper left to lower right: H_2TPP, FeTPP, CoTPP, NiTPP, CuTPP, ZnTPP.

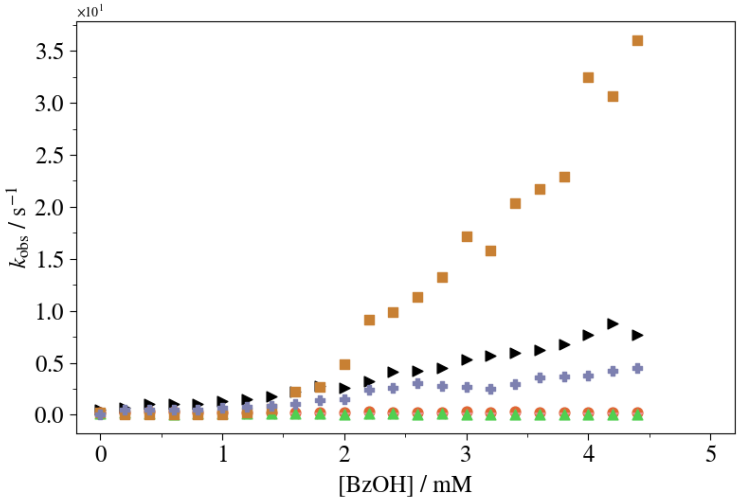


Figure S60. k_{obs} obtained from the fit in Figure S59.

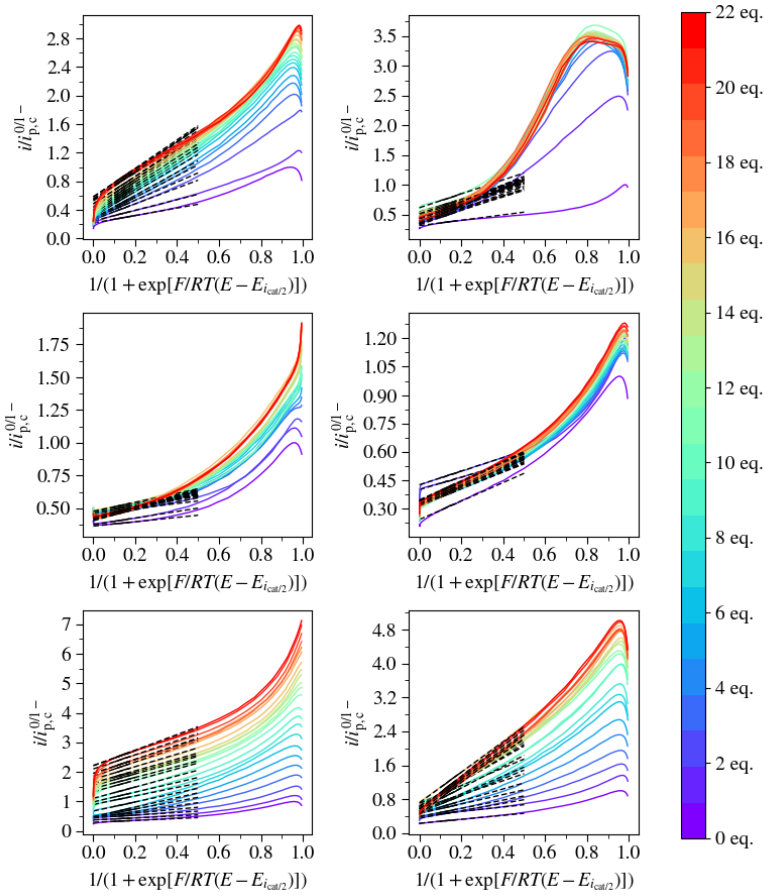


Figure S61. Linear fit of the FOWA plot in Figure S58 between $x = 0.1$ and $x = 0.2$. From upper left to lower right: H_2TPP, FeTPP, CoTPP, NiTPP, CuTPP, ZnTPP.

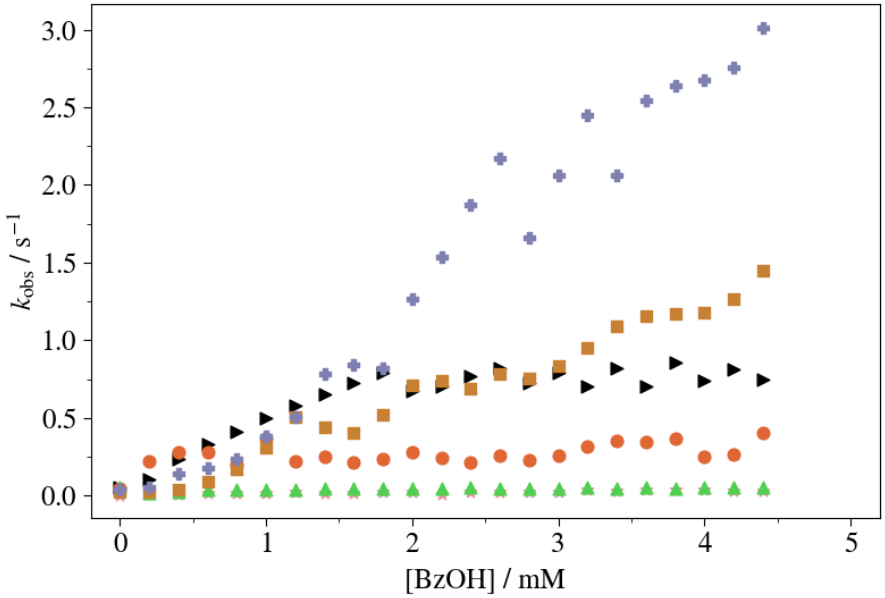


Figure S62. k_{obs} obtained from the fit in Figure S61.

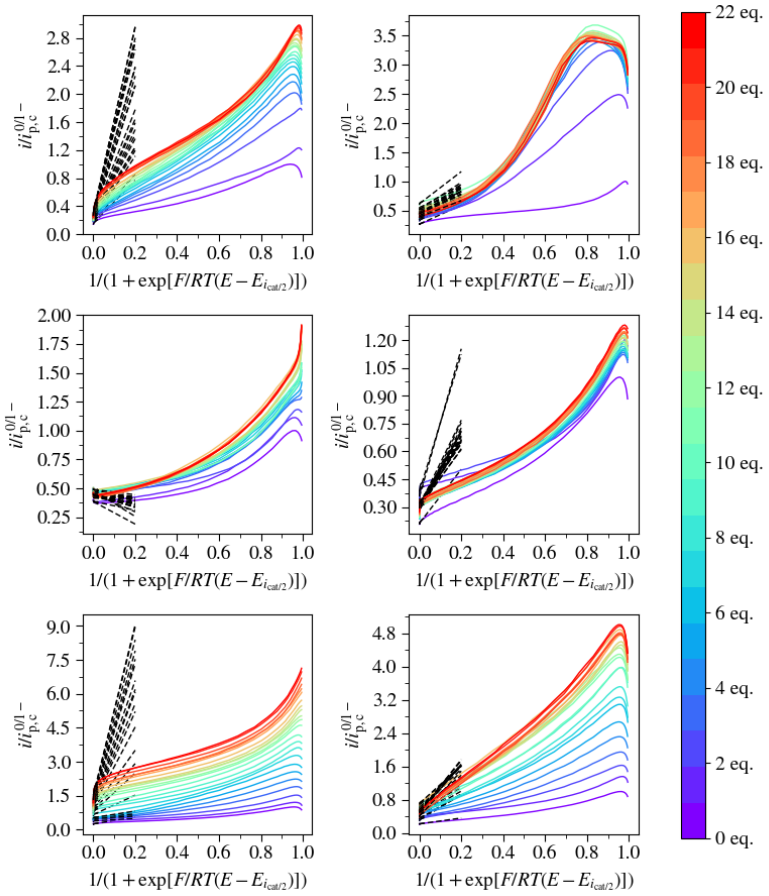


Figure S63. Linear fit of the FOWA plot in Figure S58 between $x = E_{i_{cat/2}} + 0.1$ and $x = E_{i_{cat/2}} + 0.2$. From upper left to lower right: H_2TPP, FeTPP, CoTPP, NiTPP, CuTPP, ZnTPP.

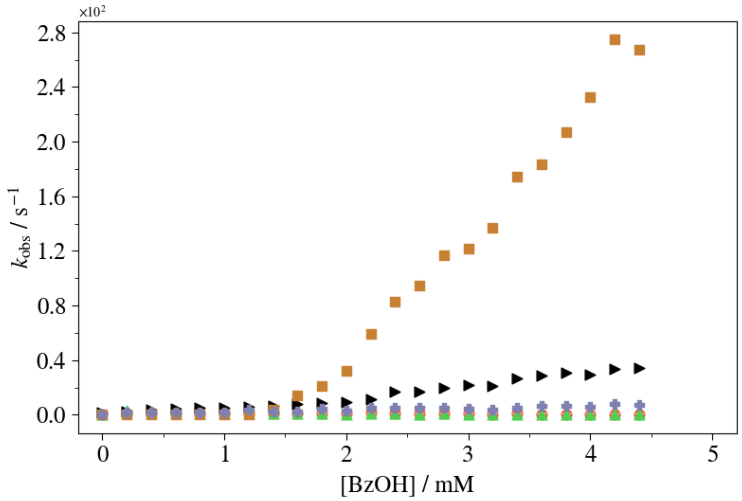


Figure S64. k_{obs} obtained from the fit in Figure S63.

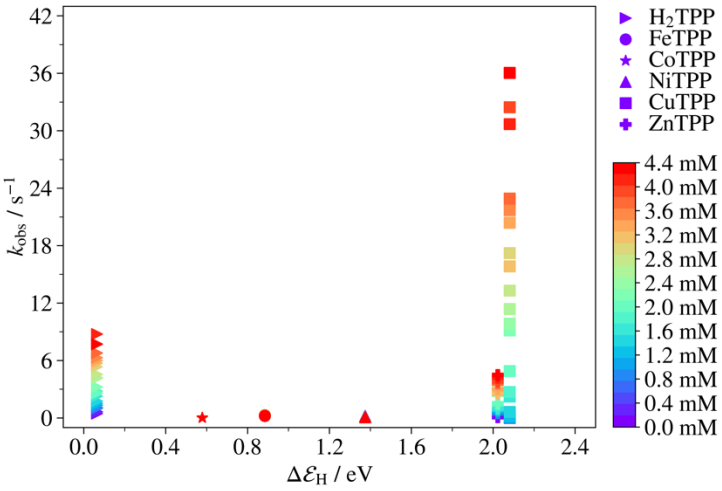


Figure S65. k_{obs} obtained from the interval $x = 0.002$ and $x = 0.05$ using $E_{cat/2} \approx E_{i_{cat/2}}$.

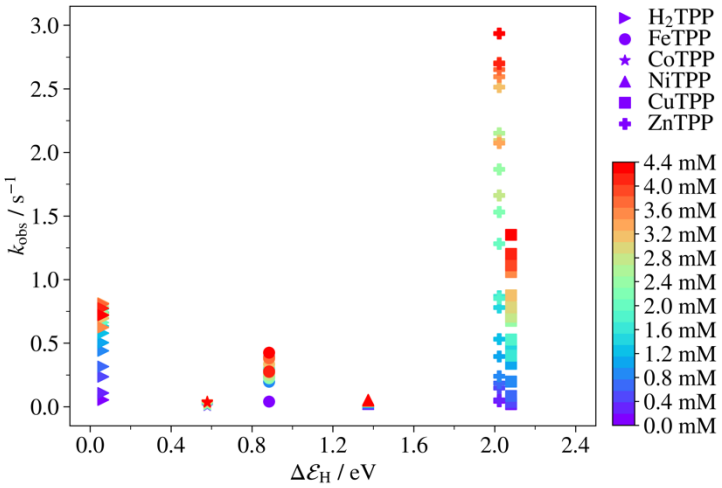


Figure S66. k_{obs} obtained from the interval $x = [0.1, 0.2]$ using $E_{cat/2} \approx E_{i_{cat/2}}$.

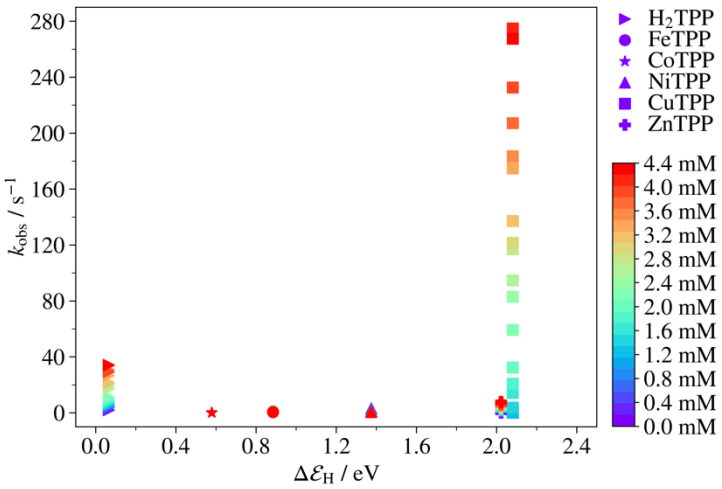


Figure S67. k_{obs} obtained from the interval $x = [E_{i_{cat/2}} + 0.1, E_{i_{cat/2}} + 0.2]$ using $E_{cat/2} \approx E_{i_{cat/2}}$.

References

1 R. Guilard, A. Zrineh, A. Tabard, A. Endo, B. Han, C. Lecomte, M. Souhassou, A. Habbou, M. Ferhat and K. Kadish, *Inorg. Chem.*, 1990, **29**, 4476–4482.

2 T. Kohshin, K. Horino, T. Komura and K. Murata, *Bull. Chem. Soc. Jpn.*, 1993, **66**, 733–738.

3 F. Zaar, S. Olsson, R. Emanuelsson, M. Strømme and M. Sjödin, *Electrochim. Acta*, 2022, **424**, 140616.

4 K. Kadish, X. Lin, J. Ding, Y. Wu and C. Araullo, *Inorg. Chem.*, 1986, **25**, 3236–3242.

5 A. Giraudeau, A. Louati, H. Callot and M. Gross, *Inorg. Chem*, 1981, **20**, 769–772.

6 A. Antipas, D. Dolphin, M. Gouterman and E. Johnson, *J. Am. Chem. Soc.*, 1978, **100**, 7705–7709.

7 Y. Fang, F. Mandoj, L. Zeng, R. Pudi, M. Stefanelli, R. Paolesse and K. Kadish, *J. Porphyr. Phthalocyanines*, 2015, **19**, 1–10.

8 S. Jones and H. Po, *Inorganica Chim. Acta*, 1980, **42**, 95–99.

9 A. Stanienda and G. Biebl, *Z. Phys. Chem.*, 1967, **52**, 254–275.

10 K. Kadish and L. Shiue, *Inorg. Chem*, 1982, **21**, 3623–3630.

11 R. Felton and H. Linschitz, *J. Am. Chem. Soc.*, 1966, **88**, 1113–1116.

12 L. Ye, Y. Fang, Z. Ou, S. Xue and K. Kadish, *Inorg. Chem.*, 2017, **56**, 13613–13626.

13 A. Wolberg, *Isr. J. Chem.*, 1974, **12**, 1031–1035.

14 A. Wolberg and J. Manassen, *J. Am. Chem. Soc.*, 1970, **92**, 2982–2991.

15 A. Giraudeau, H. Callot, J. Jordan, I. Ezhar and M. Gross, *J. Am. Chem. Soc.*, 1979, **101**, 3857–3862.

16 L. Truxillo and D. Davis, *Anal. Chem.*, 1975, **47**, 2260–2267.

17 A. Wahab, M. Bhattacharya, S. Ghosh, A. Samuelson and P. Das, *J. Phys. Chem. B*, 2008, **112**, 2842–2847.

18 D. Guldi, P. Hambright, D. Lexa, P. Neta and J.-M. Savéant, *J. Phys. Chem*, 1992, **96**, 4459–4466.

19 C. Newton and D. Davis, *J . Magn. Reson.*, 1975, **20**, 446–457.

20 L. Bottomley and K. Kadish, *Inorg. Chem.*, 1983, **22**, 342–349.

21 S. Cheung, C. Grimes, J. Wong and C. Reed, *J. Am. Chem. Soc.*, 1976, **98**, 5028–5030.

22 Y. Murakami, Y. Matsuda and S. Yamada, *J. Chem. Soc., Dalton Trans.*, 1981, 855–861.

23 A. Giraudeau, H. Callot and M. Gross, *Inorg. Chem.*, 1979, **18**, 201–206.

24 H. Callat, A. Giraudeau and M. Gross, *J. Chem. Soc., Perkin Trans. 2*, 1975, 1321–1324.

25 K. Kadish, G. Larson, D. Lexa and M. Momenteau, *J. Am. Chem. Soc.*, 1975, **97**, 282–288.

26 R. Felton and G. Owen, *Ann. N. Y. Acad. Sci.*, 1973, **206**, 506–515.

27 K. Kadish, M. Morrison, L. Constant, L. Dickens and D. Davis, *J. Am. Chem. Soc.*, 1976, **98**, 8387–8390.

28 M. Autret, Z. Ou, A. Antonini, T. Boschi, P. Tagliatesta and K. Kadish, *J. Chem. Soc., Dalton Trans.*, 1996, 2793–2787.

29 K. Kadish, J.-L. Cornillon, A. Coutsolelos and R. Guilard, *Inorg. Chem.*, 1987, **26**, 4167–4173.

30 G. Brown, F. Hopf, J. Ferguson, T. Meyer and D. Whitten, *J. Am. Chem. Soc.*, 1973, **95**, 5939–5942.

31 C. Paliteiro and A. Sobral, *Electrochim. Acta*, 2005, **50**, 2445–2451.

32 Y. Fang, P. Bhyrappa, Z. Ou and K. Kadish, *Chem. Eur. J.*, 2014, **20**, 524–532.

33 H. Kageyama, M. Hidai and Y. Uchida, *Bull. Chem. Soc. Jpn.*, 1972, **45**, 2898–2902.

34 S. Schmidt and G. Schuster, *J. Am. Chem. Soc*, 1980, **102**, 7100–7103.

35 A. Ghosh, S. Mobin, R. Fröhlich, R. Butcher, D. Maity and M. Ravikanth, *Inorg. Chem.*, 2010, **49**, 8287–8297.

36 M. Perrée-Fauvet, A. Gaudemer, J. Bonvoisin, J. Girerd, C. Boucly-Goester and P. Boucly, *Inorg. Chem.*, 1989, **28**, 3533–3538.

37 Y. Fang, L. Wang, W. Xu, Z. Ou, M. Chen, L. Cong, W. Shan, X. Ke and K. Kadish, *Inorg. Chem.*, 2019, **58**, 2576–2587.

38 S. Kelly and K. Kadish, *Inorg. Chem.*, 1984, **23**, 679–687.

39 X. Jiang, C. Gros, Y. Chang, N. Desbois, L. Zeng, Y. Cui and K. Kadish, *Inorg. Chem.*, 2017, **56**, 8045–8057.

40 D. Dolphin, T. Niem, R. Felton and I. Fujita, *J. Am. Chem. Soc.*, 1975, **97**, 5288–5290.

41 D. Chang, T. Malinski, A. Ulman and K. Kadish, *Inorg. Chem.*, 1984, **23**, 817–824.

42 Y. Fang, X. Jiang, Z. Ou, C. Michelin, N. Desbois, C. Gros and K. Kadish, *J. Porphyr. Phthalocyanines*, 2014, **18**, 832–841.

43 J. Schneider, K. Vuong, J. Calladine, X. Sun, A. Whitwood, M. George and R. Perutz, *Inorg. Chem.*, 2011, **50**, 11877–11889.

44 T. Malinski, D. Chang, J.-M. Latour, J.-C. Marchon, M. Gross, A. Giraudeau and K. Kadish, *Inorg. Chem.*, 1984, **23**, 3947–3955.

45 D. Clack and N. Hush, *J. Am. Chem. Soc.*, 1965, **87**, 4238–4242.

46 Q. Wang, X. Zhao, J. Zhang and X. Zhang, *J. Electroanal. Chem.*, 2015, **755**, 210–214.

47 V. Birss, K. Dang, J. E. Wong and R. P. C. Wong, *J. Electroanal. Chem.*, 2003, **550–551**, 67–79.

48 T. Nam, S. Son, B. Koo, H. V. Hoa Tran, J. R. Kim, Y. Choi and S. P. Jung, *Int. J. Hydrog. Energy*, 2017, **42**, 27677–27684.

Appendix 1

This appendix contains all optimized geometries used in this study, with the porphyrins listed in alphabetical order.

AgTPP, total charge 0									
	Doublet			Quartet			Sextet		
N	-1.49758	1.48755	-0.00563	-0.13235	2.11823	-0.02921	2.12553	0.00000	-0.07141
N	1.48634	1.49729	-0.04758	2.12382	0.13277	-0.06196	0.00000	-2.12584	0.00000
N	1.49568	-1.48794	0.04763	0.13047	-2.11602	0.04485	-2.12553	0.00000	0.07141
N	-1.48824	-1.49688	0.00567	-2.12440	-0.12998	0.02074	0.00000	2.12584	0.00000
C	-2.84788	1.25481	-0.02237	-1.29319	2.84940	-0.04293	2.92402	1.11675	-0.00400
C	-3.52629	2.53767	-0.04603	-0.96073	4.23502	-0.06342	4.30094	0.68618	0.10661
C	-2.56404	3.50742	-0.05253	0.42586	4.32144	-0.07196	4.30094	-0.68617	0.10661
C	-1.27539	2.83963	-0.01732	0.92849	2.98824	-0.03573	2.92402	-1.11674	-0.00400
C	-0.01339	3.47900	0.00434	2.32238	2.60531	-0.00310	2.47447	-2.47511	0.00386
C	1.25254	2.84623	0.01701	2.84758	1.29826	0.00745	1.11704	-2.92665	0.00148
C	2.53246	3.52049	0.13271	4.25332	0.94964	0.14032	0.68615	-4.30794	-0.00719
C	3.50191	2.55787	0.13360	4.33873	-0.41081	0.14157	-0.68613	-4.30794	0.00720
C	2.83682	1.27295	0.01843	2.98772	-0.93303	0.00757	-1.11703	-2.92666	-0.00147
C	3.47748	0.01089	-0.00001	2.62801	-2.29514	-0.01324	-2.47446	-2.47512	-0.00386
C	2.84472	-1.25515	-0.01842	1.28948	-2.84368	-0.05201	-2.92402	-1.11675	0.00399
C	3.51785	-2.53587	-0.13360	0.95454	-4.21920	-0.21255	-4.30094	-0.68618	-0.10663
C	2.55446	-3.50455	-0.13263	-0.43244	-4.30474	-0.20496	-4.30094	0.68617	-0.10663
C	1.27033	-2.83832	-0.01693	-0.93190	-2.98042	-0.04099	-2.92402	1.11674	0.00399
C	0.00839	-3.47900	-0.00425	-2.32688	-2.60041	-0.00548	-2.47447	2.47511	-0.00386
C	-1.25759	-2.84754	0.01737	-2.85288	-1.29437	0.02739	-1.11704	2.92665	-0.00147
C	-2.54203	-3.52337	0.05263	-4.26397	-0.94317	0.07217	-0.68614	4.30794	0.00721
C	-3.51034	-2.55967	0.04601	-4.34726	0.41732	0.06336	0.68613	4.30794	-0.00719
C	-2.83997	-1.27259	0.02236	-2.98915	0.93733	0.03678	1.11703	2.92666	0.00147
C	-3.47855	-0.01088	-0.00002	-2.62856	2.29750	-0.00258	2.47446	2.47512	0.00386
H	-4.59775	2.67544	-0.05640	-1.66386	5.05450	-0.06409	5.15408	1.34161	0.19852
H	-2.71105	4.57721	-0.08066	1.02105	5.22179	-0.10162	5.15408	-1.34160	0.19852
H	2.66811	4.58855	0.22139	5.06341	1.65639	0.24380	1.34071	-5.16640	-0.02207
H	4.56867	2.70146	0.22485	5.23088	-1.00988	0.24876	-1.34069	-5.16640	0.02210
H	4.58548	-2.67278	-0.22488	1.65597	-5.03105	-0.33463	-5.15407	-1.34161	-0.19855
H	2.69680	-4.57174	-0.22131	-1.03041	-5.19641	-0.32079	-5.15408	1.34160	-0.19855
H	-2.68235	-4.59407	0.08082	-5.08128	-1.64821	0.10610	-1.34070	5.16640	0.02210
H	-4.58091	-2.70414	0.05636	-5.24452	1.01842	0.07032	1.34069	5.16640	-0.02207
C	4.97428	0.01556	-0.00007	3.73937	-3.28829	-0.00068	-3.53204	-3.52579	-0.03190
C	5.69201	-0.48941	1.09622	3.86816	-4.20296	1.05929	-4.41421	-3.68203	1.05105
C	5.68878	0.52493	-1.09643	4.67610	-3.33244	-1.04737	-3.67236	-4.37682	-1.14159
C	7.08911	-0.48393	1.09768	4.91503	-5.12592	1.07903	-5.40653	-4.66478	1.02741
H	5.14614	-0.88125	1.94957	3.14587	-4.17775	1.86950	-4.31171	-3.03043	1.91399
C	7.08589	0.52802	-1.09805	5.71651	-4.26445	-1.03370	-4.66781	-5.35632	-1.16846
H	5.14042	0.91340	-1.94973	4.57629	-2.63731	-1.87566	-2.99945	-4.25941	-1.98603
C	7.79062	0.02419	-0.00023	5.84161	-5.16169	0.03117	-5.53750	-5.50476	-0.08319
H	7.62833	-0.87340	1.95670	5.00729	-5.81700	1.91213	-6.07466	-4.77573	1.87692
H	7.62262	0.92078	-1.95713	6.42650	-4.29036	-1.85554	-4.76597	-6.00021	-2.03801
H	8.87690	0.02752	-0.00028	6.65272	-5.88410	0.04416	-6.31044	-6.26772	-0.10297
C	-0.01526	4.97641	0.02844	3.30802	3.72483	0.03530	3.53205	-3.52578	0.03190
C	-0.47900	5.67466	1.15474	3.36277	4.59322	1.13883	3.67238	-4.37680	1.14159
C	0.45070	5.70905	-1.07482	4.19990	3.92930	-1.03054	4.41421	-3.68203	-1.05106
C	-0.47691	7.07169	1.17812	4.29445	5.63219	1.17994	4.66783	-5.35629	1.16846
H	-0.83647	5.11416	2.01373	2.67511	4.44214	1.96540	2.99948	-4.25938	1.98604
C	0.45092	7.10616	-1.05422	5.12482	4.97573	-0.99429	5.40653	-4.66478	-1.02742
H	0.80889	5.17518	-1.95034	4.15765	3.26661	-1.88990	4.31169	-3.03044	-1.91400
C	-0.01254	7.79190	0.07297	5.17701	5.82858	0.11229	5.53752	-5.50474	0.08319
H	-0.83471	7.59613	2.05976	4.33142	6.28760	2.04554	4.76601	-6.00018	2.03803
H	0.81049	7.65757	-1.91853	5.80228	5.12438	-1.83045	6.07465	-4.77573	-1.87694
H	-0.01158	8.87805	0.09015	5.89839	6.64014	0.14267	6.31046	-6.26770	0.10297
C	-4.97744	-0.01556	-0.00010	-3.74388	3.29042	0.00059	3.53204	3.52579	0.03190
C	-5.69080	-0.35868	1.15873	-4.55701	3.45074	1.13410	3.67237	4.37681	1.14159

C	-5.69281	0.32312	-1.15900	-3.99590	4.08296	-1.13143	4.41420	3.68204	-1.05106
C	-7.08829	-0.36288	1.15968	-5.60035	4.38010	1.13532	4.66782	5.35630	1.16846
H	-5.14257	-0.61894	2.05968	-4.36183	2.84663	2.01531	2.99947	4.25939	1.98604
C	-7.09030	0.31864	-1.16008	-5.04430	5.00540	-1.13344	5.40652	4.66479	-1.02742
H	-5.14612	0.58681	-2.05989	-3.36824	3.96608	-2.00984	4.31169	3.03045	-1.91400
C	-7.79221	-0.02431	-0.00023	-5.84884	5.15827	0.00071	5.53750	5.50476	0.08319
H	-7.62559	-0.62779	2.06605	-6.21659	4.49614	2.02246	4.76599	6.00019	2.03802
H	-7.62916	0.58022	-2.06649	-5.23259	5.60391	-2.02032	6.07464	4.77574	-1.87694
H	-8.87849	-0.02769	-0.00028	-6.66174	5.87878	0.00015	6.31044	6.26771	0.10297
C	0.01589	-4.97640	-0.02830	-3.30618	-3.72561	-0.02631	-3.53205	3.52578	-0.03190
C	0.48625	-5.70608	1.07505	-3.36370	-4.63857	1.04061	-4.41422	3.68202	1.05105
C	-0.44339	-5.67756	-1.15462	-4.18075	-3.89902	-1.11188	-3.67237	4.37681	-1.14159
C	0.49507	-7.10317	1.05454	-4.28386	-5.68841	1.02906	-5.40654	4.66477	1.02742
H	0.84101	-5.16997	1.95059	-2.68620	-4.51402	1.87996	-4.31171	3.03042	1.91399
C	-0.43269	-7.07455	-1.17791	-5.09383	-4.95627	-1.12866	-4.66782	5.35630	-1.16845
H	-0.80422	-5.11933	-2.01368	-4.13331	-3.20477	-1.94561	-2.99947	4.25940	-1.98603
C	0.03597	-7.79183	-0.07266	-5.15079	-5.85209	-0.05680	-5.53752	5.50474	-0.08319
H	0.85793	-7.65230	1.91892	-4.32337	-6.37851	1.86715	-6.07467	4.77571	1.87693
H	-0.78715	-7.60124	-2.05956	-5.75766	-5.08039	-1.97962	-4.76599	6.00020	-2.03801
H	0.04364	-8.87795	-0.08978	-5.86298	-6.67221	-0.06788	-6.31046	6.26770	-0.10297
Ag	-0.00070	0.00000	0.00002	-0.00052	0.00128	-0.00279	0.00000	0.00000	0.00000

AgTPP, total charge 1

	Singlet			Triplet			Quintet		
N	0.00026	-2.08926	0.11632	2.11562	-0.00001	-0.10204	0.32267	-2.09213	-0.03648
N	-2.08922	-0.00026	-0.11601	-2.11562	0.00001	0.10204	-2.09389	-0.32337	-0.06685
N	-0.00026	2.08926	0.11632	-0.00001	-2.11559	0.00000	-0.32015	2.08957	0.06155
N	2.08922	0.00026	-0.11601	0.00001	2.11559	0.00000	2.09431	0.31933	0.02231
C	1.11352	-2.86095	-0.15499	2.91032	1.11134	-0.01721	1.54244	-2.71392	-0.05374
C	0.68388	-4.16440	-0.59051	4.28496	0.68385	0.12600	1.33469	-4.13973	-0.08156
C	-0.68280	-4.16455	-0.59063	4.28495	-0.68389	0.12599	-0.02449	-4.34901	-0.09394
C	-1.11278	-2.86121	-0.15511	2.91031	-1.11137	-0.01721	-0.65231	-3.05233	-0.04553
C	-2.45529	-2.45590	-0.00005	2.46305	-2.46377	-0.00245	-2.08092	-2.80723	-0.00341
C	-2.86097	-1.11352	0.15512	1.11179	-2.91381	-0.00097	-2.70798	-1.54884	0.01414
C	-4.16447	-0.68389	0.59048	0.68378	-4.29565	-0.01013	-4.15105	-1.32710	0.17505
C	-4.16461	0.68280	0.59061	-0.68382	-4.29565	0.01011	-4.35777	0.01048	0.18053
C	-2.86123	1.11278	0.15525	-1.11182	-2.91380	0.00097	-3.04956	0.65886	0.02032
C	-2.45591	2.45528	0.00015	-2.46307	-2.46374	0.00245	-2.82883	2.04767	-0.00488
C	-1.11352	2.86095	-0.15499	-2.91032	-1.11134	0.01722	-1.53663	2.70583	-0.05671
C	-0.68389	4.16440	-0.59050	-4.28496	-0.68385	-0.12597	-1.32496	4.11658	-0.25748
C	0.68280	4.16455	-0.59062	-4.28495	0.68389	-0.12597	0.03492	4.32517	-0.25038
C	1.11278	2.86121	-0.15511	-2.91031	1.11137	0.01722	0.65762	3.04182	-0.04752
C	2.45529	2.45590	-0.00005	-2.46305	2.46377	0.00245	2.08689	2.80085	-0.00535
C	2.86097	1.11351	0.15512	-1.11179	2.91381	0.00096	2.71496	1.54369	0.03362
C	4.16447	0.68389	0.59048	-0.68378	4.29565	0.01011	4.16632	1.31908	0.08516
C	4.16462	-0.68280	0.59060	0.68382	4.29565	-0.01014	4.37063	-0.01848	0.06612
C	2.86123	-1.11278	0.15525	1.11182	2.91380	-0.00097	3.05176	-0.66500	0.03480
C	2.45590	-2.45528	0.00015	2.46307	2.46374	-0.00244	2.83035	-2.05172	-0.00778
H	1.34568	-4.96299	-0.89160	5.13553	1.33768	0.24521	2.11309	-4.88728	-0.08552
H	-1.34439	-4.96327	-0.89182	5.13552	-1.33773	0.24521	-0.54090	-5.29583	-0.13167
H	-4.96310	-1.34569	0.89145	1.33633	-5.15499	-0.03427	-4.88631	-2.10767	0.30047
H	-4.96338	1.34439	0.89167	-1.33638	-5.15498	0.03424	-5.29424	0.53088	0.31351
H	-1.34569	4.96299	-0.89159	-5.13554	-1.33768	-0.24518	-2.10026	4.85229	-0.40774
H	1.34439	4.96327	-0.89181	-5.13552	1.33773	-0.24518	0.55605	5.25922	-0.39508
H	4.96310	1.34569	0.89144	-1.33633	5.15499	0.03423	4.91227	2.09820	0.12856
H	4.96339	-1.34439	0.89166	1.33638	5.15498	-0.03427	5.31533	-0.54110	0.07057
C	-3.50623	3.50523	0.00017	-3.52046	-3.51145	-0.03168	-4.01956	2.93759	0.00975
C	-3.42515	4.59664	0.88481	-4.43738	-3.62744	1.02836	-4.19483	3.87615	1.04368
C	-4.59765	3.42372	-0.88442	-3.62083	-4.39224	-1.12345	-4.98529	2.85979	-1.01017
C	-4.41749	5.57725	0.89009	-5.42482	-4.61320	1.00187	-5.31776	4.70376	1.06425
H	-2.59347	4.65954	1.58000	-4.36052	-2.95501	1.87752	-3.45748	3.93956	1.83846
C	-5.57876	4.41557	-0.88952	-4.62281	-5.36298	-1.15616	-6.09998	3.70019	-0.99546
H	-4.66024	2.59205	-1.57965	-2.92505	-4.29887	-1.95185	-4.84707	2.15312	-1.82325
C	-5.49351	5.49155	0.00033	-5.52298	-5.47962	-0.09183	-6.27126	4.62049	0.04338
H	-4.35230	6.40569	1.58880	-6.11652	-4.70408	1.83378	-5.44960	5.41177	1.87679
H	-6.40724	4.35001	-1.58816	-4.70103	-6.02640	-2.01206	-6.83089	3.63869	-1.79600
H	-6.26145	6.25910	0.00040	-6.29695	-6.24065	-0.11508	-7.14088	5.27033	0.05693
C	-3.50526	-3.50621	-0.00028	3.52042	-3.51148	0.03168	-2.95848	-4.00956	0.02967
C	-3.42386	-4.59772	0.88420	3.62078	-4.39228	1.12344	-2.90237	-4.90714	1.11094
C	-4.59657	-3.42502	-0.88504	4.43736	-3.62747	-1.02835	-3.85844	-4.26176	-1.02064

C	-4.41574	-5.57880	0.88911	4.62276	-5.36303	1.15615	-3.73723	-6.02492	1.14477
H	-2.59227	-4.66038	1.57952	2.92500	-4.29892	1.95184	-2.21614	-4.71534	1.93060
C	-5.57720	-4.41734	-0.89052	5.42478	-4.61324	-1.00187	-4.68249	-5.38882	-0.99110
H	-4.65938	-2.59326	-1.58014	4.36051	-2.95503	-1.87751	-3.89686	-3.58062	-1.86585
C	-5.49162	-5.49345	-0.00085	5.52293	-5.47967	0.09183	-4.62636	-6.27054	0.09258
H	-4.35027	-6.40735	1.58767	4.70096	-6.02646	2.01204	-3.69541	-6.70211	1.99247
H	-6.40556	-4.35206	-1.58932	6.11650	-4.70412	-1.83377	-5.36468	-5.57842	-1.81426
H	-6.25918	-6.26137	-0.00108	6.29689	-6.24070	0.11508	-5.27045	-7.14418	0.11744
C	3.50623	-3.50523	0.00017	3.52046	3.51145	0.03168	4.02764	-2.94009	0.00435
C	3.42516	-4.59664	0.88481	3.62082	4.39225	1.12345	4.85574	-3.00357	1.13770
C	4.59766	-3.42371	-0.88441	4.43740	3.62743	-1.02835	4.34078	-3.72724	-1.11715
C	4.41750	-5.57725	0.89009	4.62280	5.36299	1.15616	5.97532	-3.83875	1.14874
H	2.59348	-4.65954	1.58000	2.92503	4.29889	1.95184	4.61119	-2.40812	2.01269
C	5.57877	-4.41556	-0.88952	5.42483	4.61319	-1.00186	5.46735	-4.55172	-1.10792
H	4.66024	-2.59204	-1.57964	4.36054	2.95499	-1.87751	3.70805	-3.67924	-1.99872
C	5.49353	-5.49154	0.00033	5.52298	5.47962	0.09184	6.28520	-4.61161	0.02557
H	4.35231	-6.40569	1.58881	4.70101	6.02642	2.01205	6.60210	-3.88660	2.03408
H	6.40725	-4.35000	-1.58816	6.11655	4.70406	-1.83376	5.70698	-5.14490	-1.98525
H	6.26147	-6.25909	0.00040	6.29695	6.24065	0.11509	7.15787	-5.25744	0.03320
C	3.50526	3.50620	-0.00028	-3.52042	3.51148	-0.03168	2.95477	4.00997	-0.03132
C	3.42385	4.59773	0.88419	-4.43735	3.62749	1.02836	2.89045	4.95063	1.01245
C	4.59658	3.42500	-0.88502	-3.62079	4.39227	-1.12346	3.84049	4.23576	-1.09959
C	4.41572	5.57881	0.88910	-5.42477	4.61325	1.00187	3.70702	6.08220	0.99494
H	2.59225	4.66040	1.57950	-4.36049	2.95505	1.87753	2.21095	4.78218	1.84282
C	5.57721	4.41733	-0.89050	-4.62277	5.36302	-1.15617	4.64587	5.37628	-1.12176
H	4.65940	2.59324	-1.58012	-2.92502	4.29889	-1.95186	3.88104	3.52458	-1.91954
C	5.49162	5.49345	-0.00085	-5.52293	5.47967	-0.09184	4.58427	6.29935	-0.07321
H	4.35025	6.40737	1.58765	-6.11648	4.70414	1.83378	3.65939	6.79286	1.81447
H	6.40558	4.35204	-1.58929	-4.70098	6.02644	-2.01206	5.31705	5.54478	-1.95844
H	6.25918	6.26137	-0.00108	-6.29689	6.24070	-0.11509	5.21410	7.18354	-0.08883
Ag	0.00000	0.00000	0.00041	0.00000	0.00000	0.00000	0.00050	-0.00182	0.00145

AgTPP, total charge -1

		Singlet			Triplet			Quintet	
N	-0.00001	-2.14060	-0.00008	0.07237	-2.12325	-0.03947	2.13631	0.00007	-0.07623
N	-2.16077	0.00002	-0.42700	-2.11800	-0.07413	0.01960	0.00008	-2.13685	0.00002
N	0.00000	2.14060	0.00010	-0.07370	2.12521	0.01282	-2.13631	-0.00007	0.07624
N	2.16076	-0.00001	0.42701	2.11837	0.07668	0.09127	-0.00007	2.13685	0.00001
C	1.11612	-2.92770	0.04920	1.21776	-2.87694	0.06783	2.93576	1.11901	-0.00690
C	0.68720	-4.31166	0.02775	0.83950	-4.24638	0.24052	4.29743	0.69309	0.10945
C	-0.68725	-4.31166	-0.02766	-0.54612	-4.29498	0.23349	4.29748	-0.69280	0.10946
C	-1.11615	-2.92770	-0.04925	-1.01776	-2.95446	0.05701	2.93584	-1.11881	-0.00689
C	-2.46782	-2.45794	-0.11251	-2.39471	-2.54135	0.01583	2.47462	-2.47516	0.00200
C	-2.92048	-1.11548	-0.16616	-2.87441	-1.22283	-0.01250	1.11934	-2.93877	0.00202
C	-4.27233	-0.68170	0.18672	-4.27644	-0.82575	-0.08984	0.69306	-4.30530	-0.00694
C	-4.27232	0.68173	0.18673	-4.32173	0.53599	-0.08497	-0.69278	-4.30534	0.00679
C	-2.92047	1.11551	-0.16613	-2.94924	1.02362	-0.02603	-1.11914	-2.93884	-0.00206
C	-2.46781	2.45797	-0.11246	-2.56061	2.36924	0.00707	-2.47445	-2.47532	-0.00199
C	-1.11612	2.92770	-0.04920	-1.22088	2.88259	0.04778	-2.93576	-1.11901	0.00696
C	-0.68721	4.31166	-0.02775	-0.84593	4.26329	0.09840	-4.29745	-0.69309	-0.10929
C	0.68724	4.31166	0.02766	0.53962	4.31278	0.10716	-4.29749	0.69280	-0.10929
C	1.11614	2.92770	0.04925	1.01438	2.96275	0.04234	-2.93584	1.11881	0.00696
C	2.46782	2.45795	0.11250	2.39014	2.54639	0.00668	-2.47462	2.47515	-0.00197
C	2.92048	1.11548	0.16616	2.86898	1.22706	0.00087	-1.11934	2.93877	-0.00205
C	4.27232	0.68170	-0.18672	4.26516	0.83266	-0.15027	-0.69307	4.30530	0.00679
C	4.27232	-0.68173	-0.18672	4.31309	-0.52877	-0.14744	0.69277	4.30535	-0.00695
C	2.92047	-1.11551	0.16614	2.94874	-1.01963	0.00615	1.11914	2.93885	0.00201
C	2.46780	-2.45797	0.11247	2.56164	-2.36781	0.02628	2.47445	2.47532	0.00198
H	1.33168	-5.17719	0.09727	1.51956	-5.07593	0.37305	5.15521	1.34311	0.20564
H	-1.33174	-5.17718	-0.09709	-1.16786	-5.16987	0.36056	5.15530	-1.34276	0.20565
H	-5.08976	-1.33313	0.46505	-5.11464	-1.50582	-0.14580	1.34202	-5.16892	-0.02390
H	-5.08975	1.33316	0.46509	-5.20348	1.16042	-0.12040	-1.34169	-5.16901	0.02367
H	-1.33169	5.17719	-0.09727	-1.52802	5.10132	0.12338	-5.15523	-1.34311	-0.20541
H	1.33173	5.17719	0.09709	1.15873	5.19715	0.15681	-5.15532	1.34276	-0.20541
H	5.08975	1.33313	-0.46506	5.09539	1.51431	-0.27044	-1.34204	5.16892	0.02368
H	5.08974	-1.33316	-0.46508	5.18914	-1.15053	-0.26696	1.34168	5.16901	-0.02392
C	-3.53509	3.49993	-0.01154	-3.65352	3.39179	-0.00038	-3.53189	-3.52518	-0.03221
C	-3.61843	4.36172	1.09733	-3.92752	4.16051	1.14366	-4.43307	-3.67094	1.03763
C	-4.50246	3.63258	-1.02388	-4.43143	3.61262	-1.14909	-3.66080	-4.39336	-1.13103
C	-4.62845	5.32213	1.18979	-4.95042	5.11238	1.14376	-5.42627	-4.65303	1.01311

H	-2.88392	4.26319	1.89083	-3.32827	4.00002	2.03525	-4.34355	-3.00365	1.88962
C	-5.51421	4.59227	-0.93533	-5.45901	4.56096	-1.15263	-4.65587	-5.37353	-1.16045
H	-4.44922	2.97096	-1.88350	-4.22149	3.02922	-2.04102	-2.97164	-4.28769	-1.96345
C	-5.58189	5.44346	0.17258	-5.72291	5.31582	-0.00544	-5.54329	-5.50939	-0.08727
H	-4.67519	5.97155	2.06061	-5.14765	5.69175	2.04249	-6.10733	-4.75098	1.85499
H	-6.24786	4.67655	-1.73340	-6.04938	4.71277	-2.05305	-4.74028	-6.02888	-2.02391
H	-6.36837	6.19054	0.24380	-6.52023	6.05479	-0.00643	-6.31689	-6.27280	-0.10843
C	-3.53513	-3.49988	-0.01157	-3.40770	-3.63902	0.01919	3.53213	-3.52494	0.03220
C	-4.50242	-3.63261	-1.02397	-4.31963	-3.78763	1.07931	3.66101	-4.39324	1.13094
C	-3.61858	-4.36155	1.09739	-3.47214	-4.56327	-1.03958	4.43342	-3.67054	-1.03758
C	-5.51420	-4.59227	-0.93540	-5.27168	-4.81140	1.07584	4.65615	-5.37334	1.16034
H	-4.44910	-2.97108	-1.88365	-4.27137	-3.08919	1.90967	2.97177	-4.28770	1.96331
C	-4.62863	-5.32193	1.18987	-4.41958	-5.58919	-1.04595	5.42668	-4.65255	-1.01307
H	-2.88414	-4.26295	1.89094	-2.76806	-4.46359	-1.86044	4.34393	-3.00316	-1.88951
C	-5.58198	-5.44335	0.17259	-5.32690	-5.71788	0.01254	5.54367	-5.50902	0.08722
H	-6.24778	-4.67662	-1.73352	-5.96520	-4.90440	1.90821	4.74053	-6.02877	2.02375
H	-4.67545	-5.97127	2.06075	-4.45314	-6.28618	-1.87991	6.10782	-4.75037	-1.85490
H	-6.36848	-6.19040	0.24382	-6.06517	-6.51582	0.00881	6.31732	-6.27237	0.10838
C	3.53509	-3.49992	0.01155	3.65016	-3.38974	0.00595	3.53189	3.52518	0.03217
C	4.50242	-3.63260	1.02392	4.60082	-3.46199	1.03988	3.66074	4.39348	1.13091
C	3.61848	-4.36168	-1.09735	3.75330	-4.31422	-1.04976	4.43316	3.67083	-1.03763
C	5.51418	-4.59228	0.93537	5.62566	-4.41247	1.01448	4.65581	5.37365	1.16028
H	4.44916	-2.97101	1.88356	4.52468	-2.76229	1.86704	2.97152	4.28790	1.96329
C	4.62851	-5.32208	-1.18980	4.77426	-5.26639	-1.07818	5.42635	4.65291	-1.01315
H	2.88399	-4.26313	-1.89087	3.02151	-4.27251	-1.85102	4.34369	3.00345	-1.88955
C	5.58190	-5.44344	-0.17256	5.71806	-5.31997	-0.04531	5.54331	5.50939	0.08715
H	6.24780	-4.67658	1.73347	6.34749	-4.44759	1.82697	4.74017	6.02908	2.02369
H	4.67527	-5.97148	-2.06064	4.83666	-5.96424	-1.90973	6.10747	4.75077	-1.85498
H	6.36839	-6.19051	-0.24377	6.51326	-6.06089	-0.06625	6.31691	6.27279	0.10829
C	3.53513	3.49988	0.01155	3.40858	3.63823	-0.04250	-3.53213	3.52494	-0.03217
C	3.61861	4.36151	-1.09744	3.47038	4.52224	-1.13514	-4.43332	3.67063	1.03768
C	4.50240	3.63264	1.02397	4.33530	3.81431	1.00036	-3.66112	4.39313	-1.13098
C	4.62867	5.32188	-1.18993	4.42756	5.53777	-1.18879	-5.42658	4.65264	1.01318
H	2.88419	4.26288	-1.89101	2.75764	4.39898	-1.94520	-4.34374	3.00332	1.88966
C	5.51418	4.59229	0.93539	5.29716	4.82760	0.94957	-4.65625	5.37323	-1.16037
H	4.44906	2.97114	1.88367	4.29164	3.14429	1.85412	-2.97195	4.28752	-1.96341
C	5.58199	5.44334	-0.17263	5.34813	5.69531	-0.14580	-5.54368	5.50901	-0.08718
H	4.67551	5.97118	-2.06083	4.45893	6.20331	-2.04812	-6.10765	4.75053	1.85506
H	6.24775	4.67666	1.73352	6.00235	4.94226	1.76934	-4.74072	6.02859	-2.02383
H	6.36850	6.19038	-0.24387	6.09405	6.48505	-0.18666	-6.31733	6.27236	-0.10833
Ag	0.00000	0.00000	0.00001	0.00023	0.00082	0.01515	0.00000	0.00000	0.00002

H-AgTPP, total charge 0

		Singlet			**Triplet**			**Quintet**	
N	0.00040	2.21955	-0.40212	-2.11182	-0.00001	-0.07616	2.12554	0.00000	-0.10002
N	2.07307	0.03130	0.01712	-0.00114	2.11125	-0.02456	0.00137	-2.13114	-0.01866
N	-0.00038	-2.13742	-0.13879	2.11061	0.00001	0.02802	-2.12339	0.00000	0.05732
N	-2.07307	0.03200	0.01715	-0.00113	-2.11125	-0.02456	0.00137	2.13114	-0.01866
C	-1.14368	2.95167	-0.13349	-2.90511	-1.11641	-0.03201	2.92374	1.11324	-0.02480
C	-0.68758	4.24071	0.29268	-4.28873	-0.68310	0.03329	4.28050	0.69536	0.08821
C	0.68905	4.24047	0.29270	-4.28873	0.68307	0.03329	4.28051	-0.69535	0.08821
C	1.14472	2.95129	-0.13347	-2.90512	1.11640	-0.03201	2.92374	-1.11323	-0.02480
C	2.47288	2.48102	-0.18739	-2.46056	2.45919	-0.02318	2.45654	-2.48210	-0.01744
C	2.86801	1.11716	-0.24326	-1.11778	2.90452	-0.02777	1.12020	-2.92662	-0.02125
C	4.19640	0.67155	-0.62306	-0.68485	4.28957	-0.05210	0.68426	-4.31376	-0.04805
C	4.17890	-0.69125	-0.58780	0.68135	4.29017	-0.04468	-0.67914	-4.31484	-0.03721
C	2.83943	-1.09457	-0.19002	1.11533	2.90517	-0.03182	-1.11685	-2.92787	-0.02944
C	2.43286	-2.45345	-0.10320	2.45785	2.45959	-0.03282	-2.45299	-2.48264	-0.02811
C	1.09955	-2.93041	-0.02763	2.90207	1.11635	-0.02782	-2.91845	-1.11326	-0.03409
C	0.68186	-4.31528	0.17359	4.28349	0.68309	-0.13199	-4.27103	-0.69512	-0.19341
C	-0.68335	-4.31505	0.17360	4.28349	-0.68306	-0.13199	-4.27103	0.69511	-0.19341
C	-1.10057	-2.93004	-0.02762	2.90207	-1.11633	-0.02782	-2.91846	1.11325	-0.03409
C	-2.43372	-2.45261	-0.10317	2.45787	-2.45957	-0.03282	-2.45300	2.48264	-0.02811
C	-2.83982	-1.09359	-0.18999	1.11534	-2.90516	-0.03182	-1.11686	2.92787	-0.02944
C	-4.17915	-0.68981	-0.58779	0.68137	-4.29016	-0.04468	-0.67915	4.31483	-0.03721
C	-4.19617	0.67300	-0.62306	-0.68483	-4.28958	-0.05210	0.68425	4.31376	-0.04805
C	-2.86762	1.11814	-0.24326	-1.11776	-2.90453	-0.02777	1.12019	2.92662	-0.02125
C	-2.47201	2.48187	-0.18742	-2.46054	-2.45921	-0.02318	2.45653	2.48210	-0.01744
H	-1.33915	5.03757	0.61911	-5.14501	-1.33951	0.08692	5.13812	1.34572	0.17467
H	1.34089	5.03712	0.61914	-5.14502	1.33948	0.08692	5.13813	-1.34570	0.17467

H	5.01111	1.31383	-0.92533	-1.34137	5.14704	-0.07792	1.33882	-5.17218	-0.07919
H	4.97997	-1.36414	-0.85757	1.33698	5.14861	-0.05046	-1.33202	-5.17497	-0.03715
H	1.33745	-5.16230	0.31825	5.13680	1.33993	-0.21833	-5.12318	-1.34657	-0.31821
H	-1.33923	-5.16185	0.31827	5.13681	-1.33990	-0.21833	-5.12318	1.34655	-0.31821
H	-4.98045	-1.36242	-0.85756	1.33701	-5.14860	-0.05046	-1.33203	5.17496	-0.03715
H	-5.01065	1.31556	-0.92534	-1.34134	-5.14705	-0.07792	1.33881	5.17219	-0.07919
C	3.51659	-3.48134	-0.12680	3.52040	3.51496	-0.05730	-3.51801	-3.52688	-0.05198
C	3.56168	-4.46021	-1.13451	4.34197	3.72413	1.06152	-4.40548	-3.65983	1.02960
C	4.51483	-3.49175	0.86286	3.71747	4.30851	-1.19838	-3.66183	-4.38603	-1.15404
C	4.57572	-5.42046	-1.15330	5.33589	4.70605	1.04160	-5.40043	-4.63904	1.01619
H	2.80089	-4.45460	-1.90934	4.19311	3.11439	1.94804	-4.30406	-2.99417	1.88144
C	5.52575	-4.45526	0.84928	4.71274	5.28895	-1.22073	-4.66469	-5.35849	-1.17225
H	4.48662	-2.74106	1.64715	3.08863	4.14788	-2.06937	-2.98863	-4.27956	-1.99953
C	5.56038	-5.42278	-0.16002	5.52451	5.49123	-0.10009	-5.53463	-5.49058	-0.08577
H	4.59870	-6.16363	-1.94552	5.96016	4.85837	1.91761	-6.07091	-4.73644	1.86539
H	6.28408	-4.45141	1.62732	4.85538	5.89138	-2.11352	-4.76708	-6.00965	-2.03580
H	6.34783	-6.17102	-0.17300	6.29781	6.25395	-0.11661	-6.31231	-6.24885	-0.09811
C	3.54381	3.51653	-0.15429	-3.52008	3.51767	0.00070	3.51721	-3.53077	0.01027
C	4.57571	3.45249	0.79995	-3.71225	4.31044	1.14315	3.65407	-4.38443	1.11749
C	3.54500	4.58497	-1.06938	-4.34010	3.73397	-1.11787	4.40270	-3.67810	-1.07098
C	5.57590	4.42569	0.83832	-4.70201	5.29640	1.16736	4.64974	-5.36407	1.14197
H	4.58017	2.63749	1.51731	-3.08366	4.14488	2.01338	2.98052	-4.26822	1.96139
C	4.54671	5.55704	-1.03405	-5.32858	4.72136	-1.09606	5.39054	-4.66446	-1.05121
H	2.76062	4.63892	-1.81850	-4.19435	3.12570	-2.00595	4.30526	-3.01846	-1.92799
C	5.56583	5.48151	-0.07914	-5.51283	5.50525	0.04726	5.51884	-5.50940	0.05649
H	6.35993	4.36220	1.58769	-4.84093	5.89816	2.06116	4.74691	-6.01083	2.00940
H	4.53493	6.36883	-1.75599	-5.95179	4.87915	-1.97187	6.05971	-4.77288	-1.90012
H	6.34504	6.23782	-0.05056	-6.28182	6.27228	0.06523	6.29093	-6.27327	0.07370
C	-3.54257	3.51775	-0.15433	-3.52005	-3.51769	0.00070	3.51720	3.53078	0.01027
C	-4.57451	3.45406	0.79989	-3.71221	-4.31047	1.14314	3.65406	4.38444	1.11749
C	-3.54338	4.58620	-1.06941	-4.34008	-3.73399	-1.11787	4.40269	3.67811	-1.07098
C	-5.57436	4.42761	0.83826	-4.70197	-5.29643	1.16735	4.64972	5.36408	1.14197
H	-4.57926	2.63906	1.51726	-3.08363	-4.14491	2.01337	2.98050	4.26823	1.96138
C	-4.54475	5.55861	-1.03409	-5.32855	-4.72138	-1.09605	5.39053	4.66447	-1.05121
H	-2.75897	4.63987	-1.81852	-4.19434	-3.12572	-2.00595	4.30525	3.01847	-1.92799
C	-5.56391	5.48343	-0.07920	-5.51280	-5.50528	0.04726	5.51882	5.50941	0.05649
H	-6.35843	4.36439	1.58761	-4.84088	-5.89820	2.06115	4.74689	6.01084	2.00940
H	-4.53267	6.37040	-1.75603	-5.95177	-4.87917	-1.97187	6.05970	4.77289	-1.90012
H	-6.34285	6.24001	-0.05062	-6.28179	-6.27231	0.06523	6.29091	6.27329	0.07370
C	-3.51780	-3.48013	-0.12676	3.52042	-3.51494	-0.05730	-3.51802	3.52687	-0.05198
C	-3.56324	-4.45899	-1.13447	4.34200	-3.72410	1.06152	-4.40549	3.65982	1.02960
C	-4.51605	-3.49019	0.86289	3.71749	-4.30849	-1.19838	-3.66184	4.38602	-1.15404
C	-4.57761	-5.41889	-1.15325	5.33593	-4.70601	1.04160	-5.40044	4.63903	1.01619
H	-2.80245	-4.45365	-1.90930	4.19314	-3.11435	1.94804	-4.30407	2.99415	1.88144
C	-5.52730	-4.45335	0.84932	4.71277	-5.28893	-1.22073	-4.66470	5.35848	-1.17225
H	-4.48758	-2.73950	1.64718	3.08864	-4.14787	-2.06937	-2.98864	4.27956	-1.99952
C	-5.56227	-5.42087	-0.15997	5.52455	-5.49119	-0.10009	-5.53464	5.49056	-0.08577
H	-4.60085	-6.16206	-1.94547	5.96020	-4.85832	1.91761	-6.07092	4.73642	1.86539
H	-6.28563	-4.44923	1.62736	4.85540	-5.89136	-2.11351	-4.76709	6.00964	-2.03579
H	-6.34998	-6.16883	-0.17294	6.29784	-6.25391	-0.11661	-6.31233	6.24883	-0.09810
Ag	-0.00003	-0.12452	0.99876	-0.00437	0.00000	0.17220	0.00526	0.00000	0.12966
H	0.00017	1.32249	-0.86966	-0.07544	-0.00001	2.04788	0.09796	0.00000	2.04391

H-AgTPP, total charge 1

		Doublet			Quartet			Sextet	
N	2.10415	-0.00048	0.09876	2.11961	-0.00579	-0.12605	2.12298	-0.00002	-0.12462
N	-0.00048	-2.09482	-0.13224	-0.00481	-2.11901	-0.01653	0.00182	-2.11813	-0.02454
N	-2.10415	0.00048	0.09875	-2.11785	0.00574	0.09362	-2.11858	0.00003	0.07336
N	0.00048	2.09482	-0.13224	0.00706	2.11898	-0.01632	0.00187	2.11813	-0.02453
C	2.86712	1.11205	-0.17993	2.91637	1.10383	-0.04442	2.91742	1.11723	-0.05144
C	4.16471	0.68277	-0.63731	4.29069	0.67237	0.08508	4.31434	0.67679	0.05821
C	4.16439	-0.68466	-0.63734	4.28687	-0.69605	0.08496	4.31432	-0.67689	0.05821
C	2.86662	-1.11336	-0.17993	2.91014	-1.11976	-0.04460	2.91740	-1.11730	-0.05144
C	2.45561	-2.45673	-0.01753	2.45833	-2.47106	-0.02517	2.48793	-2.45613	-0.02619
C	1.11241	-2.86472	0.14374	1.10559	-2.91741	-0.02721	1.11285	-2.91589	-0.03875
C	0.68261	-4.16599	0.58814	0.67438	-4.29776	-0.05689	0.69084	-4.29298	-0.07770
C	-0.68453	-4.16568	0.58812	-0.69370	-4.29526	-0.03470	-0.68500	-4.29438	-0.05551
C	-1.11372	-2.86421	0.14374	-1.11896	-2.91264	-0.02275	-1.10873	-2.91731	-0.03443
C	-2.45673	-2.45560	-0.01754	-2.46899	-2.45809	-0.01571	-2.48342	-2.45651	-0.02531
C	-2.86713	-1.11205	-0.17994	-2.91186	-1.10393	-0.00184	-2.91134	-1.11733	-0.00478

C	-4.16472	-0.68276	-0.63732	-4.28267	-0.67234	-0.16708	-4.30640	-0.67673	-0.13805
C	-4.16441	0.68468	-0.63728	-4.27890	0.69580	-0.16711	-4.30639	0.67683	-0.13805
C	-2.86661	1.11336	-0.17994	-2.90571	1.11981	-0.00195	-2.91131	1.11739	-0.00478
C	-2.45560	2.45672	-0.01754	-2.45531	2.47151	-0.01582	-2.48337	2.45657	-0.02531
C	-1.11241	2.86472	0.14374	-1.10282	2.91865	-0.02263	-1.10866	2.91734	-0.03443
C	-0.68263	4.16601	0.58808	-0.67006	4.29890	-0.03430	-0.68490	4.29439	-0.05552
C	0.68452	4.16569	0.58811	0.69804	4.29399	-0.05634	0.69094	4.29297	-0.07771
C	1.11371	2.86421	0.14375	1.12172	2.91132	-0.02678	1.11292	2.91586	-0.03875
C	2.45673	2.45560	-0.01752	2.47207	2.45753	-0.02480	2.48798	2.45607	-0.02619
H	4.95791	1.34377	-0.95418	5.14518	1.32306	0.19275	5.16475	1.33485	0.15468
H	4.95729	-1.34602	-0.95424	5.13772	-1.35150	0.19254	5.16471	-1.33497	0.15468
H	1.34276	-4.96403	0.89440	1.32513	-5.15785	-0.09938	1.34607	-5.14940	-0.12178
H	-1.34505	-4.96343	0.89436	-1.34751	-5.15389	-0.02652	-1.33848	-5.15312	-0.05646
H	-4.95792	-1.34375	-0.95420	-5.13215	-1.32411	-0.30456	-5.15326	-1.33586	-0.25682
H	-4.95732	1.34604	-0.95413	-5.12479	1.35222	-0.30453	-5.15324	1.33597	-0.25682
H	-1.34278	4.96407	0.89428	-1.31917	5.16109	-0.02600	-1.33836	5.15315	-0.05648
H	1.34503	4.96344	0.89435	1.35342	5.15056	-0.09862	1.34619	5.14937	-0.12179
C	-3.50711	-3.50386	-0.01696	-3.53144	-3.50025	-0.05019	-3.53692	-3.50838	-0.05257
C	-4.61115	-3.40767	0.85107	-4.44961	-3.60857	1.00979	-4.42922	-3.64533	1.02525
C	-3.41572	-4.60856	-0.88465	-3.63813	-4.38128	-1.14131	-3.65915	-4.37329	-1.15472
C	-5.59319	-4.39831	0.85756	-5.44326	-4.58803	0.98460	-5.41986	-4.62933	1.00269
H	-4.68163	-2.56633	1.53366	-4.36845	-2.93542	1.85795	-4.33214	-2.98903	1.88529
C	-4.40979	-5.58704	-0.88975	-4.64633	-5.34552	-1.17271	-4.65927	-5.34631	-1.18085
H	-2.57540	-4.68230	-1.56818	-2.94305	-4.29233	-1.97075	-2.98079	-4.26732	-1.99626
C	-5.49752	-5.48702	-0.01566	-5.54692	-5.45528	-0.10794	-5.53921	-5.47934	-0.10103
H	-6.43072	-4.32189	1.54416	-6.13565	-4.67322	1.81654	-6.09513	-4.73251	1.84665
H	-4.33705	-6.42513	-1.57608	-4.72937	-6.00899	-2.02811	-4.75326	-5.99806	-2.04417
H	-6.26661	-6.25342	-0.01515	-6.32575	-6.21136	-0.13021	-6.31255	-6.24111	-0.12029
C	3.50551	-3.50547	-0.01696	3.51051	-3.52335	0.01125	3.53586	-3.51274	0.01377
C	4.60955	-3.40983	0.85113	3.59965	-4.40683	1.10207	3.62998	-4.38268	1.11495
C	3.41367	-4.61007	-0.88474	4.43195	-3.64376	-1.04460	4.44559	-3.65544	-1.04870
C	5.59115	-4.40091	0.85760	4.59569	-5.38343	1.13857	4.62136	-5.36399	1.15667
H	4.68037	-2.56857	1.53378	2.90000	-4.31040	1.92683	2.93595	-4.27422	1.94326
C	4.40731	-5.58899	-0.88985	5.41320	-4.63545	-1.01442	5.42738	-4.64772	-1.01082
H	2.57337	-4.68338	-1.56832	4.36257	-2.97072	-1.89392	4.36851	-2.99770	-1.90968
C	5.49504	-5.48952	-0.01569	5.50072	-5.50378	0.07877	5.51995	-5.50122	0.09290
H	6.42867	-4.32491	1.54426	4.66547	-6.04858	1.99384	4.69368	-6.01924	2.01941
H	4.33423	-6.42700	-1.57624	6.10818	-4.72984	-1.84321	6.11630	-4.75517	-1.84315
H	6.26378	-6.25627	-0.01519	6.27002	-6.26943	0.10487	6.28652	-6.26941	0.12406
C	3.50711	3.50386	-0.01694	3.53002	3.50400	0.01171	3.53594	3.51267	0.01377
C	3.41570	4.60857	-0.88463	3.62405	4.38696	1.10254	3.63008	4.38260	1.11495
C	4.61115	3.40767	0.85107	4.45217	3.61928	-1.04411	4.44567	3.65534	-1.04870
C	4.40978	5.58705	-0.88974	4.62553	5.35797	1.13909	4.62148	5.36388	1.15667
H	2.57538	4.68231	-1.56815	2.92388	4.29439	1.92729	2.93605	4.27416	1.94326
C	5.59320	4.39830	0.85755	5.43894	4.60548	-1.01389	5.42748	4.64760	-1.01082
H	4.68165	2.56632	1.53364	4.37907	2.94664	-1.89344	4.36858	2.99760	-1.90968
C	5.49752	5.48702	-0.01566	5.53126	5.47328	0.07932	5.52007	5.50110	0.09290
H	4.33703	6.42514	-1.57606	4.69902	6.02269	1.99438	4.69382	6.01913	2.01941
H	6.43073	4.32187	1.54414	6.13446	4.69600	-1.84265	6.11641	4.75503	-1.84315
H	6.26660	6.25342	-0.01515	6.30482	6.23463	0.10547	6.28667	6.26927	0.12406
C	-3.50550	3.50546	-0.01696	-3.51192	3.51952	-0.05075	-3.53684	3.50846	-0.05257
C	-4.60967	3.40969	0.85095	-4.42971	3.63304	1.00902	-4.42914	3.64542	1.02526
C	-3.41351	4.61019	-0.88455	-3.61330	4.40119	-1.14187	-3.65905	4.37338	-1.15471
C	-5.59127	4.40076	0.85742	-5.41774	4.61816	0.98364	-5.41976	4.62945	1.00270
H	-4.68061	2.56830	1.53343	-4.35254	2.95935	1.85715	-4.33207	2.98912	1.88529
C	-4.40715	5.58913	-0.88966	-4.61599	5.37114	-1.17348	-4.65915	5.34641	-1.18084
H	-2.57309	4.68362	-1.56797	-2.91850	4.30833	-1.97114	-2.98070	4.26739	-1.99625
C	-5.49501	5.48952	-0.01569	-5.51619	5.48601	-0.10891	-5.53909	5.47946	-0.10102
H	-6.42890	4.32466	1.54393	-6.10980	4.70732	1.81544	-6.09503	4.73264	1.84666
H	-4.33395	6.42724	-1.57590	-4.69510	6.03508	-2.02889	-4.75313	5.99818	-2.04415
H	-6.26375	6.25627	-0.01518	-6.29070	6.24651	-0.13137	-6.31241	6.24125	-0.12028
Ag	0.00000	0.00000	0.07972	0.00603	0.00001	0.11470	0.00719	0.00000	0.12392
H	0.00000	0.00000	2.12068	0.14189	0.00050	2.07733	0.12250	0.00001	2.06543

H-AgTPP, total charge -1

		Doublet			Quartet			Sextet	
N	-2.11036	-0.00151	-0.31594	0.00574	-2.12570	-0.08183	-0.29566	2.11955	-0.08445
N	-0.00992	2.09753	0.02273	-2.11796	-0.00684	-0.05329	2.12016	0.29704	-0.05179
N	2.09769	0.00155	0.11615	-0.00581	2.12522	0.01779	0.29915	-2.11810	0.00072
N	-0.00672	-2.09755	0.02268	2.11789	0.00467	-0.05347	-2.11766	-0.29724	0.03320

C	-2.90725	-1.09845	-0.19469	1.12614	-2.91996	-0.03329	-1.51400	2.75332	0.00966
C	-4.30213	-0.68452	-0.02032	0.70494	-4.28623	0.03878	-1.27890	4.15579	0.16125
C	-4.30316	0.67810	-0.02020	-0.68168	-4.29001	0.03878	0.09530	4.34774	0.15452
C	-2.90894	1.09419	-0.19470	-1.11033	-2.92605	-0.03323	0.70372	3.06276	0.00123
C	-2.46226	2.44047	-0.14951	-2.47013	-2.46427	-0.02414	2.11146	2.79422	-0.02715
C	-1.11668	2.88818	-0.09353	-2.90903	-1.13358	-0.02750	2.75653	1.51633	-0.07564
C	-0.69871	4.28022	-0.22121	-4.30005	-0.69570	-0.02847	4.16654	1.28281	-0.15593
C	0.66634	4.29029	-0.18548	-4.30490	0.66653	-0.02637	4.35938	-0.09019	-0.14561
C	1.09227	2.90255	-0.05037	-2.91689	1.11468	-0.04613	3.06662	-0.70139	-0.08329
C	2.43679	2.45501	-0.06273	-2.48531	2.44797	-0.05241	2.79660	-2.10583	-0.02535
C	2.88115	1.10807	-0.05362	-1.12619	2.91524	-0.06599	1.52030	-2.75226	0.01964
C	4.24924	0.68644	-0.31917	-0.70497	4.27491	-0.21766	1.29076	-4.16451	0.03946
C	4.25025	-0.68010	-0.31923	0.68166	4.27864	-0.21803	-0.08224	-4.35951	0.04878
C	2.88281	-1.10380	-0.05363	1.11028	2.92132	-0.06597	-0.69684	-3.06743	0.01059
C	2.44050	-2.45142	-0.06276	2.47191	2.46142	-0.05238	-2.10330	-2.79729	-0.02543
C	1.09665	-2.90097	-0.05040	2.91070	1.13050	-0.04618	-2.74644	-1.51734	-0.06339
C	0.67272	-4.28933	-0.18538	4.30113	0.68995	-0.02684	-4.14552	-1.28507	-0.25338
C	-0.69235	-4.28126	-0.22111	4.30371	-0.67228	-0.02869	-4.33905	0.08814	-0.25916
C	-1.11234	-2.88981	-0.09356	2.91508	-1.11775	-0.02769	-3.05941	0.69990	-0.07008
C	-2.45856	-2.44406	-0.14953	2.48341	-2.45080	-0.02428	-2.79467	2.10851	-0.02418
H	-5.14946	-1.34037	0.12643	1.35877	-5.14478	0.09743	-2.03935	4.91482	0.27484
H	-5.15149	1.33264	0.12665	-1.33079	-5.15214	0.09741	0.62032	5.28589	0.26249
H	-1.35408	5.12965	-0.35560	-5.15923	-1.35154	-0.03407	4.92938	2.04535	-0.21908
H	1.31539	5.15161	-0.26017	-5.16898	1.31563	-0.01326	5.30393	-0.61382	-0.17718
H	5.08415	1.34300	-0.52177	-1.35932	5.12677	-0.33720	2.05579	-4.92760	0.03343
H	5.08615	-1.33540	-0.52187	1.33136	5.13401	-0.33783	-0.60284	-5.30580	0.07397
H	1.32301	-5.14972	-0.25998	5.16165	1.34378	-0.01395	-4.89700	-2.04848	-0.39528
H	-1.34648	-5.13164	-0.35541	5.16646	-1.32341	-0.03434	-5.27240	0.61245	-0.40576
C	3.50457	3.49924	-0.16676	-3.53799	3.50882	-0.06399	3.98647	-3.00565	-0.02024
C	4.41026	3.70098	0.88853	-3.67676	4.39389	1.01993	4.30117	-3.77565	1.11280
C	3.64464	4.28818	-1.32126	-4.40921	3.65988	-1.15660	4.82018	-3.10828	-1.14714
C	5.41961	4.66331	0.79734	-4.65963	5.38619	1.01872	5.41479	-4.61948	1.12114
H	4.31276	3.09257	1.78300	-3.00317	4.29087	1.86560	3.66158	-3.70319	1.98743
C	4.65232	5.25161	-1.41653	-5.39581	4.65053	-1.16120	5.93314	-3.95319	-1.14283
H	2.95608	4.13273	-2.14659	-4.30234	2.99047	-2.00525	4.58379	-2.51815	-2.02760
C	5.54465	5.44433	-0.35637	-5.52620	5.51862	-0.07276	6.23625	-4.71253	-0.00760
H	6.10677	4.80378	1.62809	-4.75197	6.05399	1.87181	5.64222	-5.20202	2.01052
H	4.74392	5.84741	-2.32137	-6.05768	4.74746	-2.01844	6.56141	-4.02062	-2.02762
H	6.32945	6.19293	-0.42949	-6.29170	6.29047	-0.07497	7.10237	-5.36941	-0.00267
C	-3.51974	3.49689	-0.14226	-3.52146	-3.52743	0.00507	3.00765	3.98388	0.00738
C	-3.64391	4.38970	0.93716	-4.34499	-3.70231	1.13016	3.89340	4.19193	1.08013
C	-4.42386	3.62178	-1.21191	-3.70909	-4.38484	-1.09297	2.98978	4.93224	-1.03133
C	-4.63525	5.37398	0.94728	-5.33291	-4.69138	1.15370	4.73094	5.30932	1.11496
H	-2.95584	4.29673	1.77211	-4.20055	-3.05191	1.98798	3.91365	3.46688	1.88811
C	-5.41572	4.60580	-1.20599	-4.69309	-5.37625	-1.07285	3.82988	6.04791	-1.00161
H	-4.33620	2.93781	-2.05090	-3.07323	-4.26178	-1.96488	2.30912	4.78146	-1.86385
C	-5.52632	5.48755	-0.12545	-5.51170	-5.53336	0.05162	4.70454	6.24290	0.07300
H	-4.71502	6.04878	1.79604	-5.95835	-4.80714	2.03557	5.40183	5.45265	1.95844
H	-6.10009	4.68565	-2.04708	-4.82383	-6.02350	-1.93672	3.80322	6.76363	-1.81967
H	-6.29814	6.25304	-0.11881	-6.27829	-6.30395	0.06848	5.35723	7.11182	0.09833
C	-3.51449	-3.50204	-0.14231	3.54038	-3.50836	0.00495	-3.98566	3.00059	-0.02000
C	-3.63732	-4.39507	0.93706	4.36460	-3.67909	1.13017	-4.94477	2.92081	1.00709
C	-4.41844	-3.62819	-1.21196	3.73251	-4.36482	-1.09305	-4.18904	3.94600	-1.04264
C	-4.62723	-5.38082	0.94715	5.35755	-4.66311	1.15384	-6.06289	3.75745	1.01487
H	-2.94937	-4.30115	1.77200	4.21668	-3.02950	1.98802	-4.79847	2.19531	1.80148
C	-5.40885	-4.61367	-1.20607	4.72154	-5.35121	-1.07281	-5.30971	4.77950	-1.04048
H	-4.33180	-2.94404	-2.05090	3.09610	-4.24504	-1.96502	-3.45772	4.01504	-1.84217
C	-5.51814	-5.49564	-0.12557	5.54080	-5.50414	0.05177	-6.25253	4.69110	-0.01023
H	-4.70599	-6.05578	1.79587	5.98341	-4.77572	2.03581	-6.78502	3.68243	1.82423
H	-6.09313	-4.69448	-2.04715	4.85568	-5.99779	-1.93665	-5.44866	5.49590	-1.84651
H	-6.28884	-6.26225	-0.11896	6.31127	-6.27085	0.06875	-7.12384	5.34106	-0.00636
C	3.50987	-3.49402	-0.16677	3.51902	3.52777	-0.06400	-3.00669	-3.98168	-0.05365
C	4.41580	-3.69443	0.88856	3.65328	4.41352	1.01993	-2.97766	-4.89346	-1.12425
C	3.65123	-4.28268	-1.32131	4.38978	3.68296	-1.15641	-3.92054	-4.21356	0.99031
C	5.42662	-4.65522	0.79741	4.63122	5.41067	1.01881	-3.83106	-5.99919	-1.15069
H	4.31732	-3.08620	1.78305	2.98013	4.30716	1.86553	-2.27953	-4.72149	-1.93789
C	4.66039	-5.24458	-1.41654	5.37145	4.67849	-1.16092	-4.77140	-5.32108	0.96900
H	2.96252	-4.12823	-2.14669	4.28648	3.01286	-2.00495	-3.95309	-3.51352	1.81974
C	5.55293	-5.43600	-0.35632	5.49731	5.54733	-0.07253	-4.73152	-6.21986	-0.10280
H	6.11393	-4.79467	1.62820	4.72014	6.07896	1.87188	-3.79530	-6.68634	-1.99255

H	4.75296	-5.84019	-2.32141	6.03305	4.77857	-2.01801	-5.46419	-5.48337	1.79109
H	6.33886	-6.18341	-0.42942	6.25901	6.32293	-0.07465	-5.39466	-7.08099	-0.12159
Ag	0.05036	-0.00011	1.05916	-0.00002	-0.00386	0.18670	0.00323	0.00330	0.13980
H	-0.98907	-0.00040	2.31656	0.00034	-0.07629	2.03111	0.04350	0.05397	2.01709

	AlTPP, total charge 0			**AlTPP, total charge 1**			**H-AlTPP, total charge 0**		
	Doublet			**Singlet**			**Singlet**		
N	0.00355	-1.95416	0.15436	0.00355	-1.95416	0.15436	0.00037	2.00370	0.02511
N	-1.94185	-0.00346	-0.14818	-1.94185	-0.00346	-0.14818	1.99683	-0.00037	0.00992
N	-0.00354	1.95424	0.15460	-0.00354	1.95424	0.15460	-0.00037	-2.00370	0.02511
N	1.94186	0.00357	-0.14817	1.94186	0.00357	-0.14817	-1.99683	0.00037	0.00992
C	1.11434	-2.79671	0.29722	1.11434	-2.79671	0.29722	-1.09877	2.84317	0.03899
C	0.69918	-4.10532	0.63008	0.69918	-4.10532	0.63008	-0.68006	4.22063	0.09400
C	-0.68470	-4.10793	0.62896	-0.68470	-4.10793	0.62896	0.68161	4.22038	0.09414
C	-1.10426	-2.80089	0.29544	-1.10426	-2.80089	0.29544	1.09982	2.84276	0.03921
C	-2.43767	-2.42492	0.01064	-2.43767	-2.42492	0.01064	2.43789	2.43922	-0.00723
C	-2.79234	-1.11985	-0.25931	-2.79234	-1.11985	-0.25931	2.83288	1.09876	-0.06667
C	-4.12655	-0.68605	-0.58998	-4.12655	-0.68605	-0.58998	4.20204	0.68003	-0.22699
C	-4.12915	0.67158	-0.58866	-4.12915	0.67158	-0.58866	4.20178	-0.68155	-0.22714
C	-2.79654	1.10988	-0.25755	-2.79654	1.10988	-0.25755	2.83246	-1.09980	-0.06689
C	-2.44665	2.41597	0.01376	-2.44665	2.41597	0.01376	2.43698	-2.44012	-0.00762
C	-1.11433	2.79678	0.29732	-1.11433	2.79678	0.29732	1.09877	-2.84317	0.03899
C	-0.69919	4.10537	0.63032	-0.69919	4.10537	0.63032	0.68006	-4.22063	0.09399
C	0.68472	4.10801	0.62907	0.68472	4.10801	0.62907	-0.68161	-4.22038	0.09415
C	1.10426	2.80096	0.29556	1.10426	2.80096	0.29556	-1.09982	-2.84277	0.03921
C	2.43769	2.42502	0.01069	2.43769	2.42502	0.01069	-2.43789	-2.43922	-0.00724
C	2.79236	1.11996	-0.25931	2.79236	1.11996	-0.25931	-2.83288	-1.09876	-0.06667
C	4.12658	0.68615	-0.58988	4.12658	0.68615	-0.58988	-4.20204	-0.68003	-0.22698
C	4.12914	-0.67148	-0.58872	4.12914	-0.67148	-0.58872	-4.20178	0.68155	-0.22714
C	2.79655	-1.10977	-0.25752	2.79655	-1.10977	-0.25752	-2.83246	1.09980	-0.06689
C	2.44664	-2.41587	0.01373	2.44664	-2.41587	0.01373	-2.43698	2.44012	-0.00762
H	1.36321	-4.93603	0.81639	1.36321	-4.93603	0.81639	-1.34587	5.06980	0.13168
H	-1.34591	-4.94113	0.81420	-1.34591	-4.94113	0.81420	1.34773	5.06930	0.13197
H	-4.95474	-1.35297	-0.77884	-4.95474	-1.35297	-0.77884	5.04375	1.34686	-0.34053
H	-4.95987	1.33572	-0.77620	-4.95987	1.33572	-0.77620	5.04324	-1.34868	-0.34082
H	-1.36319	4.93608	0.81670	-1.36319	4.93608	0.81670	1.34587	-5.06980	0.13167
H	1.34590	4.94123	0.81429	1.34590	4.94123	0.81429	-1.34772	-5.06931	0.13198
H	4.95478	1.35309	-0.77862	4.95478	1.35309	-0.77862	-5.04375	-1.34687	-0.34052
H	4.95987	-1.33560	-0.77635	4.95987	-1.33560	-0.77635	-5.04324	1.34868	-0.34083
C	-3.49943	3.47491	0.00184	-3.49943	3.47491	0.00184	3.50038	-3.49217	-0.01845
C	-4.52267	3.47926	0.96321	-4.52267	3.47926	0.96321	3.69366	-4.30626	-1.14534
C	-3.48415	4.48904	-0.96991	-3.48415	4.48904	-0.96991	4.32649	-3.67820	1.10090
C	-5.51000	4.46847	0.95108	-5.51000	4.46847	0.95108	4.69088	-5.28509	-1.15358
H	-4.53638	2.70245	1.72234	-4.53638	2.70245	1.72234	3.06010	-4.16361	-2.01612
C	-4.47155	5.47668	-0.98577	-4.47155	5.47668	-0.98577	5.32232	-4.65842	1.09503
H	-2.69384	4.49397	-1.71496	-2.69384	4.49397	-1.71496	4.17948	-3.05206	1.97622
C	-5.48794	5.46970	-0.02437	-5.48794	5.46970	-0.02437	5.50764	-5.46443	-0.03265
H	-6.29268	4.45808	1.70455	-6.29268	4.45808	1.70455	4.83084	-5.90439	-2.03518
H	-4.44888	6.24934	-1.74926	-4.44888	6.24934	-1.74926	5.95063	-4.79319	1.97099
H	-6.25522	6.23862	-0.03538	-6.25522	6.23862	-0.03538	6.28237	-6.22585	-0.03807
C	-3.48623	-3.48804	-0.00339	-3.48623	-3.48804	-0.00339	3.50169	3.49086	-0.01778
C	-4.51017	-3.49778	0.95716	-4.51017	-3.49778	0.95716	4.32773	3.67641	1.10170
C	-3.46589	-4.50101	-0.97627	-3.46589	-4.50101	-0.97627	3.69545	4.30502	-1.14455
C	-5.49339	-4.49106	0.94305	-5.49339	-4.49106	0.94305	5.32395	4.65623	1.09608
H	-4.52768	-2.72198	1.71724	-4.52768	-2.72198	1.71724	4.18036	3.05022	1.97692
C	-4.44917	-5.49270	-0.99411	-4.44917	-5.49270	-0.99411	4.69307	5.28345	-1.15252
H	-2.67493	-4.50179	-1.72066	-2.67493	-4.50179	-1.72066	3.06196	4.16273	-2.01543
C	-5.46639	-5.49103	-0.03356	-5.46639	-5.49103	-0.03356	5.50975	5.46232	-0.03147
H	-6.27671	-4.48482	1.69591	-6.27671	-4.48482	1.69591	5.95220	4.79064	1.97215
H	-4.42269	-6.26440	-1.75846	-4.42269	-6.26440	-1.75846	4.83339	5.90280	-2.03403
H	-6.23045	-6.26313	-0.04609	-6.23045	-6.26313	-0.04609	6.28479	6.22343	-0.03669
C	3.49937	-3.47488	0.00182	3.49937	-3.47488	0.00182	-3.50037	3.49217	-0.01845
C	4.52239	-3.47950	0.96340	4.52239	-3.47950	0.96340	-4.32648	3.67820	1.10091
C	3.48413	-4.48889	-0.97007	3.48413	-4.48889	-0.97007	-3.69367	4.30625	-1.14535
C	5.50963	-4.46881	0.95129	5.50963	-4.46881	0.95129	-5.32231	4.65842	1.09503
H	4.53602	-2.70285	1.72269	4.53602	-2.70285	1.72269	-4.17947	3.05207	1.97623
C	4.47142	-5.47661	-0.98592	4.47142	-5.47661	-0.98592	-4.69089	5.28508	-1.15358
H	2.69395	-4.49358	-1.71527	2.69395	-4.49358	-1.71527	-3.06011	4.16359	-2.01613

C	5.48765	-5.46986	-0.02433	5.48765	-5.46986	-0.02433	-5.50764	5.46443	-0.03265
H	6.29217	-4.45863	1.70492	6.29217	-4.45863	1.70492	-5.95061	4.79320	1.97100
H	4.44886	-6.24917	-1.74952	4.44886	-6.24917	-1.74952	-4.83085	5.90437	-2.03518
H	6.25484	-6.23888	-0.03532	6.25484	-6.23888	-0.03532	-6.28237	6.22585	-0.03807
C	3.48629	3.48807	-0.00337	3.48629	3.48807	-0.00337	-3.50169	-3.49086	-0.01778
C	4.51048	3.49755	0.95694	4.51048	3.49755	0.95694	-3.69546	-4.30502	-1.14455
C	3.46587	4.50119	-0.97608	3.46587	4.50119	-0.97608	-4.32773	-3.67641	1.10170
C	5.49378	4.49074	0.94280	5.49378	4.49074	0.94280	-4.69308	-5.28345	-1.15252
H	4.52811	2.72158	1.71685	4.52811	2.72158	1.71685	-3.06196	-4.16273	-2.01543
C	4.44923	5.49281	-0.99396	4.44923	5.49281	-0.99396	-5.32395	-4.65623	1.09609
H	2.67474	4.50220	-1.72030	2.67474	4.50220	-1.72030	-4.18036	-3.05021	1.97692
C	5.46665	5.49089	-0.03363	5.46665	5.49089	-0.03363	-5.50976	-5.46231	-0.03146
H	6.27728	4.48428	1.69547	6.27728	4.48428	1.69547	-4.83340	-5.90280	-2.03402
H	4.42263	6.26463	-1.75818	4.42263	6.26463	-1.75818	-5.95220	-4.79063	1.97215
H	6.23079	6.26291	-0.04620	6.23079	6.26291	-0.04620	-6.28479	-6.22342	-0.03668
Al	0.00001	-0.00004	0.00090	0.00001	-0.00004	0.00090	0.00000	0.00000	0.49828
H							0.00000	0.00000	2.09151

BaTPP, total charge 0

	Singlet			Triplet			Quintet		
N	-2.10447	-0.00003	0.02392	-2.16991	-0.00810	-0.05013	-0.00031	-2.09428	-0.08988
N	-0.00307	2.11470	0.10878	-0.00804	2.09835	0.11768	-2.18533	0.00030	0.09784
N	2.11878	0.00003	0.18517	2.16990	0.00826	-0.05013	0.00029	2.09424	-0.08981
N	-0.00300	-2.11470	0.10878	0.00809	-2.09835	0.11822	2.18533	-0.00033	0.09788
C	-2.90750	-1.10819	-0.07419	-2.88114	-1.11440	0.33892	1.10764	-2.89665	0.08372
C	-4.29493	-0.68302	-0.18356	-4.08985	-0.70960	0.98137	0.68629	-4.23440	0.44793
C	-4.29495	0.68290	-0.18355	-4.09508	0.67911	0.98104	-0.68749	-4.23422	0.44791
C	-2.90753	1.10810	-0.07419	-2.88945	1.09263	0.33833	-1.10848	-2.89634	0.08374
C	-2.45897	2.45564	-0.09858	-2.45803	2.46525	0.15494	-2.46468	-2.47044	-0.12982
C	-1.11130	2.90331	-0.07171	-1.12036	2.90034	-0.01392	-2.88170	-1.10621	-0.32154
C	-0.68712	4.27273	-0.31816	-0.69798	4.26338	-0.31116	-4.08233	-0.68550	-1.01387
C	0.67842	4.27632	-0.30319	0.66615	4.26843	-0.31066	-4.08216	0.68665	-1.01383
C	1.10468	2.90571	-0.06335	1.09842	2.90860	-0.01325	-2.88138	1.10701	-0.32155
C	2.45019	2.45409	-0.08513	2.43920	2.48352	0.15647	-2.46396	2.47111	-0.12983
C	2.89756	1.10746	-0.04020	2.88118	1.11454	0.33884	-1.10765	2.89663	0.08375
C	4.25106	0.68266	-0.36280	4.08990	0.70977	0.98128	-0.68630	4.23443	0.44777
C	4.25108	-0.68253	-0.36280	4.09508	-0.67894	0.98106	0.68748	4.23423	0.44780
C	2.89760	-1.10737	-0.04021	2.88946	-1.09249	0.33835	1.10846	2.89631	0.08379
C	2.45026	-2.45402	-0.08513	2.45808	-2.46515	0.15515	2.46465	2.47041	-0.12976
C	1.10477	-2.90568	-0.06335	1.12039	-2.90033	-0.01347	2.88169	1.10619	-0.32151
C	0.67854	-4.27630	-0.30318	0.69801	-4.26334	-0.31077	4.08236	0.68551	-1.01378
C	-0.68700	-4.27275	-0.31815	-0.66612	-4.26840	-0.31026	4.08217	-0.68664	-1.01380
C	-1.11122	-2.90335	-0.07171	-1.09841	-2.90858	-0.01283	2.88137	-1.10703	-0.32156
C	-2.45889	-2.45571	-0.09858	-2.43918	-2.48343	0.15672	2.46396	-2.47113	-0.12987
H	-5.15226	-1.33638	-0.25958	-4.82805	-1.36825	1.41687	1.34132	-5.06186	0.68032
H	-5.15230	1.33623	-0.25957	-4.83824	1.33243	1.41611	-1.34275	-5.06150	0.68030
H	-1.34267	5.10977	-0.51223	-1.35389	5.10022	-0.50455	-4.79815	-1.34569	-1.48246
H	1.33141	5.12065	-0.47062	1.31599	5.11014	-0.50348	-4.79781	1.34706	-1.48238
H	5.07291	1.33944	-0.61041	4.82810	1.36845	1.41672	-1.34134	5.06194	0.68001
H	5.07295	-1.33929	-0.61041	4.83820	-1.33224	1.41625	1.34274	5.06155	0.68006
H	1.33157	-5.12062	-0.47061	1.35392	-5.10018	-0.50419	4.79820	1.34572	-1.48229
H	-1.34251	-5.10982	-0.51222	-1.31595	-5.11009	-0.50315	4.79783	-1.34704	-1.48235
C	3.51365	3.49203	-0.28297	3.49734	3.52322	0.23411	-3.51339	3.51026	-0.24379
C	4.40917	3.79973	0.75321	3.39328	4.61028	1.12274	-4.72122	3.39177	0.47470
C	3.65382	4.15933	-1.51052	4.65099	3.42642	-0.56829	-3.35338	4.63071	-1.08496
C	5.41312	4.75522	0.57279	4.40039	5.57477	1.19547	-5.72132	4.35867	0.36795
H	4.31410	3.28249	1.70398	2.52575	4.68031	1.77140	-4.86416	2.53378	1.12498
C	4.65742	5.11378	-1.69475	5.65056	4.39727	-0.50617	-4.35645	5.59398	-1.19758
H	2.97308	3.91831	-2.32179	4.75198	2.58246	-1.24376	-2.44194	4.72740	-1.66649
C	5.53998	5.41629	-0.65273	5.52986	5.47633	0.37718	-5.54421	5.46598	-0.46893
H	6.09502	4.98188	1.38787	4.30564	6.39878	1.89723	-6.63874	4.24907	0.93985
H	4.75287	5.61656	-2.65324	6.52590	4.31064	-1.14396	-4.21417	6.44171	-1.86224
H	6.32078	6.15798	-0.79559	6.31218	6.22804	0.43203	-6.32377	6.21745	-0.55562
C	-3.50671	3.51665	-0.24194	-3.52438	3.49653	0.23080	-3.51443	-3.50927	-0.24372
C	-3.75413	4.42319	0.80145	-3.42958	4.58555	1.11811	-4.72211	-3.39049	0.47498
C	-4.25267	3.63875	-1.42570	-4.67691	3.38947	-0.57197	-3.35491	-4.62966	-1.08506
C	-4.72414	5.42051	0.67018	-4.44441	5.54204	1.18909	-5.72252	-4.35708	0.36829
H	-3.17819	4.34137	1.71909	-2.56305	4.66334	1.76722	-4.86468	-2.53254	1.12539

C	-5.22198	4.63584	-1.56080	-5.68427	4.35233	-0.51156	-4.35830	-5.59261	-1.19762
H	-4.06126	2.94852	-2.24211	-4.77087	2.54386	-1.24638	-2.44362	-4.72656	-1.66678
C	-5.46230	5.52977	-0.51237	-5.57267	5.43350	0.37040	-5.54589	-5.46434	-0.46874
H	-4.90299	6.11039	1.49042	-4.35661	6.36767	1.88985	-6.63981	-4.24727	0.94036
H	-5.78547	4.71701	-2.48627	-6.55860	4.25781	-1.14964	-4.21640	-6.44030	-1.86242
H	-6.21570	6.30538	-0.61692	-6.36102	6.17898	0.42392	-6.32570	-6.21556	-0.55540
C	-3.50660	-3.51676	-0.24194	-3.49738	-3.52306	0.23422	3.51342	-3.51025	-0.24380
C	-3.75401	-4.42330	0.80145	-3.39351	-4.61013	1.12288	4.72120	-3.39175	0.47477
C	-4.25256	-3.63888	-1.42570	-4.65090	-3.42623	-0.56836	3.35355	-4.63062	-1.08511
C	-4.72398	-5.42065	0.67018	-4.40067	-5.57457	1.19546	5.72135	-4.35859	0.36803
H	-3.17807	-4.34147	1.71910	-2.52609	-4.68019	1.77168	4.86404	-2.53380	1.12513
C	-5.22184	-4.63600	-1.56081	-5.65053	-4.39703	-0.50638	4.35668	-5.59383	-1.19771
H	-4.06117	-2.94864	-2.24211	-4.75175	-2.58229	-1.24386	2.44218	-4.72730	-1.66674
C	-5.46213	-5.52993	-0.51237	-5.53002	-5.47609	0.37699	5.54437	-5.46584	-0.46894
H	-4.90282	-6.11053	1.49042	-4.30606	-6.39858	1.89723	6.63872	-4.24899	0.94001
H	-5.78532	-4.71718	-2.48628	-6.52576	-4.31036	-1.14432	4.21450	-6.44150	-1.86247
H	-6.21552	-6.30557	-0.61693	-6.31237	-6.22777	0.43174	6.32397	-6.21726	-0.55564
C	3.51376	-3.49193	-0.28297	3.52446	-3.49639	0.23091	3.51439	3.50925	-0.24368
C	4.40929	-3.79959	0.75320	4.67689	-3.38934	-0.57201	3.35471	4.62977	-1.08481
C	3.65394	-4.15923	-1.51052	3.42976	-4.58544	1.11822	4.72218	3.39036	0.47479
C	5.41327	-4.75505	0.57278	5.68426	-4.35219	-0.51173	4.35808	5.59274	-1.19739
H	4.31421	-3.28235	1.70398	4.77077	-2.54372	-1.24642	2.44330	4.72677	-1.66633
C	4.65757	-5.11364	-1.69475	4.44459	-5.54193	1.18906	5.72258	4.35695	0.36808
H	2.97319	-3.91824	-2.32178	2.56332	-4.66323	1.76744	4.86486	2.53230	1.12503
C	5.54015	-5.41613	-0.65273	5.57277	-5.43338	0.37023	5.54580	5.46435	-0.46875
H	6.09518	-4.98169	1.38786	6.55850	-4.25766	-1.14991	4.21605	6.44054	-1.86202
H	4.75303	-5.61642	-2.65323	4.35688	-6.36757	1.88981	6.63997	4.24705	0.93996
H	6.32097	-6.15778	-0.79559	6.36111	-6.17887	0.42364	6.32559	6.21558	-0.55542
Ba	-0.04935	0.00000	1.61729	-0.00003	-0.00036	-1.48550	-0.00001	-0.00005	1.52202

BaTPP, total charge 1

		Doublet			Quartet			Sextet	
N	-1.47654	1.46522	-0.05164	-0.00006	-2.08672	0.05125	2.08180	0.02655	-0.00340
N	1.49503	1.51937	0.07593	-2.16266	0.00005	0.10585	-0.00126	-2.15405	0.12865
N	1.48574	-1.47114	0.09805	0.00005	2.08671	-0.05125	-2.08172	0.02902	-0.00337
N	-1.50225	-1.52838	0.15691	2.16265	-0.00006	0.10586	0.00133	2.21409	0.11358
C	-2.82979	1.25366	0.02029	1.10636	-2.90263	0.03455	2.90444	1.10489	0.12094
C	-3.51607	2.51941	0.19037	0.67693	-4.28699	0.28514	4.25190	0.67669	0.43457
C	-2.55525	3.49309	0.17938	-0.67718	-4.28695	0.28510	4.23768	-0.69749	0.44391
C	-1.28203	2.82196	0.00338	-1.10653	-2.90257	0.03453	2.89137	-1.10626	0.13566
C	-0.01747	3.47625	-0.13473	-2.43915	-2.48028	-0.14050	2.46123	-2.44744	-0.11323
C	1.25676	2.83721	-0.20639	-2.84654	-1.09759	-0.34024	1.10315	-2.85436	-0.28915
C	2.48446	3.47207	-0.64753	-4.01619	-0.68705	-1.07867	0.67700	-4.07220	-0.97879
C	3.45707	2.51238	-0.62049	-4.01616	0.68726	-1.07866	-0.68184	-4.07140	-0.97877
C	2.81982	1.28507	-0.18585	-2.84648	1.09773	-0.34024	-1.10652	-2.85305	-0.28912
C	3.46433	0.02020	-0.09352	-2.43902	2.48040	-0.14048	-2.46410	-2.44452	-0.11317
C	2.83942	-1.25109	0.05403	-1.10637	2.90262	0.03454	-2.89264	-1.10283	0.13571
C	3.54299	-2.51877	0.03640	-0.67696	4.28699	0.28508	-4.23850	-0.69246	0.44384
C	2.58972	-3.49778	0.04605	0.67716	4.28695	0.28512	-4.25109	0.68173	0.43444
C	1.30102	-2.82834	0.04608	1.10652	2.90257	0.03454	-2.90309	1.10833	0.12097
C	0.03597	-3.47396	-0.09765	2.43914	2.48028	-0.14048	-2.49287	2.48201	-0.10427
C	-1.23850	-2.83246	-0.16812	2.84653	1.09758	-0.34022	-1.14380	2.91503	-0.30212
C	-2.42960	-3.45007	-0.71564	4.01616	0.68705	-1.07868	-0.73395	4.10546	-0.92292
C	-3.40262	-2.48995	-0.72691	4.01612	-0.68727	-1.07869	0.73883	4.10458	-0.92295
C	-2.80680	-1.28574	-0.18582	2.84647	-1.09774	-0.34022	1.14728	2.91368	-0.30212
C	-3.46484	-0.02032	-0.11436	2.43901	-2.48041	-0.14047	2.49585	2.47906	-0.10429
H	-4.58071	2.65354	0.31275	1.33465	-5.12701	0.45420	5.09382	1.32625	0.62461
H	-2.70228	4.55722	0.29076	-1.33495	-5.12694	0.45413	5.06835	-1.35980	0.63879
H	2.58360	4.49738	-0.97199	-4.71593	-1.35051	-1.56570	1.34001	-4.78727	-1.44348
H	4.49402	2.61893	-0.90301	-4.71586	1.35077	-1.56568	-1.34571	-4.78568	-1.44344
H	4.61533	-2.64401	-0.00248	-1.33468	5.12701	0.45408	-5.06996	-1.35379	0.63862
H	2.75031	-4.56539	0.03628	1.33491	5.12694	0.45416	-5.09227	1.33230	0.62433
H	-2.49763	-4.45813	-1.09717	4.71588	1.35051	-1.56573	-1.37236	4.86238	-1.35546
H	-4.40477	-2.57526	-1.12045	4.71580	-1.35077	-1.56574	1.37813	4.86072	-1.35553
C	4.95242	0.00784	-0.25753	-3.51621	3.49364	-0.23965	-3.50251	-3.49266	-0.26996
C	5.78466	-0.13262	0.86268	-4.68626	3.35538	0.53381	-3.41923	-4.69211	0.46383
C	5.52888	0.12123	-1.53166	-3.41947	4.58615	-1.12351	-4.57497	-3.32763	-1.16827
C	7.17379	-0.15146	0.71188	-5.71125	4.29694	0.45009	-4.38417	-5.68897	0.31480
H	5.34389	-0.22363	1.85163	-4.78001	2.51083	1.21026	-2.59953	-4.83240	1.16272
C	6.91772	0.09653	-1.68084	-4.45263	5.51968	-1.21665	-5.53231	-4.33025	-1.32545

H	4.88736	0.22113	-2.40248	-2.54484	4.68153	-1.75956	-4.63822	-2.41935	-1.75935
C	7.74286	-0.03785	-0.55996	-5.59786	5.38254	-0.42583	-5.44341	-5.51172	-0.58148
H	7.80886	-0.25541	1.58659	-6.59894	4.18366	1.06514	-4.31055	-6.60203	0.89802
H	7.35325	0.18016	-2.67206	-4.36740	6.34829	-1.91325	-6.34424	-4.19225	-2.03323
H	8.82210	-0.05528	-0.67712	-6.39984	6.11093	-0.49727	-6.19138	-6.28948	-0.70204
C	-0.02914	4.95617	-0.26889	-3.51641	-3.49345	-0.23968	3.49838	-3.49684	-0.27003
C	0.72733	5.75644	0.60794	-4.68642	-3.35516	0.53384	3.41380	-4.69608	0.46397
C	-0.78142	5.58268	-1.28036	-3.41980	-4.58590	-1.12362	4.57088	-3.33325	-1.16856
C	0.71655	7.14638	0.48824	-5.71147	-4.29665	0.45012	4.37752	-5.69411	0.31493
H	1.31152	5.28321	1.39151	-4.78008	-2.51065	1.21035	2.59406	-4.83528	1.16303
C	-0.77333	6.97155	-1.41175	-4.45302	-5.51937	-1.21677	5.52698	-4.33704	-1.32574
H	-1.35036	4.97357	-1.97586	-2.54521	-4.68129	-1.75974	4.63510	-2.42516	-1.75983
C	-0.03047	7.75735	-0.52433	-5.59820	-5.38220	-0.42588	5.43681	-5.51828	-0.58156
H	1.29206	7.75149	1.18221	-6.59912	-4.18335	1.06522	4.30292	-6.60699	0.89832
H	-1.34395	7.43981	-2.20802	-4.36789	-6.34792	-1.91343	6.33895	-4.20013	-2.03370
H	-0.03098	8.83860	-0.62327	-6.40023	-6.11054	-0.49733	6.18383	-6.29695	-0.70213
C	-4.94215	-0.03472	-0.26445	3.51622	-3.49364	-0.23965	3.55064	3.50733	-0.26568
C	-5.73262	-0.83523	0.58247	4.68619	-3.35547	0.53396	3.49915	4.70526	0.47629
C	-5.57758	0.72918	-1.26216	3.41960	-4.58603	-1.12367	4.61317	3.32792	-1.17319
C	-7.12110	-0.85376	0.44984	5.71119	-4.29701	0.45024	4.48017	5.68582	0.32301
H	-5.25229	-1.43017	1.35342	4.77985	-2.51101	1.21053	2.69418	4.85389	1.19088
C	-6.96440	0.69166	-1.40723	4.45278	-5.51954	-1.21681	5.58695	4.31402	-1.33411
H	-4.97614	1.32851	-1.93839	2.54506	-4.68132	-1.75986	4.65990	2.41899	-1.76503
C	-7.74037	-0.09322	-0.54757	5.59792	-5.38250	-0.42584	5.52687	5.49443	-0.58474
H	-7.71870	-1.46269	1.12142	6.59880	-4.18380	1.06540	4.43113	6.59495	0.91497
H	-7.43889	1.27134	-2.19319	4.36765	-6.34805	-1.91354	6.39068	4.16370	-2.04872
H	-8.82038	-0.11549	-0.65716	6.39991	-6.11087	-0.49729	6.28914	6.25773	-0.70742
C	0.03442	-4.94964	-0.28995	3.51640	3.49345	-0.23967	-3.54647	3.51149	-0.26569
C	0.73008	-5.54562	-1.35773	3.41984	4.58584	-1.12368	-4.60935	3.33312	-1.17299
C	-0.69543	-5.77162	0.58827	4.68638	3.35521	0.53392	-3.49349	4.70948	0.47607
C	0.69840	-6.92892	-1.53845	4.45306	5.51930	-1.21684	-5.58202	4.32031	-1.33395
H	1.27297	-4.91787	-2.05753	2.54529	4.68118	-1.75986	-4.65724	2.42412	-1.76462
C	-0.70814	-7.15661	0.41821	5.71143	4.29670	0.45019	-4.47340	5.69114	0.32275
H	-1.24222	-5.31952	1.41048	4.78000	2.51075	1.21049	-2.68824	4.85730	1.19051
C	-0.01377	-7.73850	-0.64734	5.59820	5.38219	-0.42588	-5.52045	5.50080	-0.58481
H	1.22609	-7.37376	-2.37668	4.36797	6.34781	-1.91357	-6.38604	4.17079	-2.04840
H	-1.26243	-7.77987	1.11341	6.59905	4.18344	1.06534	-4.42323	6.60032	0.91454
H	-0.03155	-8.81531	-0.78539	6.40024	6.11052	-0.49734	-6.28186	6.26496	-0.70751
Ba	-0.01780	0.04823	1.63763	0.00000	0.00000	1.59892	0.00001	-0.03716	1.63448

H-BaTPP, total charge 0

		Doublet			**Quartet**			**Sextet**	
N	-0.06842	2.09832	0.01305	-2.08249	-0.00013	0.06772	-2.18737	-0.00052	-0.11433
N	2.12532	0.07433	0.08252	-0.00300	-2.19384	-0.13960	0.00048	-2.09323	0.07493
N	0.07383	-2.11093	0.12622	2.07448	0.00013	0.04940	2.18726	0.00048	-0.11393
N	-2.13266	-0.07456	0.15988	-0.00329	2.19385	-0.13959	-0.00048	2.09317	0.07506
C	-1.20048	2.86721	-0.04299	-2.85991	1.10325	-0.19576	-2.88109	1.10568	0.31049
C	-0.82672	4.27352	-0.07684	-4.14023	0.69506	-0.68178	-4.07737	0.68505	1.00984
C	0.53834	4.32039	-0.08328	-4.14014	-0.69558	-0.68178	-4.07706	-0.68701	1.00980
C	1.00771	2.94318	-0.05305	-2.85977	-1.10361	-0.19575	-2.88056	-1.10706	0.31050
C	2.37098	2.53836	-0.12490	-2.44714	-2.46840	0.09546	-2.46320	-2.47125	0.12049
C	2.86479	1.20367	-0.14252	-1.11081	-2.89829	0.26281	-1.10746	-2.89590	-0.09651
C	4.22936	0.82719	-0.47956	-0.68338	-4.11572	0.93713	-0.68599	-4.23363	-0.45964
C	4.27901	-0.53759	-0.46480	0.68037	-4.11485	0.93726	0.68796	-4.23332	-0.45962
C	2.94092	-1.00388	-0.13514	1.10612	-2.89779	0.26130	1.10881	-2.89540	-0.09643
C	2.53595	-2.36559	-0.10514	2.44090	-2.46902	0.08569	2.46434	-2.47012	0.12063
C	1.20796	-2.86521	-0.01858	2.84906	-1.10580	-0.21985	2.88101	-1.10575	0.31079
C	0.84068	-4.26169	-0.19556	4.11980	-0.69638	-0.72108	4.07739	-0.68515	1.01000
C	-0.52369	-4.31600	-0.18649	4.11972	0.69692	-0.72105	4.07710	0.68690	1.01000
C	-0.99930	-2.94966	-0.02084	2.84892	1.10617	-0.21984	2.88052	1.10699	0.31081
C	-2.35940	-2.54135	-0.09991	2.44058	2.46933	0.08572	2.46322	2.47117	0.12068
C	-2.85332	-1.20653	-0.11264	1.10574	2.89793	0.26132	1.10749	2.89582	-0.09642
C	-4.19069	-0.83424	-0.54617	0.67984	4.11494	0.93726	0.68604	4.23348	-0.45977
C	-4.23848	0.53060	-0.55524	-0.68391	4.11563	0.93715	-0.68793	4.23317	-0.45981
C	-2.93085	1.00078	-0.12645	-1.11119	2.89816	0.26281	-1.10879	2.89531	-0.09652
C	-2.53177	2.36757	-0.11423	-2.44746	2.46810	0.09546	-2.46435	2.47007	0.12051
H	-1.50847	5.11140	-0.09376	-4.94916	1.34968	-0.97570	-4.78988	1.34528	1.48335
H	1.16129	5.20272	-0.10759	-4.94898	-1.35031	-0.97571	-4.78928	-1.34759	1.48327
H	5.02880	1.50996	-0.72936	-1.34011	-4.83689	1.40262	-1.34110	-5.06125	-0.69128
H	5.12981	-1.16481	-0.68853	1.33810	-4.83483	1.40311	1.34346	-5.06064	-0.69123

H	1.53008	-5.08153	-0.33917	4.92463	-1.35095	-1.02625	4.78996	-1.34540	1.48339
H	-1.14319	-5.19247	-0.30806	4.92446	1.35159	-1.02621	4.78938	1.34747	1.48339
H	-4.96553	-1.52075	-0.85616	1.33748	4.83502	1.40310	1.34117	5.06107	-0.69148
H	-5.05896	1.15673	-0.87528	-1.34073	4.83672	1.40264	-1.34342	5.06046	-0.69156
C	3.61261	-3.39348	-0.28322	3.52021	-3.46723	0.27032	3.51287	-3.50926	0.24072
C	4.04293	-4.16544	0.80644	3.45948	-4.72406	-0.36406	4.72390	-3.39211	-0.47266
C	4.19528	-3.61488	-1.54068	4.63288	-3.18850	1.09007	3.34894	-4.62825	1.08312
C	5.03867	-5.13298	0.64548	4.47197	-5.66840	-0.18512	5.72328	-4.35905	-0.35996
H	3.59326	-4.00297	1.78201	2.61597	-4.94809	-1.00987	4.86984	-2.53522	-1.12371
C	5.18908	-4.58343	-1.70399	5.63730	-4.13696	1.27874	4.35131	-5.59150	1.20167
H	3.86013	-3.02624	-2.38981	4.68935	-2.22779	1.59145	2.43517	-4.72351	1.66119
C	5.61475	-5.34475	-0.61077	5.56401	-5.38024	0.63915	5.54224	-5.46495	0.47794
H	5.36290	-5.71980	1.50039	4.40953	-6.62714	-0.69250	6.64324	-4.25058	-0.92799
H	5.62745	-4.74488	-2.68488	6.47723	-3.90788	1.92867	4.20605	-6.43800	1.86724
H	6.38759	-6.09753	-0.73727	6.35061	-6.11573	0.78196	6.32127	-6.21640	0.56933
C	3.39247	3.62039	-0.27179	-3.52242	-3.47242	0.27578	-3.51121	-3.51090	0.24066
C	4.36464	3.82030	0.72249	-3.45973	-4.72248	-0.37156	-4.72234	-3.39437	-0.47263
C	3.41379	4.44583	-1.40853	-4.63171	-3.20713	1.10433	-3.34665	-4.62980	1.08306
C	5.32608	4.82499	0.58999	-4.46709	-5.67311	-0.19686	-5.72123	-4.36181	-0.35985
H	4.35888	3.18410	1.60285	-2.61846	-4.93642	-1.02368	-4.86876	-2.53756	-1.12369
C	4.37913	5.44590	-1.54597	-5.63092	-4.16195	1.28898	-4.34853	-5.59355	1.20170
H	2.67372	4.29032	-2.18788	-4.69035	-2.25153	1.61515	-2.43278	-4.72460	1.66106
C	5.33692	5.64091	-0.54563	-5.55578	-5.39825	0.63632	-5.53957	-5.46760	0.47805
H	6.06529	4.96966	1.37288	-4.40313	-6.62641	-0.71420	-6.64128	-4.25381	-0.92781
H	4.38505	6.06943	-2.43564	-6.46834	-3.94314	1.94566	-4.20279	-6.43997	1.86727
H	6.08631	6.42016	-0.65126	-6.33835	-6.13864	0.77595	-6.31822	-6.21945	0.56951
C	-3.62692	3.37034	-0.28339	-3.52288	3.47196	0.27575	-3.51280	3.50927	0.24066
C	-4.64389	3.47882	0.68028	-3.46036	4.72203	-0.37160	-3.34863	4.62835	1.08291
C	-3.67859	4.20691	-1.41141	-4.63216	3.20651	1.10425	-4.72394	3.39217	-0.47253
C	-5.67658	4.40695	0.52854	-4.46786	5.67251	-0.19693	-4.35090	5.59170	1.20150
H	-4.61616	2.83187	1.55229	-2.61910	4.93609	-1.02370	-2.43475	4.72360	1.66081
C	-4.71522	5.12950	-1.56872	-5.63151	4.16118	1.28888	-5.72322	4.35920	-0.35977
H	-2.90616	4.11926	-2.16953	-4.69068	2.25090	1.61506	-4.87006	2.53523	-1.12348
C	-5.71598	5.23535	-0.59740	-5.55653	5.39750	0.63622	-5.54195	5.46517	0.47798
H	-6.44935	4.48199	1.28845	-4.40403	6.62582	-0.71427	-4.20545	6.43827	1.86696
H	-4.74338	5.76176	-2.45177	-6.46892	3.94225	1.94552	-6.64327	4.25076	-0.92765
H	-6.52094	5.95462	-0.71852	-6.33921	6.13777	0.77583	-6.32091	6.21671	0.56941
C	-3.38309	-3.61432	-0.30208	3.51975	3.46768	0.27036	3.51124	3.51082	0.24077
C	-3.41718	-4.37358	-1.48327	4.63249	3.18906	1.09006	4.72244	3.39414	-0.47240
C	-4.35117	-3.86125	0.68486	3.45881	4.72455	-0.36394	3.34662	4.62989	1.08294
C	-4.38978	-5.35874	-1.66967	5.63678	4.13766	1.27874	5.72133	4.36159	-0.35971
H	-2.68182	-4.17840	-2.25817	4.68912	2.22833	1.59137	4.86890	2.53721	-1.12328
C	-5.32011	-4.85125	0.50320	4.47117	5.66902	-0.18498	4.34850	5.59365	1.20147
H	-4.33767	-3.27250	1.59765	2.61524	4.94849	-1.00969	2.43270	4.72482	1.66082
C	-5.34266	-5.60317	-0.67549	5.56328	5.38097	0.63924	5.53961	5.46755	0.47796
H	-4.40553	-5.93144	-2.59276	6.47677	3.90866	1.92862	6.64143	4.25347	-0.92757
H	-6.05681	-5.03322	1.28069	4.40857	6.62779	-0.69229	4.20271	6.44021	1.86686
H	-6.09787	-6.37055	-0.81957	6.34978	6.11657	0.78206	6.31826	6.21941	0.56934
Ba	0.02259	0.03346	1.67095	-0.01506	0.00000	-1.56607	0.00010	-0.00002	-1.53879
H	0.15252	0.17150	4.42278	1.33846	0.00006	2.10224	-0.01485	0.00548	2.02715

CdTPP, total charge 0

		Singlet			Triplet			Quintet	
N	2.15008	0.00002	-0.10236	0.00004	-2.17326	0.20394	-0.60881	-2.08169	-0.16311
N	0.00002	-2.14899	0.00000	2.15875	-0.00004	0.10597	-2.08169	0.60881	0.16311
N	-2.15008	-0.00002	0.10236	-0.00004	-2.17326	-0.20393	0.60881	2.08169	-0.16311
N	-0.00002	2.14900	0.00000	-2.15875	0.00004	0.10598	2.08169	-0.60881	0.16311
C	2.93282	1.12134	-0.02097	-1.12028	2.94203	0.01996	0.25122	-3.12849	0.08938
C	4.31443	0.68462	0.10516	-0.68248	4.28218	0.37759	-0.53502	-4.27602	0.48567
C	4.31444	-0.68455	0.10516	0.68264	4.28216	0.37759	-1.85362	-3.89036	0.48542
C	2.93284	-1.12130	-0.02097	1.12039	2.94198	0.01996	-1.89744	-2.50005	0.08901
C	2.46884	-2.46898	-0.00888	2.46054	2.49022	-0.03750	-3.07920	-1.68562	-0.00037
C	1.12187	-2.93478	-0.00575	2.92001	1.11584	-0.15189	-3.12849	-0.25122	-0.08938
C	0.68467	-4.32182	-0.00807	4.21682	0.69559	-0.56480	-4.27602	0.53502	-0.48567
C	-0.68460	-4.32183	0.00806	4.21680	-0.69575	-0.56480	-3.89036	1.85362	-0.48542
C	-1.12182	-2.93480	0.00575	2.91997	-1.11595	-0.15189	-2.50005	1.89744	-0.08901
C	-2.46880	-2.46902	0.00888	2.46044	-2.49031	-0.03750	-1.68562	3.07920	0.00037
C	-2.93282	-1.12135	0.02097	1.12028	-2.94203	0.01996	-0.25122	3.12849	0.08938

C	-4.31443	-0.68462	-0.10516	0.68248	-4.28219	0.37759	0.53502	4.27602	0.48567
C	-4.31444	0.68455	-0.10516	-0.68264	-4.28216	0.37759	1.85362	3.89036	0.48542
C	-2.93284	1.12130	0.02097	-1.12039	-2.94198	0.01996	1.89744	2.50005	0.08901
C	-2.46884	2.46898	0.00888	-2.46054	-2.49022	-0.03750	3.07920	1.68562	-0.00037
C	-1.12187	2.93478	0.00575	-2.92001	-1.11584	-0.15189	3.12849	0.25122	-0.08938
C	-0.68467	4.32182	0.00807	-4.21682	-0.69559	-0.56481	4.27602	-0.53502	-0.48567
C	0.68460	4.32183	-0.00807	-4.21679	0.69575	-0.56481	3.89036	-1.85362	-0.48542
C	1.12182	2.93480	-0.00575	-2.91997	1.11595	-0.15189	2.50005	-1.89744	-0.08901
C	2.46880	2.46902	-0.00888	-2.46044	2.49031	-0.03750	1.68562	-3.07920	0.00037
H	5.17122	1.33516	0.20669	-1.33397	5.10347	0.63874	-0.13545	-5.23922	0.76754
H	5.17124	-1.33507	0.20670	1.33416	5.10342	0.63874	-2.70935	-4.48641	0.76704
H	1.33411	-5.18514	-0.02447	5.03047	1.34661	-0.85039	-5.23922	0.13545	-0.76754
H	-1.33402	-5.18516	0.02445	5.03042	-1.34680	-0.85039	-4.48641	2.70935	-0.76704
H	-5.17122	-1.33516	-0.20669	1.33397	-5.10347	0.63873	0.13545	5.23922	0.76754
H	-5.17124	1.33507	-0.20669	-1.33416	-5.10342	0.63874	2.70935	4.48641	0.76704
H	-1.33411	5.18514	0.02446	-5.03046	-1.34661	-0.85041	5.23922	-0.13545	-0.76754
H	1.33402	5.18516	-0.02446	-5.03041	1.34680	-0.85041	4.48641	-2.70935	-0.76704
C	-3.53140	-3.52447	-0.02568	3.52634	-3.52539	0.00954	-2.39856	4.38137	0.00077
C	-4.39191	-3.70753	1.06885	3.52474	-4.60756	-0.89032	-2.04803	5.39883	-0.90835
C	-3.69209	-4.34639	-1.15295	4.56783	-3.44023	0.95329	-3.44437	4.63369	0.91029
C	-5.38565	-4.68926	1.03928	4.52852	-5.57709	-0.84438	-2.72064	6.62161	-0.91046
H	-4.27281	-3.07713	1.94532	2.73833	-4.67259	-1.63603	-1.25077	5.21598	-1.62251
C	-4.68718	-5.32657	-1.18556	5.56270	-4.41643	1.00805	-4.11220	5.85908	0.91322
H	-3.03468	-4.20712	-2.00627	4.58167	-2.60720	1.64911	-3.71959	3.86311	1.62411
C	-5.53684	-5.50186	-0.08870	5.54866	-5.48792	0.10763	-3.75482	6.85840	0.00159
H	-6.03900	-4.82021	1.89741	4.51587	-6.39855	-1.55522	-2.44057	7.38800	-1.62785
H	-4.80044	-5.94972	-2.06831	6.34950	-4.34143	1.75339	-4.90856	6.03561	1.63091
H	-6.31007	-6.26444	-0.11303	6.32784	-6.24382	0.14598	-4.27649	7.81115	0.00190
C	3.53146	-3.52441	0.02568	3.52648	3.52526	0.00954	-4.38137	-2.39856	-0.00077
C	3.69216	-4.34634	1.15295	4.56796	3.44006	0.95328	-5.39883	-2.04803	0.90835
C	4.39198	-3.70746	-1.06885	3.52491	4.60743	-0.89032	-4.63369	-3.44437	-0.91029
C	4.68727	-5.32649	1.18555	5.56287	4.41623	1.00804	-6.62161	-2.72064	0.91046
H	3.03475	-4.20708	2.00627	4.58177	2.60702	1.64910	-5.21598	-1.25077	1.62251
C	5.38573	-4.68917	-1.03928	4.52873	5.57692	-0.84439	-5.85908	-4.11220	-0.91322
H	4.27286	-3.07705	-1.94532	2.73850	4.67249	-1.63603	-3.86311	-3.71959	-1.62411
C	5.53693	-5.50177	0.08870	5.54887	5.48771	0.10763	-6.85840	-3.75482	-0.00159
H	4.80053	-5.94965	2.06830	6.34967	4.34119	1.75339	-7.38800	-2.44057	1.62785
H	6.03909	-4.82010	-1.89741	4.51611	6.39838	-1.55522	-6.03561	-4.90856	-1.63091
H	6.31018	-6.26434	0.11302	6.32808	6.24358	0.14597	-7.81115	-4.27649	-0.00190
C	3.53140	3.52447	0.02568	-3.52634	3.52539	0.00954	2.39857	-4.38137	0.00077
C	3.69209	4.34639	1.15295	-4.56783	3.44023	0.95329	3.44437	-4.63369	0.91029
C	4.39191	3.70753	-1.06885	-3.52474	4.60756	-0.89032	2.04803	-5.39883	-0.90835
C	4.68718	5.32657	1.18555	-5.56270	4.41644	1.00805	4.11220	-5.85908	0.91322
H	3.03468	4.20713	2.00627	-4.58167	2.60720	1.64911	3.71959	-3.86311	1.62411
C	5.38565	4.68926	-1.03928	-4.52852	5.57709	-0.84438	2.72064	-6.62161	-0.91046
H	4.27281	3.07713	-1.94532	-2.73833	4.67259	-1.63603	1.25077	-5.21598	-1.62251
C	5.53684	5.50186	0.08870	-5.54866	5.48792	0.10764	3.75483	-6.85840	0.00159
H	4.80044	5.94973	2.06830	-6.34950	4.34143	1.75339	4.90856	-6.03561	1.63091
H	6.03900	4.82021	-1.89741	-4.51587	6.39855	-1.55522	2.44057	-7.38800	-1.62785
H	6.31007	6.26444	0.11303	-6.32784	6.24382	0.14598	4.27649	-7.81115	0.00190
C	-3.53146	3.52441	-0.02568	-3.52648	-3.52526	0.00954	4.38137	2.39857	-0.00077
C	-4.39197	3.70746	1.06885	-3.52492	-4.60742	-0.89033	4.63369	3.44437	-0.91029
C	-3.69216	4.34633	-1.15295	-4.56796	-3.44007	0.95329	5.39883	2.04803	0.90835
C	-5.38573	4.68917	1.03928	-4.52874	-5.57691	-0.84439	5.85908	4.11220	-0.91322
H	-4.27286	3.07706	1.94532	-2.73851	-4.67248	-1.63604	3.86311	3.71959	-1.62411
C	-4.68727	5.32649	-1.18555	-5.56286	-4.41623	1.00805	6.62161	2.72064	0.91046
H	-3.03475	4.20708	-2.00627	-4.58176	-2.60704	1.64912	5.21598	1.25077	1.62251
C	-5.53693	5.50177	-0.08870	-5.54887	-5.48771	0.10763	6.85840	3.75482	-0.00159
H	-6.03908	4.82011	1.89741	-4.51612	-6.39836	-1.55524	6.03561	4.90856	-1.63091
H	-4.80053	5.94965	-2.06830	-6.34966	-4.34120	1.75340	7.38800	2.44057	1.62785
H	-6.31018	6.26434	-0.11303	-6.32808	-6.24358	0.14597	7.81115	4.27649	-0.00190
Cd	0.00000	0.00000	0.00000	0.00000	0.00000	0.02287	0.00000	0.00000	0.00000

CdTPP, total charge 1

		Doublet			Quartet			Sextet	
N	-2.15558	-0.00001	-0.16672	2.16067	0.00011	-0.13572	1.50866	1.54361	-0.24011
N	-0.00008	2.15409	0.00108	0.00011	-2.15888	0.18770	1.51849	-1.49551	-0.06241
N	2.15534	0.00001	0.16541	-2.16067	-0.00011	-0.13572	-1.50762	-1.50649	0.06207
N	-0.00006	-2.15409	0.00108	-0.00011	2.15888	0.18770	-1.51954	1.53252	0.23894
C	-2.93814	-1.11569	-0.04100	2.91070	1.11222	0.14936	1.26444	2.86358	0.03887

C	-4.30752	-0.68546	0.15797	4.20968	0.68902	0.60583	2.52464	3.49287	0.34848
C	-4.30753	0.68542	0.15797	4.20975	-0.68860	0.60584	3.50942	2.51176	0.30876
C	-2.93815	1.11566	-0.04100	2.91081	-1.11193	0.14936	2.87826	1.27989	-0.00341
C	-2.47185	2.47302	-0.02118	2.46013	-2.49296	0.03217	3.52240	-0.00034	-0.04849
C	-1.11667	2.94399	-0.01267	1.11927	-2.93265	-0.02215	2.87974	-1.27184	-0.11136
C	-0.68531	4.32725	-0.01916	0.67806	-4.29230	-0.35746	3.53849	-2.55711	-0.20230
C	0.68540	4.32724	0.01389	-0.67764	-4.29237	-0.35743	2.56870	-3.52227	-0.15152
C	1.11664	2.94392	0.01189	-1.11897	-2.93277	-0.02215	1.28637	-2.85480	-0.07340
C	2.47177	2.47294	0.02125	-2.45988	-2.49320	0.03217	0.01260	-3.50074	0.00000
C	2.93820	1.11569	0.04208	-2.91070	-1.11222	0.14936	-1.26581	-2.86400	0.07330
C	4.30815	0.68546	-0.15316	-4.20968	-0.68902	0.60582	-2.54335	-3.54069	0.15161
C	4.30816	-0.68541	-0.15316	-4.20975	0.68860	0.60583	-3.51999	-2.58253	0.20245
C	2.93821	-1.11566	0.04207	-2.91081	1.11193	0.14936	-2.87045	-1.29253	0.11117
C	2.47179	-2.47291	0.02125	-2.46013	2.49296	0.03217	-3.52216	-0.02569	0.04822
C	1.11667	-2.94391	0.01189	-1.11927	2.93265	-0.02215	-2.88716	1.25906	0.00293
C	0.68545	-4.32723	0.01389	-0.67807	4.29230	-0.35745	-3.52732	2.48652	-0.30933
C	-0.68527	-4.32725	-0.01916	0.67764	4.29237	-0.35744	-2.54985	3.47450	-0.34925
C	-1.11664	-2.94400	-0.01267	1.11897	2.93277	-0.02215	-1.28508	2.85427	-0.03961
C	-2.47183	-2.47304	-0.02118	2.45988	2.49320	0.03216	-0.01269	3.51977	-0.00030
H	-5.15570	-1.33423	0.31770	5.00724	1.34597	0.91993	2.65865	4.54346	0.56088
H	-5.15571	1.33418	0.31770	5.00737	-1.34546	0.91995	4.56139	2.64317	0.51156
H	-1.33180	5.19113	-0.05313	1.33357	-5.11309	-0.60827	4.60447	-2.70485	-0.28419
H	1.33197	5.19117	0.04470	-1.33307	-5.11323	-0.60823	2.70891	-4.59231	-0.17934
H	5.15680	1.33423	-0.31032	-5.00725	-1.34597	0.91991	-2.67587	-4.61171	0.17959
H	5.15682	-1.33418	-0.31033	-5.00738	1.34546	0.91993	-4.58486	-2.73790	0.28452
H	1.33202	-5.19116	0.04470	-1.33358	5.11309	-0.60825	-4.58023	2.61023	-0.51207
H	-1.33175	-5.19114	-0.05313	1.33306	5.11323	-0.60825	-2.69133	4.52404	-0.56195
C	3.53122	3.51758	-0.02481	-3.52930	-3.52003	-0.00409	0.01795	-4.99013	0.00005
C	4.47506	3.61469	1.01415	-3.52172	-4.60411	0.89494	-0.41154	-5.70555	1.13226
C	3.61145	4.41407	-1.10619	-4.58245	-3.41961	-0.93477	0.45252	-5.70253	-1.13212
C	5.46577	4.59657	0.97885	-4.53490	-5.56304	0.85953	-0.39912	-7.10132	1.13380
H	4.41524	2.93061	1.85529	-2.73216	-4.67568	1.63703	-0.73933	-5.16277	2.01413
C	4.61711	5.38030	-1.14903	-5.58554	-4.38725	-0.97778	0.45008	-7.09836	-1.13358
H	2.89770	4.33467	-1.92054	-4.59728	-2.59069	-1.63609	0.77641	-5.15747	-2.01402
C	5.54238	5.47820	-0.10443	-5.56631	-5.46033	-0.07945	0.02800	-7.80109	0.00013
H	6.17719	4.67252	1.79552	-4.52244	-6.38559	1.56819	-0.72036	-7.64152	2.01922
H	4.67914	6.05470	-1.99765	-6.38110	-4.30577	-1.71218	0.77518	-7.63630	-2.01896
H	6.31923	6.23605	-0.13515	-6.35213	-6.20892	-0.10898	0.03188	-8.88678	0.00017
C	-3.53124	3.51758	0.02460	3.52966	-3.51968	-0.00408	5.00831	0.00859	0.01638
C	-3.60931	4.41674	1.10398	3.52224	-4.60371	0.89500	5.68845	-0.63138	1.06884
C	-4.47733	3.61215	-1.01262	4.58276	-3.41919	-0.93481	5.75934	0.66710	-0.97542
C	-4.61496	5.38295	1.14661	4.53552	-5.56253	0.85960	7.08263	-0.61102	1.12838
H	-2.89391	4.33931	1.91706	2.73272	-4.67533	1.63714	5.11835	-1.12930	1.84767
C	-5.46799	4.59405	-0.97764	5.58595	-4.38672	-0.97782	7.15380	0.67541	-0.92109
H	-4.41916	2.92612	-1.85227	4.59747	-2.59031	-1.63618	5.24373	1.15654	-1.79657
C	-5.54241	5.47828	0.10369	5.56688	-5.45976	-0.07944	7.81921	0.03908	0.13215
H	-4.67532	6.05936	1.99376	4.52318	-6.38504	1.56830	7.59338	-1.09816	1.95354
H	-6.18109	4.66804	-1.79302	6.38147	-4.30520	-1.71226	7.72019	1.17504	-1.70124
H	-6.31924	6.23614	0.13421	6.35277	-6.20827	-0.10896	8.90395	0.04992	0.17667
C	-3.53120	-3.51761	0.02460	3.52930	3.52003	-0.00409	-0.01809	5.00091	0.00003
C	-3.60926	-4.41678	1.10398	3.52174	4.60410	0.89496	-0.76672	5.71774	0.95471
C	-4.47730	-3.61219	-1.01261	4.58244	3.41962	-0.93479	0.72528	5.72362	-0.95433
C	-4.61490	-5.38300	1.14661	4.53492	5.56302	0.85955	-0.76555	7.11269	0.95859
H	-2.89385	-4.33935	1.91706	2.73219	4.67565	1.63707	-1.33193	5.17405	1.70628
C	-5.46796	-4.59410	-0.97763	5.58552	4.38726	-0.97780	0.71392	7.11852	-0.95758
H	-4.41914	-2.92615	-1.85226	4.59725	2.59072	-1.63613	1.29437	5.18440	-1.70619
C	-5.54236	-5.47833	0.10369	5.56632	5.46033	-0.07945	-0.02837	7.81764	0.00066
H	-4.67524	-6.05941	1.99375	4.52248	6.38555	1.56822	-1.33567	7.64947	1.71081
H	-6.18105	-4.66809	-1.79301	6.38108	4.30580	-1.71221	1.28008	7.65979	-1.70958
H	-6.31918	-6.23621	0.13421	6.35213	6.20892	-0.10898	-0.03234	8.90331	0.00090
C	3.53125	-3.51754	-0.02481	-3.52965	3.51967	-0.00408	-5.00813	-0.02737	-0.01628
C	4.47509	-3.61465	1.01415	-4.58278	3.41916	-0.93478	-5.68393	-0.67183	-1.06879
C	3.61150	-4.41403	-1.10620	-3.52222	4.60373	0.89498	-5.76359	0.62544	0.97591
C	5.46581	-4.59652	0.97885	-5.58597	4.38670	-0.97780	-7.07825	-0.66146	-1.12795
H	4.41525	-2.93058	1.85529	-4.59751	2.59027	-1.63613	-5.11048	-1.16536	-1.84796
C	4.61717	-5.38025	-1.14904	-4.53549	5.56256	0.85957	-7.15809	0.62377	0.92194
H	2.89775	-4.33463	-1.92055	-2.73268	4.67537	1.63709	-5.25128	1.11834	1.79706
C	5.54244	-5.47815	-0.10443	-5.56687	5.45976	-0.07944	-7.81920	-0.01700	-0.13132
H	6.17722	-4.67247	1.79552	-6.38151	4.30516	-1.71221	-7.58570	-1.15199	-1.95315
H	4.67921	-6.05464	-1.99767	-4.52314	6.38508	1.56825	-7.72784	1.11910	1.70238

H	6.31929	-6.23599	-0.13515	-6.35276	6.20827	-0.10897	-8.90400	-0.01392	-0.17556
Cd	-0.00020	0.00000	0.00077	0.00000	0.00000	-0.10322	-0.00001	0.01278	-0.00015

H-CdTPP, total charge 0

		Doublet			**Quartet**			**Sextet**	
N	-2.08958	-0.00004	-0.09716	1.23486	1.60238	-0.03146	-0.00153	-2.16820	-0.17343
N	-0.00427	2.09012	-0.00974	1.68531	-1.32544	-0.12967	-2.17072	0.00153	0.15297
N	2.09189	0.00005	0.07386	-1.27079	-1.73770	-0.10474	0.00153	2.16819	-0.17344
N	-0.00418	-2.09012	-0.00976	-1.62590	1.19758	0.03676	2.17072	-0.00153	0.15297
C	-2.90162	-1.09987	-0.10079	0.88196	2.87753	0.26900	1.11672	-2.93351	0.07777
C	-4.29485	-0.68231	-0.08991	2.08270	3.72272	0.36311	0.68392	-4.25586	0.47320
C	-4.29489	0.68212	-0.08991	3.14070	2.92626	0.06435	-0.68992	-4.25488	0.47322
C	-2.90167	1.09975	-0.10079	2.60042	1.58973	-0.19082	-1.12086	-2.93193	0.07779
C	-2.45295	2.44613	-0.10139	3.35835	0.46456	-0.57981	-2.48313	-2.48104	-0.01415
C	-1.10485	2.89475	-0.09072	2.87335	-0.86561	-0.67432	-2.93054	-1.11768	-0.10779
C	-0.68885	4.28213	-0.21493	3.54394	-1.96007	-1.34831	-4.24710	-0.68400	-0.52013
C	0.67591	4.28592	-0.20003	2.74295	-3.06190	-1.20088	-4.24613	0.69000	-0.52012
C	1.09613	2.89898	-0.08574	1.60518	-2.63403	-0.40538	-2.92896	1.12181	-0.10781
C	2.44140	2.44845	-0.09115	0.47818	-3.47083	0.03452	-2.47963	2.48453	-0.01418
C	2.88913	1.10045	-0.06882	-0.84887	-2.98182	-0.36607	-1.11672	2.93351	0.07777
C	4.26177	0.68266	-0.29868	-1.85111	-3.71669	-1.11961	-0.68392	4.25585	0.47319
C	4.26179	-0.68247	-0.29868	-2.91929	-2.87185	-1.26274	0.68992	4.25488	0.47322
C	2.88918	-1.10032	-0.06882	-2.54916	-1.62144	-0.62723	1.12086	2.93193	0.07778
C	2.44151	-2.44834	-0.09115	-3.35856	-0.45886	-0.57699	2.48313	2.48104	-0.01415
C	1.09627	-2.89893	-0.08575	-2.92912	0.83648	-0.21750	2.93054	1.11768	-0.10779
C	0.67610	-4.28589	-0.20002	-3.79228	2.01527	-0.12639	4.24710	0.68400	-0.52013
C	-0.68866	-4.28216	-0.21492	-2.98428	3.06820	0.15901	4.24613	-0.69000	-0.52012
C	-1.10472	-2.89480	-0.09073	-1.61564	2.53613	0.24382	2.92896	-1.12181	-0.10781
C	-2.45284	-2.44624	-0.10140	-0.45388	3.33915	0.43747	2.47963	-2.48454	-0.01418
H	-5.15270	-1.33839	-0.07033	2.09784	4.76912	0.63065	1.33723	-5.06935	0.75304
H	-5.15277	1.33816	-0.07032	4.18616	3.19794	0.04081	-1.34438	-5.06745	0.75309
H	-1.34666	5.13274	-0.31785	4.47430	-1.88691	-1.89287	-5.05548	-1.33765	-0.81368
H	1.32982	5.14256	-0.27021	2.89264	-4.05694	-1.59698	-5.05360	1.34478	-0.81366
H	5.09991	1.34051	-0.47665	-1.73853	-4.72414	-1.49601	-1.33723	5.06935	0.75304
H	5.09997	-1.34028	-0.47666	-3.84740	-3.06195	-1.78215	1.34438	5.06744	0.75308
H	1.33005	-5.14250	-0.27019	-4.86327	2.02437	-0.26668	5.05549	1.33765	-0.81367
H	-1.34643	-5.13281	-0.31783	-3.26347	4.10475	0.28085	5.05360	-1.34478	-0.81366
C	3.50683	3.49336	-0.18453	0.66584	-4.72026	0.70904	-3.52993	3.53334	-0.01710
C	4.38606	3.70049	0.89040	-0.44171	-5.52266	1.11829	-3.47441	4.61167	-0.92207
C	3.65692	4.27001	-1.34448	1.96570	-5.19107	1.06472	-4.61097	3.47733	0.88461
C	5.38680	4.67185	0.81132	-0.25490	-6.72450	1.78816	-4.46438	5.59523	-0.92734
H	4.27581	3.10004	1.78863	-1.45094	-5.17993	0.92034	-2.65343	4.66332	-1.63086
C	4.66477	5.23358	-1.42750	2.13991	-6.39467	1.73481	-5.59710	4.46475	0.88442
H	2.98547	4.10717	-2.18234	2.83513	-4.59021	0.82356	-4.66300	2.65762	1.59487
C	5.53037	5.43970	-0.34856	1.03549	-7.18090	2.09456	-5.52961	5.52772	-0.02278
H	6.05378	4.82695	1.65457	-1.12136	-7.30900	2.08524	-4.40689	6.41195	-1.64157
H	4.77410	5.82096	-2.33476	3.14419	-6.72183	1.98982	-6.41593	4.40692	1.59620
H	6.31161	6.19172	-0.41186	1.17673	-8.12183	2.61778	-6.29866	6.29481	-0.02495
C	-3.50613	3.50629	-0.13377	4.78517	0.68718	-0.95201	-3.53490	-3.52837	-0.01704
C	-3.68201	4.36446	0.96378	5.81093	-0.00447	-0.28424	-4.61580	-3.47089	0.88475
C	-4.33224	3.66351	-1.25818	5.13110	1.58353	-1.97792	-3.48092	-4.60677	-0.92202
C	-4.66793	5.35356	0.93994	7.14848	0.20423	-0.62550	-5.60330	-4.45695	0.88460
H	-3.04683	4.24552	1.83660	5.55105	-0.69529	0.51214	-4.66665	-2.65113	1.59504
C	-5.31053	4.66015	-1.28619	6.46847	1.78356	-2.32687	-4.47225	-5.58897	-0.92723
H	-4.19716	3.00533	-2.11141	4.34357	2.11090	-2.50781	-2.66005	-4.65956	-1.63085
C	-5.48321	5.50608	-0.18603	7.48126	1.09716	-1.64956	-5.53733	-5.51999	-0.02261
H	-4.79836	6.00374	1.80032	7.92980	-0.32878	-0.09127	-6.42200	-4.39799	1.59644
H	-5.93628	4.77537	-2.16668	6.71833	2.47248	-3.12873	-4.41593	-6.40575	-1.64148
H	-6.24689	6.27826	-0.20613	8.52170	1.25588	-1.91819	-6.30744	-6.28602	-0.02475
C	-3.50597	-3.50645	-0.13378	-0.66873	4.77663	0.77390	3.52993	-3.53334	-0.01710
C	-3.68183	-4.36460	0.96378	-1.26932	5.13209	1.99391	4.61097	-3.47733	0.88461
C	-4.33206	-3.66371	-1.25820	-0.29590	5.79911	-0.11507	3.47441	-4.61167	-0.92208
C	-4.66770	-5.35375	0.93993	-1.48560	6.47339	2.31888	5.59710	-4.46476	0.88442
H	-3.04667	-4.24562	1.83661	-1.55732	4.34825	2.68870	4.66300	-2.65763	1.59488
C	-5.31031	-4.66039	-1.28621	-0.51364	7.14062	0.20806	4.46438	-5.59523	-0.92734
H	-4.19700	-3.00554	-2.11143	0.15646	5.53443	-1.06659	2.65343	-4.66332	-1.63087
C	-5.48297	-5.50632	-0.18605	-1.10837	7.48232	1.42698	5.52961	-5.52772	-0.02278
H	-4.79812	-6.00393	1.80032	-1.94498	6.72935	3.26951	6.41593	-4.40692	1.59620
H	-5.93604	-4.77566	-2.16671	-0.22406	7.91750	-0.49411	4.40689	-6.41194	-1.64158
H	-6.24662	-6.27853	-0.20615	-1.27701	8.52539	1.67893	6.29866	-6.29481	-0.02495

C	3.50699	-3.49320	-0.18453	-4.78552	-0.62526	-0.98619	3.53490	3.52837	-0.01704
C	4.38623	-3.70028	0.89041	-5.63346	-1.48114	-0.26340	4.61580	3.47089	0.88475
C	3.65711	-4.26985	-1.34447	-5.30075	0.05482	-2.10212	3.48092	4.60677	-0.92202
C	5.38701	-4.67159	0.81133	-6.96858	-1.64268	-0.63971	5.60330	4.45695	0.88460
H	4.27594	-3.09984	1.78864	-5.24057	-2.00949	0.60018	4.66665	2.65113	1.59503
C	4.66501	-5.23338	-1.42748	-6.63327	-0.11516	-2.48491	4.47224	5.58897	-0.92723
H	2.98566	-4.10705	-2.18233	-4.64718	0.70768	-2.67303	2.66005	4.65956	-1.63085
C	5.53062	-5.43945	-0.34854	-7.47186	-0.96167	-1.75287	5.53733	5.51999	-0.02261
H	6.05400	-4.82666	1.65459	-7.61443	-2.29947	-0.06398	6.42200	4.39800	1.59644
H	4.77437	-5.82076	-2.33474	-7.01446	0.41104	-3.35545	4.41592	6.40575	-1.64148
H	6.31189	-6.19143	-0.41183	-8.50909	-1.09083	-2.04837	6.30744	6.28602	-0.02474
Cd	-0.01820	-0.00001	1.06927	0.02538	-0.17505	1.11144	0.00000	0.00000	0.06922
H	-0.16795	-0.00009	2.78252	0.06573	-0.08652	2.82162	0.00014	0.00015	2.69443

CoTPP, total charge 0

		Doublet			**Quartet**			**Sextet**	
N	-1.99464	0.00001	-0.00755	0.01104	1.99538	-0.01382	-0.15012	2.04749	-0.01836
N	0.00001	1.99491	-0.00004	2.02122	-0.00004	0.00000	2.06408	0.15147	-0.00614
N	1.99463	-0.00002	0.00763	0.01096	-1.99538	0.01382	0.15150	-2.05008	0.02152
N	-0.00002	-1.99492	-0.00004	-1.97911	0.00004	0.00000	-2.06392	-0.15399	0.05004
C	-2.83346	-1.09827	0.01508	-1.05997	2.83387	0.23598	-1.31087	2.79057	0.07404
C	-4.21350	-0.67981	0.06471	-0.64360	4.18920	0.25640	-1.00111	4.16470	0.23994
C	-4.21349	0.67985	0.06486	0.71244	4.19064	-0.02507	0.38450	4.26674	0.23311
C	-2.83345	1.09830	0.01529	1.09554	2.83383	-0.17651	0.89046	2.95236	0.06456
C	-2.43580	2.43594	0.01479	2.44804	2.40719	-0.33925	2.28665	2.61512	0.01339
C	-1.09832	2.83405	0.00699	2.85899	1.08504	-0.19264	2.80725	1.31558	-0.02782
C	-0.67980	4.21490	-0.00051	4.24181	0.66364	-0.14406	4.21731	0.98991	-0.09827
C	0.67987	4.21489	-0.00003	4.24179	-0.66380	0.14407	4.31628	-0.36831	-0.08939
C	1.09836	2.83402	-0.00722	2.85894	-1.08515	0.19264	2.96751	-0.89358	-0.03788
C	2.43584	2.43590	-0.01479	2.44794	-2.40729	0.33925	2.64279	-2.25391	0.00795
C	2.83346	1.09825	-0.01506	1.09543	-2.83387	0.17650	1.31388	-2.79590	0.05663
C	4.21351	0.67979	-0.06431	0.71227	-4.19067	0.02507	1.00712	-4.17990	0.10579
C	4.21350	-0.67988	-0.06416	-0.64377	-4.18917	-0.25641	-0.37833	-4.28280	0.10997
C	2.83345	-1.09831	-0.01485	-1.06008	-2.83383	-0.23598	-0.88722	-2.96023	0.04246
C	2.43580	-2.43595	-0.01442	-2.41056	-2.40062	-0.39108	-2.28271	-2.61986	-0.00401
C	1.09832	-2.83406	-0.00701	-2.81568	-1.07865	-0.22252	-2.80240	-1.31933	-0.02485
C	0.67981	-4.21491	0.00012	-4.19907	-0.66315	-0.14704	-4.20685	-0.99543	-0.16859
C	-0.67987	-4.21491	-0.00066	-4.19904	0.66332	0.14704	-4.30766	0.36268	-0.16548
C	-1.09836	-2.83405	0.00678	-2.81564	1.07877	0.22252	-2.96651	0.88982	-0.01815
C	-2.43584	-2.43592	0.01442	-2.41046	2.40071	0.39108	-2.64298	2.25237	0.01975
H	-5.06057	-1.34823	0.10681	-1.27673	5.04013	0.45542	-1.71529	4.96459	0.36552
H	-5.06055	1.34827	0.10710	1.37631	5.04007	-0.08247	0.97533	5.16248	0.35255
H	-1.34797	5.06317	-0.00468	5.09393	1.30999	-0.28967	5.02234	1.70784	-0.14857
H	1.34806	5.06314	0.00394	5.09387	-1.31019	0.28967	5.21705	-0.96360	-0.11405
H	5.06059	1.34820	-0.10636	1.37611	-5.04013	0.08246	1.72353	-4.98731	0.12792
H	5.06057	-1.34831	-0.10607	-1.27693	-5.04008	-0.45543	-0.96650	-5.18681	0.15778
H	1.34799	-5.06318	0.00423	-5.04885	-1.31592	-0.28018	-5.00464	-1.71434	-0.28219
H	-1.34804	-5.06317	-0.00497	-5.04880	1.31612	0.28018	-5.20292	0.95599	-0.27777
C	3.49526	3.49330	-0.02768	3.46566	-3.46597	0.59379	3.76850	-3.23510	0.00375
C	4.24291	3.76766	1.12748	3.45872	-4.16568	1.81191	4.06827	-3.98053	1.15546
C	3.75926	4.22570	-1.19500	4.42353	-3.80421	-0.37576	4.54358	-3.42982	-1.15035
C	5.23277	4.75418	1.11695	4.40121	-5.16494	2.06273	5.12636	-4.89220	1.15579
H	4.04157	3.20422	2.03415	2.71185	-3.91732	2.56019	3.46991	-3.83626	2.05022
C	4.74990	5.21136	-1.20791	5.36055	-4.81078	-0.12863	5.59743	-4.34750	-1.15263
H	3.18480	4.01551	-2.09269	4.42144	-3.28148	-1.32764	4.31168	-2.86101	-2.04613
C	5.48926	5.47865	-0.05137	5.35492	-5.49128	1.09267	5.89334	-5.07967	0.00109
H	5.80111	4.95708	2.02038	4.38934	-5.68953	3.01397	5.35149	-5.45504	2.05734
H	4.94467	5.76773	-2.12053	6.09093	-5.06498	-0.89163	6.18499	-4.49013	-2.05523
H	6.25899	6.24511	-0.06052	6.08502	-6.27200	1.28594	6.71414	-5.79118	0.00062
C	-3.49521	3.49335	0.02768	3.46580	3.46583	-0.59378	3.25064	3.75268	0.02105
C	-3.75880	4.22617	1.19483	4.42368	3.80404	0.37576	4.13040	3.94311	1.09950
C	-4.24326	3.76732	-1.12732	3.45889	4.16554	-1.81191	3.28989	4.66011	-1.05135
C	-4.74943	5.21184	1.20775	5.36074	4.81057	0.12864	5.03034	5.01176	1.10429
H	-3.18403	4.01628	2.09240	4.42157	3.28130	1.32765	4.09765	3.25255	1.93705
C	-5.23310	4.75386	-1.11679	4.40142	5.16476	-2.06273	4.19691	5.72145	-1.05197
H	-4.04224	3.20357	-2.03386	2.71201	3.91721	-2.56019	2.60853	4.52217	-1.88551
C	-5.48918	5.47874	0.05137	5.35514	5.49106	-1.09266	5.06890	5.90219	0.02713
H	-4.94388	5.76853	2.12024	6.09112	5.06474	0.89164	5.69853	5.14875	1.94986

H	-5.80174	4.95646	-2.02009	4.38957	5.68935	-3.01397	4.22226	6.40719	-1.89419
H	-6.25891	6.24521	0.06052	6.08528	6.27175	-1.28594	5.77094	6.73111	0.02874
C	-3.49527	-3.49331	0.02704	-3.45380	3.42452	0.68122	-3.76438	3.23356	0.00613
C	-3.75906	-4.22626	1.19406	-4.13832	3.40764	1.90737	-4.69972	3.27016	1.05411
C	-4.24318	-3.76710	-1.12810	-3.78352	4.40933	-0.26484	-3.90509	4.14348	-1.05617
C	-4.74973	-5.21190	1.20672	-5.12705	4.35546	2.18348	-5.75042	4.19070	1.03971
H	-3.18441	-4.01650	2.09174	-3.88681	2.64929	2.64311	-4.59130	2.57772	1.88364
C	-5.23306	-4.75360	-1.11783	-4.77825	5.35070	0.00733	-4.96201	5.05508	-1.07668
H	-4.04201	-3.20324	-2.03454	-3.26161	4.42464	-1.21687	-3.18391	4.12378	-1.86759
C	-5.48933	-5.47862	0.05020	-5.45126	5.32868	1.23362	-5.88710	5.08368	-0.02731
H	-4.94432	-5.76869	2.11911	-5.64276	4.33250	3.13936	-6.45961	4.21076	1.86244
H	-5.80158	-4.95607	-2.02124	-5.02896	6.09952	-0.73877	-5.06321	5.74288	-1.91149
H	-6.25908	-6.24507	0.05915	-6.22236	6.06365	1.44621	-6.70616	5.79706	-0.04094
C	3.49522	-3.49335	-0.02704	-3.45394	-3.42438	-0.68122	-3.25220	-3.75228	-0.04194
C	4.24272	-3.76756	1.12826	-3.78370	-4.40918	0.26484	-3.29008	-4.62586	-1.14211
C	3.75939	-4.22590	-1.19423	-4.13846	-3.40747	-1.90737	-4.14599	-3.96508	1.02067
C	5.23258	-4.75408	1.11799	-4.77846	-5.35051	-0.00733	-4.20726	-5.67765	-1.18346
H	4.04125	-3.20401	2.03483	-3.26178	-4.42451	1.21687	-2.60048	-4.46872	-1.96600
C	4.75005	-5.21155	-1.20689	-5.12723	-4.35525	-2.18347	-5.05627	-5.02433	0.98450
H	3.18506	-4.01582	-2.09203	-3.88692	-2.64913	-2.64310	-4.11672	-3.29847	1.87756
C	5.48924	-5.47870	-0.05020	-5.45147	-5.32847	-1.23362	-5.09189	-5.88204	-0.11898
H	5.80079	-4.95687	2.02152	-5.02920	-6.09932	0.73877	-4.23126	-6.33695	-2.04658
H	4.94494	-5.76803	-2.11940	-5.64294	-4.33227	-3.13935	-5.73539	-5.17906	1.81821
H	6.25898	-6.24515	-0.05915	-6.22260	-6.06340	-1.44621	-5.80195	-6.70354	-0.14940
Co	0.00000	-0.00001	0.00000	0.01591	0.00000	0.00000	0.00017	-0.00132	0.00617

CoTPP, total charge 1

		Singlet			Triplet			Quintet	
N	0.38678	1.93574	0.00080	1.30496	1.51635	-0.19733	-1.33011	-1.31148	0.04010
N	1.92028	-0.39245	0.08482	1.42360	-1.23714	0.02760	-1.45255	1.43167	-0.24606
N	-0.38676	-1.93571	0.00080	-1.33218	-1.36059	0.03818	1.32053	1.54649	-0.24334
N	-1.92026	0.39247	0.08481	-1.44533	1.40470	-0.20164	1.42403	-1.18982	0.04798
C	-0.49343	2.95526	-0.35307	1.09509	2.85028	-0.00659	-1.13326	-2.57064	0.54239
C	0.22672	4.18481	-0.56238	2.24316	3.60273	-0.44529	-2.40503	-3.27876	0.61379
C	1.53120	3.93001	-0.26237	3.15540	2.69529	-0.90887	-3.34332	-2.45960	0.07176
C	1.61461	2.53346	0.07856	2.59759	1.38964	-0.68150	-2.67497	-1.22235	-0.27898
C	2.82668	1.87904	0.41433	3.28601	0.17217	-0.79105	-3.32289	-0.08136	-0.79107
C	2.93727	0.49300	0.43439	2.73058	-1.05477	-0.35368	-2.71839	1.18535	-0.78180
C	4.16403	-0.22971	0.65852	3.48184	-2.26129	-0.13619	-3.33969	2.43915	-1.12849
C	3.91845	-1.53012	0.33690	2.61633	-3.17442	0.40059	-2.48314	3.42889	-0.72720
C	2.52678	-1.61127	-0.02625	1.33125	-2.53325	0.47923	-1.33179	2.77306	-0.15476
C	1.87889	-2.82597	-0.37424	0.12708	-3.18791	0.82126	-0.14573	3.40890	0.40832
C	0.49345	-2.95523	-0.35307	-1.13557	-2.62646	0.55725	1.09462	2.87286	-0.13886
C	-0.22668	-4.18481	-0.56229	-2.39729	-3.30822	0.66759	2.19760	3.62346	-0.69213
C	-1.53117	-3.93000	-0.26234	-3.34431	-2.47652	0.13536	3.12941	2.70844	-1.10090
C	-1.61459	-2.53344	0.07855	-2.66824	-1.26545	-0.24121	2.60353	1.40547	-0.77728
C	-2.82667	-1.87903	0.41432	-3.31790	-0.10297	-0.73995	3.29908	0.18754	-0.82311
C	-2.93725	-0.49298	0.43438	-2.71303	1.15678	-0.71763	2.74616	-1.00949	-0.32974
C	-4.16401	0.22973	0.65853	-3.34579	2.40536	-1.04589	3.49614	-2.22289	-0.07400
C	-3.91844	1.53014	0.33692	-2.51454	3.39883	-0.60717	2.62928	-3.12000	0.46384
C	-2.52677	1.61129	-0.02626	-1.34167	2.75496	-0.07241	1.32432	-2.47247	0.50844
C	-1.87888	2.82600	-0.37423	-0.15476	3.41362	0.40661	0.12311	-3.13065	0.85649
H	-0.20943	5.11594	-0.89004	2.30700	4.67970	-0.48792	-2.54021	-4.26807	1.02358
H	2.36745	4.61190	-0.29445	4.11294	2.89776	-1.36413	-4.40027	-2.64508	-0.04890
H	5.08830	0.20638	1.00513	4.53370	-2.38643	-0.34462	-4.30378	2.54739	-1.60227
H	4.59908	-2.36707	0.37600	2.82142	-4.19496	0.68699	-2.60286	4.49826	-0.82484
H	0.20951	-5.11596	-0.88987	-2.54364	-4.29112	1.08838	2.23465	4.70005	-0.77559
H	-2.36741	-4.61190	-0.29441	-4.40565	-2.65200	0.04342	4.08509	2.89664	-1.56664
H	-5.08827	-0.20637	1.00515	-4.29541	2.51506	-1.54747	4.55087	-2.34872	-0.26800
H	-4.59906	2.36709	0.37603	-2.64906	4.46241	-0.73084	2.82422	-4.13344	0.78128
C	2.73454	-3.99967	-0.68299	0.21990	-4.55815	1.38920	-0.19575	4.47832	1.35595
C	2.67079	-5.17140	0.09251	-0.30886	-5.66888	0.70855	0.99571	5.05900	1.89058
C	3.64695	-3.93599	-1.75205	0.87066	-4.75596	2.62012	-1.43766	4.96714	1.86696
C	3.49856	-6.25648	-0.19973	-0.19257	-6.94927	1.25171	0.94118	6.08559	2.82165
H	1.99235	-5.21656	0.93883	-0.78573	-5.52829	-0.25662	1.96386	4.68239	1.58245
C	4.45828	-5.02993	-2.05366	0.96911	-6.03544	3.16873	-1.47862	5.99421	2.79824
H	3.70376	-3.03329	-2.35311	1.28360	-3.90224	3.14928	-2.36849	4.51938	1.53973
C	4.38804	-6.19148	-1.27682	0.43993	-7.13489	2.48527	-0.29340	6.57349	3.27625
H	3.45154	-7.14964	0.41578	-0.59153	-7.80137	0.70979	1.86497	6.50717	3.20634
H	5.14536	-4.97559	-2.89255	1.45990	-6.17340	4.12734	-2.43883	6.34481	3.16453

H	5.02653	-7.03892	-1.50685	0.52397	-8.13093	2.90907	-0.33085	7.37946	4.00216
C	4.02056	2.72204	0.68420	4.68313	0.16068	-1.29773	-4.72244	-0.22608	-1.27280
C	5.17260	2.62881	-0.11659	5.00174	-0.59496	-2.44039	-5.77665	0.47766	-0.66515
C	3.99783	3.64532	1.74524	5.70273	0.87492	-0.64425	-5.00550	-1.09531	-2.34094
C	6.27901	3.43979	0.14149	6.30807	-0.61661	-2.93064	-7.08660	0.31585	-1.11955
H	5.18729	1.93724	-0.95344	4.21925	-1.15069	-2.94851	-5.56962	1.12957	0.17818
C	5.11264	4.44051	2.01242	7.01176	0.83674	-1.12721	-6.31470	-1.24422	-2.80203
H	3.11116	3.72269	2.36753	5.47084	1.43578	0.25600	-4.19474	-1.63954	-2.81648
C	6.25420	4.34206	1.20952	7.31623	0.09704	-2.27439	-7.35771	-0.54063	-2.19158
H	7.15743	3.36919	-0.49273	6.53843	-1.19100	-3.82273	-7.89489	0.85382	-0.63361
H	5.09009	5.13655	2.84538	7.79363	1.38003	-0.60525	-6.51933	-1.90802	-3.63648
H	7.11774	4.96786	1.41308	8.33386	0.07302	-2.65203	-8.37650	-0.66153	-2.54681
C	-2.73456	3.99968	-0.68299	-0.20459	4.61166	1.24126	0.20977	-4.49623	1.44348
C	-3.64681	3.93604	-1.75219	-1.42868	5.23852	1.60396	0.77520	-4.67059	2.71812
C	-2.67106	5.17132	0.09267	0.97699	5.12473	1.84743	-0.23616	-5.62546	0.73594
C	-4.45818	5.02995	-2.05381	-1.45352	6.36414	2.41799	0.87990	-5.94579	3.27845
H	-3.70344	3.03340	-2.35336	-2.37177	4.82873	1.27416	1.12193	-3.80249	3.27181
C	-3.49888	6.25636	-0.19958	0.94643	6.24966	2.66257	-0.12614	-6.90030	1.29554
H	-1.99280	5.21643	0.93914	1.92084	4.61431	1.71339	-0.65094	-5.50355	-0.26062
C	-4.38817	6.19141	-1.27683	-0.26571	6.89246	2.93738	0.42914	-7.06305	2.56885
H	-5.14512	4.97564	-2.89282	-2.40639	6.82137	2.66576	1.31059	-6.06533	4.26803
H	-3.45205	7.14945	0.41606	1.86864	6.61297	3.10525	-0.46723	-7.76547	0.73492
H	-5.02670	7.03882	-1.50687	-0.28934	7.76865	3.57789	0.51261	-8.05440	3.00361
C	-4.02054	-2.72204	0.68419	-4.71890	-0.24457	-1.20994	4.69710	0.16075	-1.33242
C	-3.99780	-3.64529	1.74526	-5.01436	-1.13923	-2.25518	5.71077	0.90457	-0.70472
C	-5.17256	-2.62884	-0.11661	-5.76709	0.48143	-0.61604	5.01896	-0.63165	-2.44777
C	-5.11260	-4.44050	2.01245	-6.32452	-1.28377	-2.71199	7.02063	0.85666	-1.18546
H	-3.11114	-3.72264	2.36756	-4.21061	-1.70516	-2.71656	5.47378	1.49965	0.17218
C	-6.27897	-3.43984	0.14148	-7.07938	0.32005	-1.06297	6.32716	-0.66690	-2.93412
H	-5.18726	-1.93730	-0.95348	-5.55321	1.14686	0.21458	4.23900	-1.20618	-2.93900
C	-6.25415	-4.34209	1.20953	-7.36024	-0.55648	-2.11582	7.33051	0.07531	-2.30327
H	-5.09004	-5.13651	2.84542	-6.53702	-1.96413	-3.53098	7.79856	1.42505	-0.68482
H	-7.15738	-3.36927	-0.49276	-7.88208	0.87380	-0.58557	6.56171	-1.27255	-3.80417
H	-7.11769	-4.96789	1.41310	-8.38085	-0.67653	-2.46615	8.34873	0.04273	-2.67864
Co	0.00001	0.00001	-0.10860	-0.01112	0.07412	-0.04955	-0.00976	0.11357	-0.05683

CoTPP, total charge -1

		Singlet			**Triplet**			**Quintet**	
N	-1.98494	-0.00001	-0.00712	0.00002	2.01193	-0.00431	0.00021	-2.06245	-0.00001
N	0.00000	1.98555	-0.00011	2.00490	-0.00001	0.00000	-2.05518	-0.00020	-0.05170
N	1.98493	-0.00001	0.00735	-0.00001	-2.01193	0.00431	-0.00021	2.06245	0.00001
N	0.00000	-1.98558	-0.00011	-2.00488	0.00001	0.00000	2.05518	0.00020	0.05173
C	-2.83173	-1.09564	0.01548	-1.10133	2.85294	0.03281	1.10942	-2.88931	-0.00040
C	-4.21525	-0.68004	0.07083	-0.68983	4.21460	0.10946	0.69299	-4.25337	0.00650
C	-4.21524	0.68000	0.07112	0.68990	4.21459	0.10934	-0.69215	-4.25351	-0.00631
C	-2.83173	1.09562	0.01589	1.10137	2.85293	0.03264	-1.10885	-2.88952	0.00047
C	-2.43165	2.43176	0.01718	2.45425	2.43465	0.02608	-2.46631	-2.44663	0.00019
C	-1.09567	2.83260	0.01046	2.84450	1.10614	0.01520	-2.87820	-1.11419	-0.01352
C	-0.68005	4.21707	0.00104	4.22998	0.67792	0.00235	-4.26268	-0.68070	0.06188
C	0.68006	4.21707	-0.00213	4.22997	-0.67796	-0.00236	-4.26282	0.67985	0.06189
C	1.09567	2.83260	-0.01094	2.84449	-1.10617	-0.01520	-2.87842	1.11362	-0.01352
C	2.43165	2.43174	-0.01718	2.45422	-2.43468	-0.02608	-2.46681	2.44615	0.00020
C	2.83174	1.09561	-0.01540	1.10134	-2.85294	-0.03264	-1.10942	2.88931	0.00048
C	4.21527	0.67999	-0.07003	0.68985	-4.21460	-0.10933	-0.69299	4.25337	-0.00633
C	4.21527	-0.68005	-0.06974	-0.68987	-4.21459	-0.10945	0.69215	4.25351	0.00648
C	2.83173	-1.09565	-0.01499	-1.10136	-2.85293	-0.03281	1.10885	2.88952	-0.00041
C	2.43165	-2.43178	-0.01646	-2.45423	-2.43465	-0.02638	2.46632	2.44663	-0.00019
C	1.09567	-2.83263	-0.01053	-2.84448	-1.10614	-0.01537	2.87820	1.11419	0.01349
C	0.68006	-4.21710	-0.00184	-4.22996	-0.67792	-0.00248	4.26268	0.68070	-0.06201
C	-0.68006	-4.21711	0.00075	-4.22996	0.67796	0.00248	4.26282	-0.67985	-0.06201
C	-1.09568	-2.83264	0.01005	-2.84447	1.10617	0.01537	2.87842	-1.11363	0.01349
C	-2.43166	-2.43178	0.01646	-2.45421	2.43467	0.02638	2.46681	-2.44615	-0.00018
H	-5.06416	-1.34681	0.11954	-1.35244	5.06524	0.17399	1.34733	-5.11312	0.02115
H	-5.06415	1.34674	0.12010	1.35253	5.06523	0.17376	-1.34633	-5.11338	-0.02087
H	-1.34649	5.06756	-0.00356	5.08224	1.34187	-0.00178	-5.11838	-1.33740	0.13047
H	1.34651	5.06756	0.00211	5.08222	-1.34193	0.00176	-5.11866	1.33637	0.13048
H	5.06420	1.34674	-0.11866	1.35248	-5.06524	-0.17375	-1.34733	5.11312	-0.02089
H	5.06420	-1.34682	-0.11810	-1.35249	-5.06523	-0.17398	1.34632	5.11338	0.02111
H	1.34650	-5.06760	0.00268	-5.08222	-1.34187	0.00153	5.11838	1.33739	-0.13067

H	-1.34649	-5.06760	-0.00412	-5.08220	1.34193	-0.00154	5.11865	-1.33637	-0.13067
C	3.49068	3.48817	-0.03152	3.50668	-3.49463	-0.03710	-3.52411	3.50174	0.02922
C	4.27590	3.73511	1.10617	3.70640	-4.32098	1.08216	-3.69089	4.32685	1.15551
C	3.72674	4.25634	-1.18312	4.31974	-3.69902	-1.16454	-4.38204	3.69891	-1.06647
C	5.26776	4.71999	1.09518	4.69271	-5.31045	1.08055	-4.68484	5.30776	1.19030
H	4.09914	3.14416	2.00025	3.07740	-4.17529	1.95561	-3.03083	4.18577	2.00643
C	4.71672	5.24302	-1.19857	5.31026	-4.68611	-1.17013	-5.38045	4.67735	-1.03532
H	3.12372	4.07006	-2.06713	4.16670	-3.07166	-2.03800	-4.25695	3.07242	-1.94498
C	5.49220	5.47897	-0.05835	5.50137	-5.49673	-0.04684	-5.53657	5.48721	0.09389
H	5.86304	4.89599	1.98787	4.83309	-5.93347	1.96061	-4.79833	5.92882	2.07561
H	4.88416	5.82491	-2.10166	5.92852	-4.82442	-2.05388	-6.03242	4.80959	-1.89549
H	6.26290	6.24561	-0.06869	6.27002	-6.26550	-0.04939	-6.31121	6.24947	0.11993
C	-3.49067	3.48818	0.03152	3.50671	3.49459	0.03710	-3.52341	-3.50244	0.02921
C	-3.72616	4.25695	1.18284	4.31979	3.69897	1.16454	-3.69007	-4.32753	1.15552
C	-4.27648	3.73453	-1.10589	3.70644	4.32094	-1.08215	-4.38125	-3.69982	-1.06651
C	-4.71613	5.24363	1.19829	5.31032	4.68604	1.17012	-4.68382	-5.30864	1.19030
H	-3.12267	4.07114	2.06664	4.16674	3.07161	2.03800	-3.03007	-4.18628	2.00646
C	-5.26834	4.71941	-1.09491	4.69276	5.31041	-1.08055	-5.37946	-4.67846	-1.03537
H	-4.10019	3.14311	-1.99976	3.07744	4.17526	-1.95560	-4.25624	-3.07333	-1.94504
C	-5.49220	5.47899	0.05835	5.50143	5.49667	0.04684	-5.53546	-5.48830	0.09387
H	-4.88311	5.82598	2.10117	5.92858	4.82434	2.05387	-4.79723	-5.92969	2.07564
H	-5.86408	4.89495	-1.98738	4.83315	5.93343	-1.96061	-6.03137	-4.81086	-1.89556
H	-6.26289	6.24563	0.06869	6.27009	6.26543	0.04938	-6.30995	-6.25072	0.11990
C	-3.49071	-3.48819	0.03029	-3.50667	3.49462	0.03762	3.52411	-3.50175	-0.02921
C	-3.72654	-4.25722	1.18136	-4.31964	3.69886	1.16516	4.38214	-3.69883	1.06642
C	-4.27624	-3.73422	-1.10739	-3.70652	4.32108	-1.08153	3.69080	-4.32694	-1.15545
C	-4.71657	-5.24385	1.19631	-5.31017	4.68593	1.17094	5.38055	-4.67727	1.03527
H	-3.12328	-4.07165	2.06536	-4.16649	3.07141	2.03854	4.25712	-3.07227	1.94489
C	-5.26815	-4.71905	-1.09691	-4.69285	5.31053	-1.07972	4.68475	-5.30785	-1.19024
H	-4.09968	-3.14258	-2.00106	-3.07761	4.17549	-1.95506	3.03067	-4.18593	-2.00631
C	-5.49235	-5.47890	0.05610	-5.50141	5.49667	0.04776	5.53657	-5.48721	-0.09389
H	-4.88382	-5.82641	2.09900	-5.92835	4.82413	2.05477	6.03259	-4.80943	1.89540
H	-5.86366	-4.89434	-1.98958	-4.83334	5.93364	-1.95970	4.79816	-5.92898	-2.07551
H	-6.26308	-6.24550	0.06605	-6.27007	6.26542	0.05047	6.31121	-6.24948	-0.11994
C	3.49070	-3.48819	-0.03029	-3.50671	-3.49458	-0.03762	3.52341	3.50244	-0.02923
C	4.27564	-3.73481	1.10767	-3.70658	-4.32104	1.08153	3.68997	4.32761	-1.15550
C	3.72711	-4.25662	-1.18164	-4.31967	-3.69882	-1.16516	4.38136	3.69974	1.06642
C	5.26755	-4.71965	1.09719	-4.69291	-5.31048	1.07973	4.68372	5.30873	-1.19030
H	4.09862	-3.14365	2.00156	-3.07766	-4.17545	1.95507	3.02989	4.18643	-2.00638
C	4.71714	-5.24326	-1.19659	-5.31022	-4.68587	-1.17095	5.37956	4.67838	1.03526
H	3.12432	-4.07058	-2.06586	-4.16652	-3.07137	-2.03854	4.25643	3.07319	1.94492
C	5.49233	-5.47890	-0.05611	-5.50147	-5.49660	-0.04777	5.53546	5.48831	-0.09393
H	5.86260	-4.89541	1.99007	-4.83341	-5.93358	1.95970	4.79704	5.92984	-2.07560
H	4.88485	-5.82535	-2.09949	-5.92840	-4.82407	-2.05477	6.03155	4.81072	1.89541
H	6.26306	-6.24551	-0.06606	-6.27014	-6.26535	-0.05047	6.30995	6.25073	-0.11998
Co	0.00000	-0.00002	0.00000	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000

H-CoTPP, total charge 0

		Singlet			Triplet			Quintet	
N	-0.00469	-1.98603	-0.00828	-2.05314	-0.00305	-0.09596	2.03713	-0.00001	-0.02659
N	-1.98132	0.00471	-0.06311	-0.00376	2.03649	-0.03234	0.00158	-2.03618	-0.00400
N	0.00469	1.98603	-0.00828	2.05249	0.00305	0.02267	-2.03448	0.00001	0.01801
N	1.98132	-0.00471	-0.06311	0.00238	-2.03649	-0.03247	0.00160	2.03618	-0.00400
C	1.09037	-2.82705	0.06668	-2.87213	-1.10777	-0.04308	2.86390	1.10394	-0.01109
C	0.66960	-4.19797	0.21922	-4.25676	-0.68755	0.02540	4.24493	0.68195	0.02468
C	-0.68982	-4.19478	0.21778	-4.25881	0.67484	0.02533	4.24492	-0.68199	0.02468
C	-1.10382	-2.82188	0.06452	-2.87544	1.09921	-0.04319	2.86389	-1.10397	-0.01110
C	-2.43797	-2.42676	-0.02156	-2.45143	2.43848	-0.02213	2.44637	-2.44447	-0.01138
C	-2.82400	-1.09046	-0.11775	-1.11121	2.86023	-0.01347	1.10588	-2.86228	-0.01621
C	-4.19507	-0.66955	-0.26900	-0.68907	4.24223	-0.00659	0.68438	-4.24337	-0.05276
C	-4.19188	0.68977	-0.26754	0.67473	4.24362	0.00127	-0.67958	-4.24401	-0.04941
C	-2.81884	1.10392	-0.11558	1.10113	2.86254	-0.02047	-1.10220	-2.86291	-0.02705
C	-2.42647	2.43827	-0.01777	2.44477	2.44639	-0.02510	-2.44243	-2.44464	-0.03486
C	-1.09037	2.82705	0.06668	2.87344	1.10903	-0.02293	-2.85941	-1.10391	-0.03222
C	-0.66960	4.19797	0.21922	4.25549	0.68775	-0.11199	-4.23773	-0.68195	-0.12597
C	0.68982	4.19478	0.21778	4.25754	-0.67501	-0.11207	-4.23772	0.68199	-0.12597
C	1.10382	2.82188	0.06452	2.87677	-1.10046	-0.02304	-2.85940	1.10394	-0.03222
C	2.43797	2.42676	-0.02156	2.45211	-2.43909	-0.02532	-2.44240	2.44467	-0.03487
C	2.82400	1.09046	-0.11775	1.10972	-2.85925	-0.02067	-1.10218	2.86292	-0.02705
C	4.19507	0.66955	-0.26900	0.68743	-4.24159	0.00110	-0.67955	4.24401	-0.04941

C	4.19188	-0.68977	-0.26755	-0.67638	-4.24425	-0.00660	0.68442	4.24336	-0.05275
C	2.81884	-1.10392	-0.11558	-1.10261	-2.86350	-0.01344	1.10591	2.86227	-0.01620
C	2.42647	-2.43827	-0.01777	-2.44409	-2.44575	-0.02196	2.44639	2.44445	-0.01137
H	1.33610	-5.04157	0.31934	-5.10715	-1.35116	0.08211	5.09766	1.34400	0.05873
H	-1.36051	-5.03522	0.31650	-5.11117	1.33591	0.08199	5.09765	-1.34405	0.05873
H	-5.03822	-1.33634	-0.37088	-1.35056	5.09601	-0.00996	1.34668	-5.09612	-0.08056
H	-5.03188	1.36074	-0.36801	1.33420	5.09875	0.01959	-1.34099	-5.09772	-0.06375
H	-1.33610	5.04157	0.31935	5.10505	1.35069	-0.18577	-5.08754	-1.34437	-0.20139
H	1.36051	5.03522	0.31650	5.10908	-1.33539	-0.18595	-5.08753	1.34441	-0.20140
H	5.03822	1.33634	-0.37087	1.34944	-5.09476	0.01935	-1.34095	5.09773	-0.06375
H	5.03188	-1.36074	-0.36802	-1.33533	-5.09998	-0.00989	1.34673	5.09611	-0.08055
C	-3.48376	3.49603	-0.00249	3.50015	3.50820	-0.04203	-3.50406	-3.49994	-0.06311
C	-3.64983	4.35650	-1.09876	4.30296	3.73337	1.08695	-4.29197	-3.74655	1.07173
C	-4.32782	3.64518	1.10886	3.70841	4.29240	-1.18729	-3.73270	-4.25542	-1.22350
C	-4.63913	5.34327	-1.08561	5.29023	4.72220	1.07285	-5.28540	-4.72908	1.04825
H	-3.00065	4.24402	-1.96237	4.14559	3.13015	1.97649	-4.11820	-3.16534	1.97283
C	-5.31498	4.63402	1.12521	4.69749	5.27927	-1.20417	-4.72760	-5.23636	-1.24929
H	-4.20218	2.98300	1.96067	3.09260	4.12018	-2.06538	-3.12863	-4.06557	-2.10614
C	-5.47402	5.48544	0.02725	5.49079	5.49777	-0.07337	-5.50631	-5.47657	-0.11279
H	-4.75819	5.99845	-1.94403	5.90033	4.88703	1.95656	-5.88430	-4.91094	1.93625
H	-5.95734	4.73983	1.99498	4.84918	5.87464	-2.10019	-4.89523	-5.80991	-2.15663
H	-6.24224	6.25339	0.03874	6.25902	6.26569	-0.08549	-6.27918	-6.23966	-0.13196
C	-3.50013	-3.47968	-0.00902	-3.51085	3.49627	0.01120	3.50489	-3.50324	-0.00595
C	-4.34629	-3.62656	1.10104	-3.73476	4.24816	1.17487	3.73814	-4.27222	1.14465
C	-3.66859	-4.33794	-1.10665	-4.30073	3.74971	-1.12074	4.28117	-3.74373	-1.15006
C	-5.33788	-4.61099	1.11476	-4.72674	5.23181	1.20676	4.72681	-5.25973	1.15188
H	-4.21879	-2.96611	1.95392	-3.12864	4.05379	2.05508	3.14206	-4.08799	2.03387
C	-4.66231	-5.32028	-1.09613	-5.29106	4.73520	-1.09141	5.26839	-4.73277	-1.14511
H	-3.01775	-4.22723	-1.96924	-4.13098	3.17143	-2.02448	4.10297	-3.15307	-2.04414
C	-5.49930	-5.46021	0.01544	-5.50737	5.47875	0.07304	5.49445	-5.49323	0.00650
H	-5.98185	-4.71510	1.98354	-4.89057	5.80240	2.11666	4.89813	-5.84383	2.05176
H	-4.78317	-5.97379	-1.95558	-5.89126	4.92234	-1.97746	5.85821	-4.90977	-2.04017
H	-6.27097	-6.22472	0.02489	-6.27794	6.24403	0.09687	6.26243	-6.26147	0.01132
C	3.48376	-3.49602	-0.00249	-3.50032	-3.50673	0.01155	3.50492	3.50321	-0.00594
C	4.32782	-3.64518	1.10886	-3.72186	-4.25919	1.17531	3.73817	4.27218	1.14467
C	3.64983	-4.35650	-1.09876	-4.28949	-3.76270	-1.12032	4.28121	3.74369	-1.15004
C	5.31497	-4.63402	1.12521	-4.71082	-5.24586	1.20735	4.72685	5.25969	1.15190
H	4.20218	-2.98300	1.96067	-3.11628	-4.06288	2.05546	3.14209	4.08796	2.03388
C	4.63913	-5.34326	-1.08561	-5.27679	-4.75121	-1.09084	5.26843	4.73273	-1.14509
H	3.00065	-4.24401	-1.96237	-4.12154	-3.18401	-2.02414	4.10301	3.15304	-2.04412
C	5.47402	-5.48544	0.02725	-5.49075	-5.49530	0.07370	5.49450	5.49318	0.00653
H	5.95733	-4.73983	1.99498	-4.87285	-5.81686	2.11732	4.89817	5.84378	2.05178
H	4.75819	-5.99845	-1.94403	-5.87646	-4.94028	-1.97683	5.85826	4.90972	-2.04014
H	6.24224	-6.25339	0.03874	-6.25898	-6.26294	0.09765	6.26249	6.26141	0.01135
C	3.50013	3.47968	-0.00902	3.51066	-3.49773	-0.04235	-3.50403	3.49997	-0.06313
C	3.66859	4.33794	-1.10664	4.31424	-3.72051	1.08655	-4.29194	3.74659	1.07171
C	4.34630	3.62656	1.10104	3.72121	-4.28126	-1.18766	-3.73266	4.25546	-1.22352
C	4.66231	5.32028	-1.09613	5.30451	-4.70635	1.07234	-5.28537	4.72912	1.04822
H	3.01775	4.22723	-1.96924	4.15512	-3.11780	1.97613	-4.11819	3.16538	1.97281
C	5.33789	4.61098	1.11476	4.71328	-5.26512	-1.20466	-4.72754	5.23640	-1.24931
H	4.21879	2.96611	1.95392	3.10482	-4.11086	-2.06570	-3.12858	4.06561	-2.10615
C	5.49930	5.46021	0.01544	5.50732	-5.48126	-0.07392	-5.50626	5.47662	-0.11282
H	4.78317	5.97379	-1.95558	5.91517	-4.86935	1.95600	-5.88427	4.91099	1.93622
H	5.98185	4.71509	1.98354	4.86670	-5.85999	-2.10071	-4.89516	5.80996	-2.15665
H	6.27097	6.22472	0.02489	6.27788	-6.24683	-0.08614	-6.27913	6.23972	-0.13200
Co	0.00000	0.00000	0.04673	0.01713	0.00006	0.13712	0.00369	-0.00001	0.36749
H	0.00000	0.00000	1.45779	-0.41205	-0.00146	1.54656	0.02816	-0.00002	2.07061

H-CoTPP, total charge -1

		Doublet			**Quartet**			**Sextet**	
N	-0.76829	1.84043	-0.05203	-0.53794	1.99443	-0.01462	-2.04194	-0.00001	-0.06509
N	1.84167	0.77662	0.00451	2.00180	0.52912	0.01737	-0.00142	2.05198	-0.01201
N	0.76753	-1.82381	-0.02464	0.54029	-1.99333	0.01408	2.03876	0.00001	0.01631
N	-1.83535	-0.76268	0.00866	-1.99736	-0.52809	0.04265	-0.00141	-2.05198	-0.01201
C	-2.10847	2.19213	0.06878	-1.81100	2.49766	-0.01800	-2.87062	-1.11166	-0.03329
C	-2.25885	3.62703	-0.05464	-1.76310	3.94976	0.03489	-4.25553	-0.67968	0.03083
C	-1.02227	4.14142	-0.27014	-0.44451	4.29896	0.05445	-4.25553	0.67965	0.03082
C	-0.08435	3.03578	-0.21681	0.31839	3.06189	0.01216	-2.87063	1.11164	-0.03329
C	1.29187	3.19039	-0.25861	1.72943	2.98944	0.01188	-2.46348	2.44232	-0.02772
C	2.19221	2.11285	-0.06994	2.49656	1.80396	-0.01921	-1.10785	2.88190	-0.03502

C	3.59366	2.27698	0.13140	3.94667	1.76216	-0.12885	-0.69398	4.24477	-0.08372
C	4.11636	1.01732	0.34078	4.30270	0.44555	-0.14749	0.69057	4.24539	-0.07369
C	3.03278	0.10028	0.23581	3.07044	-0.32226	-0.06418	1.10483	2.88218	-0.03859
C	3.16963	-1.30597	0.27344	2.99962	-1.73041	-0.05126	2.45987	2.44185	-0.03340
C	2.10748	-2.17369	0.08551	1.81234	-2.49380	-0.01797	2.86680	1.11158	-0.01636
C	2.26563	-3.60050	-0.10727	1.76816	-3.94719	-0.05176	4.25153	0.67969	-0.08697
C	1.02962	-4.11359	-0.32931	0.45055	-4.29941	-0.03508	4.25154	-0.67966	-0.08698
C	0.08726	-3.01543	-0.23083	-0.31347	-3.06146	-0.00753	2.86681	-1.11156	-0.01637
C	-1.28829	-3.17095	-0.29133	-1.72347	-2.98768	-0.01666	2.45989	-2.44183	-0.03341
C	-2.19081	-2.09521	-0.10364	-2.48855	-1.80092	-0.03941	1.10485	-2.88217	-0.03859
C	-3.60065	-2.25257	0.03767	-3.93311	-1.76021	-0.21457	0.69059	-4.24538	-0.07369
C	-4.12413	-0.99230	0.24194	-4.28877	-0.44403	-0.23067	-0.69395	-4.24477	-0.08371
C	-3.02841	-0.08408	0.21293	-3.06204	0.32191	-0.06469	-1.10784	-2.88190	-0.03502
C	-3.16547	1.32122	0.25659	-2.99675	1.73290	-0.05110	-2.46347	-2.44233	-0.02772
H	-3.19877	4.15701	0.00111	-2.61846	4.60946	0.07055	-5.11042	-1.33822	0.08953
H	-0.75243	5.17465	-0.43233	-0.02950	5.29547	0.10926	-5.11043	1.33819	0.08953
H	4.11619	3.22247	0.13992	4.59960	2.62129	-0.19261	-1.35072	5.10174	-0.12537
H	5.14412	0.75199	0.54055	5.29978	0.03385	-0.21584	1.34690	5.10349	-0.09018
H	3.21198	-4.12212	-0.10537	2.62557	-4.60437	-0.09138	5.10553	1.33895	-0.15122
H	0.76438	-5.13908	-0.54105	0.03713	-5.29800	-0.04145	5.10554	-1.33892	-0.15122
H	-4.13006	-3.19343	0.00030	-4.57861	-2.61888	-0.33583	1.34693	-5.10348	-0.09018
H	-5.16043	-0.71602	0.37282	-5.27765	-0.03025	-0.37005	-1.35070	-5.10175	-0.12537
C	4.53354	-1.88291	0.45989	4.29307	-2.48387	-0.08791	3.51882	3.49642	-0.06310
C	4.84494	-2.62654	1.61084	4.74651	-3.18147	1.04390	4.34210	3.72397	1.05223
C	5.53569	-1.71295	-0.51119	5.08106	-2.51573	-1.25008	3.71954	4.28580	-1.20837
C	6.11303	-3.18969	1.78406	5.95091	-3.88996	1.01572	5.34201	4.70093	1.02226
H	4.07750	-2.75985	2.36783	4.14317	-3.15950	1.94678	4.18945	3.12292	1.94407
C	6.80409	-2.27311	-0.34189	6.28725	-3.22137	-1.28162	4.71594	5.26456	-1.24217
H	5.30468	-1.13947	-1.40402	4.73568	-1.98170	-2.13070	3.08515	4.11928	-2.07412
C	7.09896	-3.01521	0.80805	6.72731	-3.91246	-0.14781	5.53332	5.47610	-0.12578
H	6.33058	-3.76151	2.68292	6.28417	-4.42112	1.90385	5.96807	4.85852	1.89719
H	7.56101	-2.13535	-1.11025	6.88048	-3.23443	-2.19268	4.85746	5.85898	-2.14156
H	8.08564	-3.45189	0.94066	7.66465	-4.46249	-0.17074	6.30957	6.23675	-0.15096
C	1.87538	4.55133	-0.44057	2.48184	4.28288	0.02609	-3.51902	3.49967	-0.00562
C	1.71837	5.55526	0.53079	3.25423	4.64946	1.14130	-3.68768	4.32401	1.12047
C	2.62347	4.85718	-1.59147	2.44014	5.15971	-1.07099	-4.36844	3.69980	-1.10677
C	2.27233	6.82640	0.35111	3.96256	5.85393	1.16031	-4.67815	5.30861	1.14974
H	1.15734	5.32589	1.43206	3.28911	3.97846	1.99457	-3.03232	4.17981	1.97447
C	3.18088	6.12475	-1.77431	3.14647	6.36556	-1.05545	-5.36231	4.68303	-1.08128
H	2.76158	4.08442	-2.34223	1.84848	4.88282	-1.93876	-4.24037	3.07309	-1.98471
C	3.00587	7.11794	-0.80323	3.91159	6.71816	0.06135	-5.52186	5.49225	0.04790
H	2.13660	7.58616	1.11713	4.55074	6.11885	2.03542	-4.79460	5.92973	2.03454
H	3.74945	6.33869	-2.67616	3.10221	7.02719	-1.91709	-6.00819	4.81906	-1.94538
H	3.43862	8.10523	-0.94390	4.46180	7.65558	0.07507	-6.29336	6.25781	0.06963
C	-4.54005	1.87334	0.45351	-4.29446	2.47520	-0.08701	-3.51899	-3.49969	-0.00561
C	-5.15863	1.80832	1.71277	-5.20044	2.38627	0.98389	-3.68766	-4.32403	1.12048
C	-5.25318	2.45073	-0.60950	-4.64434	3.27494	-1.18837	-4.36842	-3.69983	-1.10676
C	-6.44609	2.31566	1.90822	-6.41604	3.07474	0.95620	-4.67812	-5.30863	1.14975
H	-4.61603	1.35514	2.53750	-4.93638	1.77286	1.84028	-3.03229	-4.17982	1.97448
C	-6.54010	2.96327	-0.41791	-5.85901	3.96529	-1.21947	-5.36228	-4.68307	-1.08127
H	-4.78639	2.49304	-1.58944	-3.95275	3.34614	-2.02280	-4.24036	-3.07312	-1.98470
C	-7.14209	2.89770	0.84267	-6.75107	3.86825	-0.14625	-5.52182	-5.49228	0.04791
H	-6.90437	2.25950	2.89260	-7.09941	2.99454	1.79795	-4.79455	-5.92975	2.03456
H	-7.07344	3.40836	-1.25442	-6.11016	4.57510	-2.08387	-6.00817	-4.81909	-1.94536
H	-8.14308	3.29409	0.99331	-7.69635	4.40455	-0.16886	-6.29333	-6.25785	0.06965
C	-1.86479	-4.52914	-0.50993	-2.48101	-4.27817	-0.03957	3.51884	-3.49640	-0.06311
C	-1.70638	-5.55549	0.43759	-2.43845	-5.12851	-1.15721	4.34213	-3.72395	1.05222
C	-2.60234	-4.81280	-1.67342	-3.26531	-4.66409	1.06055	3.71955	-4.28578	-1.20838
C	-2.24982	-6.82584	0.22361	-3.15412	-6.32880	-1.17521	5.34204	-4.70090	1.02225
H	-1.15186	-5.34440	1.34734	-1.83971	-4.83512	-2.01460	4.18948	-3.12290	1.94406
C	-3.14940	-6.07945	-1.89026	-3.98267	-5.86332	1.04612	4.71596	-5.26453	-1.24218
H	-2.74038	-4.02366	-2.40689	-3.30285	-4.01197	1.92823	3.08516	-4.11927	-2.07413
C	-2.97383	-7.09458	-0.94218	-3.92984	-6.70186	-0.07243	5.53335	-5.47607	-0.12579
H	-2.11307	-7.60306	0.97173	-3.10934	-6.96972	-2.05233	5.96811	-4.85848	1.89716
H	-3.70988	-6.27568	-2.80114	-4.58024	-6.14373	1.90997	4.85748	-5.85896	-2.14157
H	-3.39851	-8.08119	-1.10956	-4.48736	-7.63497	-0.08496	6.30961	-6.23672	-0.15098
Co	0.00119	0.00831	0.07115	0.01778	0.02199	0.55394	-0.00651	0.00000	0.36339
H	-0.00010	0.01999	1.48477	-0.04906	-0.04812	2.21403	-0.04632	0.00001	2.06743

H-CoTPP, total charge 1

	Doublet			Quartet			Sextet		
N	-1.93365	0.38310	-0.00156	-2.02962	0.35462	0.01136	-0.00010	2.04644	-0.01236
N	0.37302	1.96205	-0.02735	0.35430	2.01562	-0.02971	2.04615	0.00009	0.01163
N	1.94045	-0.36201	-0.04957	2.01922	-0.35278	-0.06230	0.00009	-2.04644	-0.01235
N	-0.36275	-1.91429	-0.02608	-0.35065	-2.01635	-0.03090	-2.04614	-0.00010	0.01162
C	-2.95466	-0.50145	-0.28533	-3.02227	-0.58902	-0.10646	-1.10096	2.86796	0.08551
C	-4.22157	0.17845	-0.30398	-4.28696	0.05531	-0.35626	-0.68446	4.22755	0.30106
C	-3.97594	1.47492	0.03983	-4.05152	1.40191	-0.35669	0.68408	4.22761	0.30103
C	-2.55272	1.59472	0.20734	-2.64322	1.57910	-0.10702	1.10070	2.86806	0.08547
C	-1.90381	2.82836	0.39316	-1.99261	2.83335	-0.00934	2.44900	2.45052	-0.01805
C	-0.51985	2.98670	0.20992	-0.59202	3.01089	0.09081	2.86126	1.10088	-0.12464
C	0.14299	4.26129	0.14884	0.05452	4.27450	0.33512	4.20963	0.68441	-0.40251
C	1.43827	4.01296	-0.19554	1.40152	4.03994	0.33107	4.20970	-0.68403	-0.40248
C	1.58404	2.58329	-0.25295	1.57915	2.63226	0.08847	2.86137	-1.10061	-0.12460
C	2.81431	1.92656	-0.42407	2.83464	1.98752	-0.02796	2.44922	-2.45030	-0.01797
C	2.96259	0.53961	-0.24273	3.01633	0.59111	-0.14543	1.10096	-2.86795	0.08552
C	4.24133	-0.09542	-0.06990	4.28815	-0.05706	-0.36432	0.68446	-4.22755	0.30107
C	3.99158	-1.39124	0.27349	4.05325	-1.40056	-0.36494	-0.68408	-4.22761	0.30104
C	2.56378	-1.55724	0.24944	2.63694	-1.57899	-0.14632	-1.10070	-2.86806	0.08547
C	1.90641	-2.78325	0.44506	1.99232	-2.83098	-0.02973	-2.44900	-2.45053	-0.01804
C	0.52321	-2.93486	0.24032	0.59253	-3.01178	0.08672	-2.86126	-1.10088	-0.12465
C	-0.13065	-4.21185	0.14871	-0.05180	-4.27588	0.32949	-4.20964	-0.68441	-0.40251
C	-1.42787	-3.96408	-0.19236	-1.39850	-4.03973	0.33461	-4.20970	0.68403	-0.40248
C	-1.56597	-2.53570	-0.28131	-1.57839	-2.63173	0.09053	-2.86136	1.10061	-0.12461
C	-2.79744	-1.88495	-0.47547	-2.83572	-1.98965	-0.00864	-2.44923	2.45030	-0.01798
H	-5.16922	-0.27263	-0.55379	-5.22394	-0.44893	-0.53730	-1.34176	5.06935	0.45675
H	-4.68152	2.28774	0.12065	-4.76184	2.19403	-0.53820	1.34131	5.06947	0.45669
H	-0.32304	5.21842	0.32304	-0.44874	5.21299	0.51117	5.04124	1.34273	-0.60289
H	2.22410	4.72985	-0.37497	2.19401	4.75322	0.49901	5.04136	-1.34228	-0.60284
H	5.19700	0.39975	-0.15052	5.22905	0.44766	-0.52197	1.34176	-5.06935	0.45676
H	4.70651	-2.15958	0.52328	4.76711	-2.19444	-0.52326	-1.34131	-5.06947	0.45670
H	0.34771	-5.16779	0.29797	0.45196	-5.21568	0.49690	-5.04124	-1.34273	-0.60290
H	-2.22372	-4.67667	-0.34621	-2.19007	-4.75193	0.51130	-5.04136	1.34228	-0.60284
C	4.03637	2.72033	-0.72375	4.05096	2.84312	-0.01535	3.50368	-3.49655	-0.02740
C	4.71634	2.51228	-1.93646	5.02744	2.68056	0.98398	3.50983	-4.49935	-1.01478
C	4.54350	3.65451	0.19596	4.23983	3.82706	-1.00274	4.51444	-3.49595	0.95197
C	5.86826	3.24280	-2.23274	6.16212	3.49247	1.00027	4.50968	-5.47222	-1.02651
H	4.33106	1.78817	-2.64831	4.88250	1.93073	1.75582	2.74276	-4.49689	-1.78321
C	5.70649	4.36897	-0.09570	5.38671	4.62180	-0.99637	5.49966	-4.48367	0.95016
H	4.03898	3.79960	1.14647	3.49536	3.95043	-1.78349	4.50911	-2.73240	1.72387
C	6.36715	4.17026	-1.31253	6.34727	4.46050	0.00763	5.50291	-5.47054	-0.04133
H	6.37641	3.08548	-3.17922	6.90037	3.36955	1.78683	4.51427	-6.22965	-1.80436
H	6.09814	5.07693	0.62835	5.53008	5.36566	-1.77413	6.26320	-4.48342	1.72202
H	7.26791	4.73194	-1.54026	7.23495	5.08558	0.01644	6.27535	-6.23348	-0.04667
C	-2.74560	4.01219	0.71361	-2.84384	4.05113	-0.01155	3.50335	3.49688	-0.02753
C	-2.88460	5.07744	-0.19286	-3.83379	4.23103	0.97229	4.51414	3.49640	0.95181
C	-3.44130	4.05437	1.93451	-2.67288	5.04016	-0.99789	3.50937	4.49964	-1.01495
C	-3.70114	6.16533	0.11987	-4.62523	5.37991	0.97522	5.49926	4.48422	0.94995
H	-2.37306	5.03790	-1.14986	-3.96299	3.47811	1.74383	4.50890	2.73288	1.72374
C	-4.24153	5.15317	2.25176	-3.48208	6.17655	-1.00547	4.50912	5.47261	-1.02673
H	-3.34053	3.23145	2.63600	-1.92002	4.90192	-1.76794	2.74228	4.49709	-1.78335
C	-4.37525	6.20921	1.34476	-4.45551	6.35212	-0.01622	5.50238	5.47106	-0.04158
H	-3.81375	6.97560	-0.59402	-5.37297	5.51617	1.75052	6.26282	4.48408	1.72178
H	-4.76167	5.18259	3.20432	-3.35322	6.92364	-1.78266	4.51362	6.23002	-1.80460
H	-5.00449	7.05960	1.58888	-5.07839	7.24140	-0.01805	6.27475	6.23408	-0.04697
C	-3.98082	-2.71564	-0.82209	-4.04968	-2.84630	-0.00971	-3.50369	3.49655	-0.02740
C	-4.00615	-3.41595	-2.04118	-4.22529	-3.83504	-0.99552	-4.51443	3.49595	0.95197
C	-5.07030	-2.83217	0.05873	-5.04121	-2.67909	0.97479	-3.50983	4.49935	-1.01479
C	-5.10954	-4.20033	-2.38042	-5.37210	-4.62942	-1.00184	-5.49965	4.48367	0.95017
H	-3.16658	-3.33031	-2.72469	-3.47082	-3.96076	-1.76613	-4.50910	2.73240	1.72388
C	-6.16313	-3.63324	-0.27558	-6.17554	-3.49124	0.97897	-4.50968	5.47222	-1.02651
H	-5.04631	-2.31344	1.01232	-4.90669	-1.92663	1.74587	-2.74277	4.49689	-1.78321
C	-6.18847	-4.31332	-1.49767	-6.34658	-4.46381	-0.01190	-5.50291	5.47054	-0.04132
H	-5.12535	-4.72379	-3.33147	-5.50502	-5.37625	-1.77860	-6.26319	4.48342	1.72203
H	-6.99223	-3.72854	0.41892	-6.92456	-3.36533	1.75478	-4.51428	6.22965	-1.80436
H	-7.04268	-4.93038	-1.75894	-7.23427	-5.08895	-0.01275	-6.27535	6.23348	-0.04666
C	2.69498	-3.98913	0.81118	2.84623	-4.04849	-0.01753	-3.50336	-3.49688	-0.02753
C	3.67459	-4.50870	-0.05302	3.81982	-4.22732	0.98185	-3.50937	-4.49965	-1.01494
C	2.44454	-4.63772	2.03346	2.69005	-5.03783	-1.00524	-4.51414	-3.49640	0.95180

C	4.38953	-5.65385	0.30084	4.61166	-5.37611	0.99782	-4.50912	-5.47262	-1.02672
H	3.85542	-4.02746	-1.00944	3.93780	-3.47309	1.75398	-2.74227	-4.49710	-1.78334
C	3.17548	-5.77118	2.39236	3.49920	-6.17459	-0.99919	-5.49927	-4.48422	0.94994
H	1.68799	-4.24097	2.70396	1.94792	-4.90104	-1.78598	-4.50892	-2.73287	1.72373
C	4.14684	-6.28335	1.52621	4.45740	-6.34918	0.00484	-5.50239	-5.47107	-0.04158
H	5.13277	-6.05571	-0.38102	5.34773	-5.51126	1.78441	-4.51362	-6.23003	-1.80459
H	2.98498	-6.25437	3.34577	3.38170	-6.92271	-1.77721	-6.26283	-4.48407	1.72177
H	4.70910	-7.16999	1.80273	5.08027	-7.23842	0.01341	-6.27475	-6.23408	-0.04697
Co	0.00416	0.01751	0.02867	-0.01623	0.00287	0.10269	0.00001	0.00001	0.30134
H	0.02873	0.01333	1.43740	0.39024	-0.07185	1.52265	0.00001	0.00002	2.02327

CrTPP, total charge 0

		Singlet			Triplet			Quintet	
N	-1.43129	1.44305	-0.01850	-2.04334	0.00000	-0.01832	2.04814	0.00000	-0.01959
N	1.44443	1.42983	0.01815	0.00000	2.04361	0.00000	0.00000	-2.04841	0.00000
N	1.43281	-1.44045	0.03722	2.04334	0.00000	0.01832	-2.04814	0.00000	0.01959
N	-1.44600	-1.42726	-0.03761	0.00000	-2.04362	0.00000	0.00000	2.04841	0.00000
C	-2.80252	1.25709	-0.02487	-2.86795	-1.10710	0.01283	2.87085	1.10760	0.01234
C	-3.47030	2.53450	-0.04506	-4.24729	-0.68190	0.07525	4.25065	0.68198	0.07598
C	-2.49886	3.49412	-0.02496	-4.24729	0.68190	0.07525	4.25065	-0.68198	0.07598
C	-1.22939	2.81131	-0.01609	-2.86795	1.10710	0.01283	2.87085	-1.10761	0.01234
C	0.01585	3.45989	0.00018	-2.44811	2.44827	0.01374	2.44895	-2.44912	0.01355
C	1.25508	2.79989	0.01602	-1.10720	2.86879	0.00634	1.10770	-2.87170	0.00629
C	2.53076	3.47103	0.02455	-0.68191	4.24945	-0.00117	0.68198	-4.25288	-0.00126
C	3.49336	2.50255	0.04401	0.68191	4.24945	0.00122	-0.68198	-4.25288	0.00121
C	2.81390	1.23131	0.02398	1.10720	2.86879	-0.00632	-1.10770	-2.87170	-0.00630
C	3.46416	-0.01326	0.00137	2.44811	2.44827	-0.01374	-2.44895	-2.44911	-0.01355
C	2.80254	-1.25213	-0.01517	2.86795	1.10710	-0.01285	-2.87085	-1.10760	-0.01232
C	3.46847	-2.52552	-0.12687	4.24729	0.68190	-0.07530	-4.25065	-0.68198	-0.07593
C	2.49704	-3.48514	-0.14065	4.24729	-0.68190	-0.07530	-4.25065	0.68198	-0.07593
C	1.22952	-2.80706	-0.02852	2.86795	-1.10711	-0.01285	-2.87085	1.10760	-0.01233
C	-0.01589	-3.45721	0.00019	2.44811	-2.44827	-0.01374	-2.44895	2.44912	-0.01355
C	-1.25529	-2.79568	0.02856	1.10720	-2.86879	-0.00631	-1.10770	2.87170	-0.00630
C	-2.52901	-3.46204	0.14072	0.68190	-4.24945	0.00122	-0.68198	4.25288	0.00121
C	-3.49158	-2.49352	0.12643	-0.68191	-4.24945	-0.00117	0.68198	4.25288	-0.00126
C	-2.81394	-1.22634	0.01454	-1.10720	-2.86879	0.00633	1.10770	2.87170	0.00629
C	-3.46415	0.01853	-0.00236	-2.44811	-2.44827	0.01374	2.44895	2.44912	0.01355
H	-4.54047	2.67834	-0.07008	-5.09938	-1.34345	0.12801	5.10306	1.34306	0.12974
H	-2.62931	4.56642	-0.02021	-5.09938	1.34345	0.12802	5.10306	-1.34306	0.12973
H	2.67102	4.54210	0.01993	-1.34310	5.10338	-0.00712	1.34269	-5.10720	-0.00739
H	4.56481	2.63656	0.06859	1.34309	5.10338	0.00719	-1.34270	-5.10719	0.00732
H	4.53667	-2.66538	-0.20486	5.09938	1.34344	-0.12810	-5.10307	-1.34306	-0.12966
H	2.62622	-4.55345	-0.23391	5.09938	-1.34345	-0.12810	-5.10307	1.34306	-0.12966
H	-2.66808	-4.52908	0.23424	1.34309	-5.10338	0.00720	-1.34270	5.10719	0.00732
H	-4.56104	-2.62351	0.20423	-1.34310	-5.10338	-0.00712	1.34270	5.10720	-0.00739
C	4.96069	-0.02265	-0.02426	3.50825	3.50559	-0.02985	-3.50917	-3.50644	-0.03005
C	5.69033	-0.45151	1.09557	4.29438	3.74532	1.10778	-4.29884	-3.74319	1.10581
C	5.66065	0.39232	-1.16805	3.73590	4.27298	-1.18270	-3.73358	-4.27695	-1.18149
C	7.08754	-0.46320	1.07393	5.28488	4.73103	1.09443	-5.28941	-4.72881	1.09212
H	5.15438	-0.77208	1.98438	4.12161	3.15566	2.00357	-4.12875	-3.15119	2.00057
C	7.05772	0.37900	-1.19236	4.72715	5.25786	-1.19850	-4.72488	-5.26176	-1.19769
H	5.10162	0.72130	-2.03938	3.13288	4.08971	-2.06742	-3.12793	-4.09613	-2.06492
C	7.77546	-0.04833	-0.07073	5.50438	5.49010	-0.05935	-5.50557	-5.49093	-0.06028
H	7.63726	-0.79398	1.95073	5.88231	4.90666	1.98471	-5.88950	-4.90201	1.98109
H	7.58408	0.69932	-2.08718	4.89328	5.84062	-2.10025	-4.88838	-5.84685	-2.09841
H	8.86155	-0.05815	-0.08868	6.27465	6.25598	-0.07074	-6.27589	-6.25675	-0.07196
C	0.02278	4.95753	0.00073	-3.50825	3.50559	0.02985	3.50917	-3.50644	0.03005
C	0.34866	5.66966	1.16521	-3.73595	4.27294	1.18272	3.73354	-4.27700	1.18147
C	-0.29640	5.67373	-1.16310	-4.29433	3.74537	-1.10781	4.29888	-3.74314	-1.10579
C	0.35475	7.06720	1.16699	-4.72719	5.25781	1.19853	4.72483	-5.26181	1.19766
H	0.59408	5.12038	2.06973	-3.13296	4.08962	2.06746	3.12785	-4.09622	2.06488
C	-0.28943	7.07127	-1.16359	-5.28483	4.73108	-1.09445	5.28945	-4.72876	-1.09210
H	-0.54688	5.12761	-2.06815	-4.12153	3.15574	-2.00361	4.12883	-3.15111	-2.00053
C	0.03593	7.77206	0.00202	-5.50437	5.49010	0.05935	5.50557	-5.49094	0.06028
H	0.60611	7.60381	2.07762	-4.89336	5.84054	2.10029	4.88830	-5.84693	2.09837
H	-0.53574	7.61104	-2.07374	-5.88222	4.90675	-1.98475	5.88958	-4.90194	-1.98105
H	0.04101	8.85835	0.00251	-6.27464	6.25598	0.07075	6.27589	-6.25676	0.07196
C	-4.96072	0.02288	0.02286	-3.50825	-3.50559	0.02984	3.50917	3.50644	0.03005
C	-5.65715	0.44414	1.16650	-3.73595	-4.27294	1.18270	3.73354	4.27700	1.18147

C	-5.69396	-0.39912	-1.09723	-4.29433	-3.74536	-1.10783	4.29889	3.74314	-1.10578
C	-7.05429	0.44370	1.19041	-4.72720	-5.25782	1.19850	4.72484	5.26180	1.19767
H	-5.09536	0.76785	2.03804	-3.13297	-4.08963	2.06745	3.12785	4.09621	2.06488
C	-7.09123	-0.39792	-1.07599	-5.28483	-4.73107	-1.09448	5.28946	4.72876	-1.09209
H	-5.16074	-0.72455	-1.98591	-4.12152	-3.15573	-2.00363	4.12883	3.15111	-2.00053
C	-7.77561	0.02315	0.06853	-5.50438	-5.49010	0.05933	5.50557	5.49093	0.06029
H	-7.57792	0.76876	2.08513	-4.89337	-5.84054	2.10027	4.88830	5.84693	2.09838
H	-7.64371	-0.72353	-1.95298	-5.88222	-4.90674	-1.98478	5.88958	4.90194	-1.98105
H	-8.86176	0.02336	0.08615	-6.27465	-6.25598	0.07071	6.27589	6.25676	0.07196
C	-0.02272	-4.95313	0.00067	3.50825	-3.50559	-0.02984	-3.50917	3.50644	-0.03005
C	0.45725	-5.67060	1.10808	4.29437	-3.74531	1.10780	-4.29884	3.74319	1.10580
C	-0.50925	-5.66704	-1.10617	3.73591	-4.27299	-1.18268	-3.73358	4.27695	-1.18149
C	0.44949	-7.06780	1.11025	5.28487	-4.73102	1.09446	-5.28941	4.72881	1.09211
H	0.83168	-5.12453	1.96916	4.12160	-3.15565	2.00359	-4.12875	3.15119	2.00056
C	-0.51439	-7.06425	-1.10719	4.72715	-5.25787	-1.19848	-4.72488	5.26176	-1.19769
H	-0.87859	-5.11824	-1.96771	3.13289	-4.08971	-2.06741	-3.12793	4.09613	-2.06492
C	-0.03571	-7.76904	0.00182	5.50438	-5.49010	-0.05932	-5.50557	5.49093	-0.06029
H	0.81958	-7.60725	1.97765	5.88230	-4.90666	1.98474	-5.88950	4.90202	1.98108
H	-0.88942	-7.60097	-1.97416	4.89328	-5.84063	-2.10022	-4.88838	5.84685	-2.09842
H	-0.04075	-8.85532	0.00227	6.27465	-6.25598	-0.07071	-6.27589	6.25676	-0.07197
Cr	-0.00004	-0.00156	-0.00015	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

CrTPP, total charge 1

		Doublet			Quartet			Sextet	
N	2.04986	0.00000	-0.04913	-2.05480	0.00002	-0.05153	2.05499	-0.00001	-0.05319
N	0.00000	-2.05055	-0.00002	0.00002	2.05547	0.00000	-0.00001	-2.05573	0.00001
N	-2.04985	0.00000	0.04916	2.05481	-0.00002	0.05153	-2.05500	0.00001	0.05317
N	0.00000	2.05054	-0.00002	-0.00002	-2.05548	0.00000	0.00001	2.05572	0.00001
C	2.87585	1.10245	0.00562	-2.87880	-1.10293	0.00429	2.87854	1.10267	0.00405
C	4.24920	0.68285	0.11393	-4.25254	-0.68291	0.11399	4.25195	0.68308	0.11634
C	4.24920	-0.68286	0.11387	-4.25253	0.68297	0.11402	4.25194	-0.68311	0.11633
C	2.87586	-1.10246	0.00555	-2.87879	1.10297	0.00433	2.87853	-1.10268	0.00404
C	2.45190	-2.45243	0.01235	-2.45275	2.45333	0.01179	2.45271	-2.45332	0.01148
C	1.10268	-2.87824	0.00678	-1.10315	2.88123	0.00660	1.10289	-2.88110	0.00633
C	0.68280	-4.25566	-0.00610	-0.68285	4.25915	-0.00601	0.68301	-4.25890	-0.00639
C	-0.68280	-4.25566	0.00572	0.68292	4.25914	0.00611	-0.68305	-4.25890	0.00664
C	-1.10267	-2.87824	-0.00693	1.10320	2.88122	-0.00656	-1.10291	-2.88109	-0.00625
C	-2.45189	-2.45243	-0.01236	2.45279	2.45329	-0.01178	-2.45274	-2.45330	-0.01149
C	-2.87585	-1.10246	-0.00541	2.87880	1.10293	-0.00437	-2.87854	-1.10267	-0.00414
C	-4.24922	-0.68287	-0.11351	4.25253	0.68291	-0.11412	-4.25193	-0.68308	-0.11658
C	-4.24922	0.68285	-0.11356	4.25252	-0.68298	-0.11409	-4.25193	0.68311	-0.11658
C	-2.87586	1.10245	-0.00548	2.87879	-1.10297	-0.00432	-2.87852	1.10268	-0.00414
C	-2.45190	2.45242	-0.01249	2.45275	-2.45334	-0.01171	-2.45271	2.45332	-0.01149
C	-1.10267	2.87823	-0.00700	1.10315	-2.88124	-0.00652	-1.10289	2.88110	-0.00624
C	-0.68281	4.25565	0.00568	0.68285	-4.25916	0.00614	-0.68301	4.25890	0.00664
C	0.68280	4.25565	-0.00604	-0.68292	-4.25915	-0.00604	0.68305	4.25890	-0.00638
C	1.10267	2.87823	0.00686	-1.10320	-2.88122	0.00655	1.10291	2.88109	0.00635
C	2.45189	2.45243	0.01249	-2.45279	-2.45330	0.01171	2.45274	2.45329	0.01150
H	5.09922	1.34100	0.20848	-5.10280	-1.34065	0.20951	5.10209	1.34061	0.21407
H	5.09922	-1.34102	0.20837	-5.10278	1.34072	0.20957	5.10208	-1.34066	0.21406
H	1.34012	-5.11122	-0.02426	-1.33974	5.11507	-0.02428	1.33967	-5.11496	-0.02559
H	-1.34012	-5.11123	0.02374	1.33982	5.11505	0.02443	-1.33971	-5.11495	0.02593
H	-5.09926	-1.34103	-0.20787	5.10279	1.34064	-0.20970	-5.10207	-1.34061	-0.21441
H	-5.09926	1.34099	-0.20798	5.10277	-1.34073	-0.20964	-5.10206	1.34066	-0.21441
H	-1.34013	5.11122	0.02365	1.33974	-5.11508	0.02448	-1.33967	5.11496	0.02593
H	1.34012	5.11122	-0.02415	-1.33982	-5.11506	-0.02436	1.33972	5.11495	-0.02557
C	-3.50816	-3.50187	-0.03562	3.50913	3.50269	-0.03569	-3.50898	-3.50233	-0.03562
C	-4.39830	-3.63588	1.04419	4.40141	3.63529	1.04258	-4.40485	-3.63148	1.04027
C	-3.63147	-4.36637	-1.13731	3.63060	4.36870	-1.13646	-3.62737	-4.37179	-1.13417
C	-5.38421	-4.62370	1.02629	5.38739	4.62301	1.02415	-5.39086	-4.61910	1.02184
H	-4.30333	-2.97516	1.90078	4.30800	2.97349	1.89849	-4.31377	-2.96730	1.89456
C	-4.63127	-5.33999	-1.16040	4.63047	5.34222	-1.16018	-4.62751	-5.34494	-1.15810
H	-2.95415	-4.26004	-1.97945	2.95176	4.26355	-1.97752	-2.94619	-4.26911	-1.97361
C	-5.50600	-5.47441	-0.07724	5.50724	5.47516	-0.07849	-5.50759	-5.47447	-0.07865
H	-6.05622	-4.72824	1.87264	6.06098	4.72637	1.86939	-6.06694	-4.71989	1.86540
H	-4.72715	-5.99189	-2.02333	4.72483	5.99521	-2.02246	-4.71959	-6.00030	-2.01882
H	-6.27837	-6.23724	-0.09333	6.27967	6.23792	-0.09503	-6.28016	-6.23708	-0.09528
C	3.50816	-3.50187	0.03562	-3.50907	3.50274	0.03569	3.50895	-3.50236	0.03561
C	3.63129	-4.36656	1.13719	-3.63058	4.36870	1.13649	3.62745	-4.37169	1.13425
C	4.39849	-3.63570	-1.04406	-4.40130	3.63541	-1.04261	4.40470	-3.63164	-1.04036

C	4.63110	-5.34017	1.16028	-4.63044	5.34224	1.16021	4.62759	-5.34485	1.15818
H	2.95384	-4.26036	1.97924	-2.95179	4.26350	1.97758	2.94636	-4.26891	1.97375
C	5.38440	-4.62352	-1.02617	-5.38727	4.62315	-1.02419	5.39071	-4.61926	-1.02192
H	4.30366	-2.97484	-1.90056	-4.30786	2.97365	-1.89856	4.31353	-2.96755	-1.89471
C	5.50601	-5.47441	0.07724	-5.50716	5.47524	0.07848	5.50755	-5.47451	0.07865
H	4.72684	-5.99221	2.02313	-4.72482	5.99519	2.02252	4.71975	-6.00011	2.01897
H	6.05654	-4.72792	-1.87242	-6.06081	4.72656	-1.86946	6.06669	-4.72015	-1.86554
H	6.27838	-6.23724	0.09334	-6.27957	6.23801	0.09502	6.28012	-6.23712	0.09529
C	3.50815	3.50187	0.03586	-3.50913	-3.50269	0.03555	3.50898	3.50233	0.03564
C	3.63121	4.36650	1.13748	-3.63070	-4.36868	1.13632	3.62749	4.37166	1.13428
C	4.39853	3.63577	-1.04376	-4.40132	-3.63530	-1.04279	4.40473	3.63161	-1.04034
C	4.63100	5.34013	1.16069	-4.63057	-5.34220	1.15997	4.62763	5.34481	1.15821
H	2.95370	4.26026	1.97949	-2.95193	-4.26353	1.97743	2.94639	4.26888	1.97378
C	5.38443	4.62360	-1.02576	-5.38732	-4.62302	-1.02443	5.39074	4.61923	-1.02189
H	4.30376	2.97496	-1.90030	-4.30785	-2.97351	-1.89871	4.31356	2.96752	-1.89469
C	5.50597	5.47443	0.07771	-5.50726	-5.47514	0.07821	5.50758	5.47447	0.07868
H	4.72668	5.99213	2.02357	-4.72500	-5.99517	2.02225	4.71979	6.00007	2.01900
H	6.05662	4.72806	-1.87197	-6.06084	-4.72638	-1.86972	6.06673	4.72012	-1.86551
H	6.27832	6.23727	0.09388	-6.27969	-6.23790	0.09470	6.28016	6.23708	0.09532
C	-3.50816	3.50187	-0.03586	3.50908	-3.50275	-0.03555	-3.50895	3.50236	-0.03563
C	-4.39836	3.63594	1.04389	4.40131	-3.63532	1.04276	-4.40483	3.63152	1.04025
C	-3.63139	4.36632	-1.13761	3.63059	-4.36878	-1.13628	-3.62733	4.37181	-1.13419
C	-5.38426	4.62377	1.02588	5.38729	-4.62306	1.02440	-5.39083	4.61914	1.02180
H	-4.30345	2.97526	1.90051	4.30788	-2.97350	1.89865	-4.31375	2.96734	1.89454
C	-4.63118	5.33994	-1.16080	4.63045	-5.34231	-1.15994	-4.62746	5.34497	-1.15813
H	-2.95402	4.25993	-1.97970	2.95178	-4.26365	-1.97737	-2.94614	4.26912	-1.97362
C	-5.50597	5.47442	-0.07770	5.50718	-5.47523	-0.07821	-5.50754	5.47452	-0.07869
H	-6.05631	4.72836	1.87218	6.06084	-4.72640	1.86967	-6.06691	4.71995	1.86536
H	-4.72700	5.99180	-2.02378	4.72483	-5.99533	-2.02220	-4.71953	6.00032	-2.01887
H	-6.27833	6.23726	-0.09388	6.27960	-6.23800	-0.09470	-6.28012	6.23713	-0.09534
Cr	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

H-CrTPP, total charge 0

		Doublet			**Quartet**			**Sextet**	
N	-2.02808	0.00197	-0.02956	-2.03766	0.00003	-0.03708	2.04820	0.00003	-0.03572
N	0.00077	2.03267	-0.01490	-0.00125	2.03611	-0.01983	-0.00007	-2.04860	-0.01590
N	2.02461	-0.00198	-0.00113	2.03402	-0.00004	-0.00288	-2.04837	-0.00011	0.00382
N	-0.00323	-2.03268	-0.01491	-0.00132	-2.03611	-0.01983	-0.00022	2.04851	-0.01597
C	-2.85968	-1.10305	-0.01008	-2.86417	-1.10575	-0.01150	2.87083	1.10765	-0.00160
C	-4.23824	-0.67735	0.02746	-4.24365	-0.68163	0.03354	4.25045	0.68211	0.06461
C	-4.23690	0.68563	0.02757	-4.24362	0.68177	0.03356	4.25050	-0.68189	0.06461
C	-2.85750	1.10863	-0.00992	-2.86413	1.10585	-0.01147	2.87090	-1.10753	-0.00160
C	-2.44360	2.44768	-0.00349	-2.44740	2.44588	-0.00653	2.44881	-2.44902	0.00065
C	-1.10383	2.86237	-0.01142	-1.10731	2.86253	-0.01745	1.10762	-2.87190	-0.00705
C	-0.67972	4.24141	-0.02969	-0.68367	4.24271	-0.03884	0.68195	-4.25303	-0.01138
C	0.68383	4.24070	-0.02819	0.67975	4.24325	-0.03676	-0.68207	-4.25302	-0.00879
C	1.10650	2.86104	-0.02462	1.10443	2.86322	-0.02995	-1.10775	-2.87194	-0.01967
C	2.44531	2.44337	-0.03172	2.44434	2.44614	-0.03330	-2.44901	-2.44919	-0.02605
C	2.85559	1.10305	-0.03760	2.86010	1.10573	-0.03630	-2.87117	-1.10774	-0.02525
C	4.23248	0.67734	-0.11547	4.23841	0.68163	-0.10990	-4.25109	-0.68219	-0.08494
C	4.23114	-0.68564	-0.11537	4.23839	-0.68178	-0.10988	-4.25114	0.68181	-0.08498
C	2.85342	-1.10864	-0.03747	2.86007	-1.10583	-0.03628	-2.87125	1.10746	-0.02530
C	2.44051	-2.44815	-0.03147	2.44426	-2.44622	-0.03326	-2.44918	2.44894	-0.02616
C	1.10088	-2.86320	-0.02447	1.10433	-2.86326	-0.02993	-1.10795	2.87178	-0.01978
C	0.67553	-4.24204	-0.02806	0.67960	-4.24328	-0.03674	-0.68236	4.25289	-0.00889
C	-0.68803	-4.24009	-0.02976	-0.68381	-4.24269	-0.03885	0.68165	4.25299	-0.01144
C	-1.10946	-2.86023	-0.01156	-1.10741	-2.86249	-0.01748	1.10742	2.87189	-0.00709
C	-2.44841	-2.44292	-0.00375	-2.44749	-2.44580	-0.00657	2.44864	2.44910	0.00065
H	-5.09066	-1.33958	0.06183	-5.09560	-1.34418	0.07306	5.10273	1.34322	0.12040
H	-5.08801	1.34953	0.06202	-5.09556	1.34436	0.07309	5.10282	-1.34294	0.12040
H	-1.34240	5.09408	-0.04340	-1.34651	5.09519	-0.05495	1.34265	-5.10737	-0.01517
H	1.34715	5.09292	-0.03163	1.34174	5.09649	-0.04174	-1.34279	-5.10732	-0.00016
H	5.08310	1.33978	-0.17873	5.08887	1.34452	-0.17080	-5.10368	-1.34329	-0.13590
H	5.08046	-1.34976	-0.17853	5.08883	-1.34470	-0.17077	-5.10378	1.34284	-0.13597
H	1.33718	-5.09554	-0.03138	1.34156	-5.09654	-0.04171	-1.34314	5.10715	-0.00029
H	-1.35236	-5.09146	-0.04354	-1.34668	-5.09515	-0.05498	1.34230	5.10738	-0.01522
C	3.50842	3.49745	-0.04380	3.50566	3.50212	-0.04396	-3.50910	-3.50669	-0.03925
C	4.28180	3.74037	1.10167	4.27834	3.74513	1.10201	-4.29702	-3.74181	1.09816
C	3.75136	4.25674	-1.19863	3.74808	4.26282	-1.19802	-3.73506	-4.27913	-1.18910
C	5.27575	4.72266	1.09376	5.27086	4.72886	1.09538	-5.28732	-4.72771	1.08757

H	4.09627	3.15631	1.99855	4.09328	3.16007	1.99834	-4.12576	-3.14827	1.99168
C	4.74638	5.23795	-1.20878	4.74166	5.24549	-1.20686	-4.72610	-5.26421	-1.20223
H	3.15783	4.07039	-2.08915	3.15534	4.07633	-2.08904	-3.13077	-4.09954	-2.07374
C	5.51108	5.47404	-0.06196	5.50556	5.48167	-0.05953	-5.50500	-5.49177	-0.06327
H	5.86360	4.90150	1.98972	5.85806	4.90773	1.99176	-5.88605	-4.89965	1.97771
H	4.92501	5.81491	-2.11184	4.91984	5.82347	-2.10937	-4.89080	-5.85083	-2.10174
H	6.28411	6.23718	-0.06895	6.27748	6.24593	-0.06552	-6.27513	-6.25783	-0.07255
C	-3.50200	3.50659	0.01400	-3.50593	3.50457	0.01402	3.50911	-3.50621	0.02061
C	-3.74444	4.25215	1.17784	-3.73775	4.25793	1.17509	3.73178	-4.27459	1.17383
C	-4.26851	3.77020	-1.13139	-4.28390	3.75996	-1.12559	4.30073	-3.74486	-1.11347
C	-4.73275	5.23996	1.19669	-4.72655	5.24515	1.19685	4.72324	-5.25914	1.19350
H	-3.15563	4.04960	2.06791	-3.14036	4.06169	2.06083	3.12456	-4.09229	2.05590
C	-5.25593	4.75904	-1.11470	-5.27173	4.74831	-1.10603	5.29146	-4.73025	-1.09634
H	-4.08332	3.19725	-2.03556	-4.10714	3.18107	-2.02764	4.13198	-3.15453	-2.00960
C	-5.49106	5.49647	0.05000	-5.49610	5.49347	0.05586	5.50587	-5.49022	0.05780
H	-4.91115	5.80619	2.10654	-4.89662	5.81727	2.10462	4.88537	-5.84257	2.09555
H	-5.83875	4.95384	-2.01064	-5.86326	4.93672	-1.99763	5.89309	-4.90496	-1.98398
H	-6.25896	6.26467	0.06393	-6.26437	6.26125	0.07204	6.27634	-6.25585	0.07216
C	-3.50890	-3.49973	0.01355	-3.50605	-3.50445	0.01394	3.50886	3.50637	0.02063
C	-3.75293	-4.24492	1.17730	-3.73792	-4.25782	1.17500	3.73147	4.27476	1.17386
C	-4.27586	-3.76168	-1.13193	-4.28401	-3.75980	-1.12569	4.30047	3.74510	-1.11345
C	-4.74323	-5.23074	1.19597	-4.72676	-5.24501	1.19673	4.72285	5.25938	1.19354
H	-3.16378	-4.04364	2.06743	-3.14054	-4.06161	2.06076	3.12427	4.09239	2.05592
C	-5.26527	-4.74853	-1.11541	-5.27188	-4.74810	-1.10616	5.29112	4.73057	-1.09630
H	-4.08945	-3.18901	-2.03602	-4.10721	-3.18090	-2.02773	4.13177	3.15477	-2.00958
C	-5.50197	-5.48560	0.04920	-5.49630	-5.49327	0.05572	5.50546	5.49054	0.05786
H	-4.92284	-5.79670	2.10575	-4.89687	-5.81713	2.10448	4.88493	5.84281	2.09560
H	-5.84842	-4.94206	-2.01141	-5.86340	-4.93648	-1.99777	5.89274	4.90534	-1.98394
H	-6.27141	-6.25226	0.06299	-6.26460	-6.26102	0.07188	6.27588	6.25623	0.07222
C	3.50155	-3.50431	-0.04338	3.50555	-3.50224	-0.04389	-3.50935	3.50636	-0.03942
C	4.27434	-3.74865	1.10219	4.27819	-3.74526	1.10211	-4.29731	3.74149	1.09796
C	3.74310	-4.26419	-1.19812	3.74796	-4.26297	-1.19793	-3.73532	4.27873	-1.18931
C	5.26635	-4.73292	1.09447	5.27068	-4.72902	1.09551	-5.28767	4.72732	1.08730
H	4.08988	-3.16414	1.99900	4.09314	-3.16018	1.99842	-4.12602	3.14800	1.99152
C	4.73617	-5.24737	-1.20807	4.74150	-5.24567	-1.20674	-4.72643	5.26375	-1.20250
H	3.15002	-4.07675	-2.08871	3.15524	-4.07647	-2.08896	-3.13101	4.09915	-2.07393
C	5.50029	-5.48487	-0.06116	5.50537	-5.48185	-0.05939	-5.50537	5.49132	-0.06358
H	5.85375	-4.91283	1.99050	5.85786	-4.90790	1.99190	-5.88643	4.89927	1.97742
H	4.91373	-5.82478	-2.11106	4.91968	-5.82367	-2.10923	-4.89115	5.85032	-2.10205
H	6.27180	-6.24954	-0.06801	6.27728	-6.24614	-0.06536	-6.27555	6.25732	-0.07291
Cr	-0.00227	0.00000	0.16409	-0.00268	0.00000	0.16580	-0.00013	-0.00005	-0.02461
H	-0.02224	0.00005	1.72639	-0.02520	0.00000	1.74295	0.02404	0.01379	3.50752

CuTPP, total charge 0

		Doublet			**Quartet**			**Sextet**	
N	2.02449	0.00002	-0.01750	-0.00322	-2.03577	-0.02860	-2.03964	-0.00001	-0.03010
N	0.00002	-2.02479	0.00000	-2.04497	0.00323	-0.00001	0.00000	2.04050	0.00001
N	-2.02449	-0.00001	0.01750	0.00321	2.03577	0.02861	2.03964	-0.00001	0.03007
N	-0.00001	2.02479	0.00000	2.04495	-0.00323	0.00001	0.00000	-2.04054	0.00001
C	2.85157	1.10240	0.01247	1.09532	-2.86995	0.02117	-2.87195	-1.10369	0.01236
C	4.23252	0.68090	0.07229	0.68608	-4.22538	0.11430	-4.24827	-0.68398	0.09506
C	4.23253	-0.68084	0.07231	-0.69945	-4.22320	0.11417	-4.24827	0.68392	0.09526
C	2.85158	-1.10235	0.01251	-1.10438	-2.86647	0.02099	-2.87196	1.10367	0.01265
C	2.44182	-2.44193	0.01324	-2.46756	-2.43290	0.01734	-2.45647	2.45686	0.01433
C	1.10248	-2.85236	0.00633	-2.87749	-1.09982	0.01035	-1.10382	2.87382	0.00801
C	0.68091	-4.23452	-0.00101	-4.26143	-0.67263	-0.00146	-0.68395	4.25251	-0.00274
C	-0.68085	-4.23453	0.00092	-4.25928	0.68609	0.00138	0.68394	4.25251	0.00294
C	-1.10244	-2.85238	-0.00636	-2.87400	1.10890	-0.01034	1.10382	2.87383	-0.00793
C	-2.44178	-2.44196	-0.01324	-2.45986	2.44068	-0.01731	2.45647	2.45686	-0.01433
C	-2.85157	-1.10239	-0.01248	-1.09533	2.86995	-0.02095	2.87196	1.10367	-0.01273
C	-4.23252	-0.68090	-0.07221	-0.68611	4.22539	-0.11410	4.24826	0.68392	-0.09546
C	-4.23253	0.68084	-0.07219	0.69942	4.22320	-0.11421	4.24826	-0.68398	-0.09526
C	-2.85158	1.10236	-0.01244	1.10436	2.86648	-0.02114	2.87195	-1.10370	-0.01244
C	-2.44182	2.44193	-0.01318	2.46754	2.43290	-0.01766	2.45647	-2.45689	-0.01379
C	-1.10248	2.85236	-0.00633	2.87747	1.09982	-0.01055	1.10383	-2.87386	-0.00764
C	-0.68091	4.23452	0.00094	4.26141	0.67263	0.00127	0.68394	-4.25254	0.00314
C	0.68085	4.23453	-0.00104	4.25926	-0.68609	-0.00132	-0.68394	-4.25254	-0.00294
C	1.10244	2.85238	0.00629	2.87398	-1.10890	0.01050	-1.10383	-2.87386	0.00772

C	2.44178	2.44196	0.01318	2.45984	-2.44067	0.01764	-2.45647	-2.45689	0.01379
H	5.08211	1.34574	0.12280	1.34332	-5.07827	0.19043	-5.09688	-1.34722	0.16681
H	5.08213	-1.34566	0.12285	-1.35940	-5.07400	0.19019	-5.09688	1.34714	0.16720
H	1.34542	-5.08580	-0.00671	-5.11520	-1.33336	-0.01130	-1.34662	5.10441	-0.01367
H	-1.34535	-5.08582	0.00657	-5.11096	1.34951	0.01116	1.34661	5.10441	0.01393
H	-5.08212	-1.34574	-0.12271	-1.34337	5.07828	-0.19008	5.09687	1.34714	-0.16746
H	-5.08214	1.34567	-0.12266	1.35935	5.07401	-0.19032	5.09686	-1.34722	-0.16707
H	-1.34543	5.08580	0.00662	5.11518	1.33336	0.01096	1.34661	-5.10445	0.01432
H	1.34535	5.08582	-0.00676	5.11094	-1.34952	-0.01100	-1.34661	-5.10445	-0.01406
C	-3.50170	-3.49921	-0.02881	-3.50580	3.50406	-0.03419	3.51291	3.50836	-0.03390
C	-4.27553	-3.75040	1.11462	-3.67832	4.34978	1.07401	4.35780	3.69380	1.07315
C	-3.74102	-4.25481	-1.18692	-4.32974	3.68238	-1.15709	3.68690	4.33069	-1.15964
C	-5.26588	-4.73631	1.10173	-4.66155	5.34127	1.06442	5.34871	4.67840	1.05695
H	-4.09355	-3.16957	2.01436	-3.03997	4.22015	1.94288	4.22846	3.06317	1.94805
C	-4.73226	-5.23975	-1.20226	-5.30692	4.68100	-1.17072	4.68078	5.31225	-1.17885
H	-3.14712	-4.06257	-2.07592	-4.19458	3.03756	-2.02051	3.04078	4.19070	-2.02147
C	-5.49734	-5.48368	-0.05734	-5.47780	5.51133	-0.05897	5.51416	5.49023	-0.06983
H	-5.85399	-4.92105	1.99636	-4.78960	5.98068	1.93330	5.98898	4.81239	1.92441
H	-4.90766	-5.81358	-2.10796	-5.93214	4.81020	-2.04971	4.80557	5.93497	-2.06033
H	-6.26754	-6.24965	-0.06836	-6.23956	6.28566	-0.06786	6.28585	6.25461	-0.08369
C	3.50175	-3.49916	0.02881	-3.51683	-3.49300	0.03420	-3.51291	3.50836	0.03390
C	3.74101	-4.25484	1.18688	-4.34128	-3.66878	1.15713	-3.68700	4.33059	1.15970
C	4.27566	-3.75026	-1.11459	-3.69203	-4.33814	-1.07401	-4.35770	3.69390	-1.07321
C	4.73226	-5.23976	1.20222	-5.32160	-4.66432	1.17075	-4.68088	5.31215	1.17890
H	3.14704	-4.06267	2.07585	-4.20409	-3.02442	2.02057	-3.04095	4.19052	2.02157
C	5.26603	-4.73616	-1.10170	-4.67838	-5.32652	-1.06444	-5.34862	4.67850	-1.05701
H	4.09373	-3.16937	-2.01430	-3.05331	-4.21046	-1.94291	-4.22829	3.06334	-1.94815
C	5.49742	-5.48360	0.05734	-5.49513	-5.49406	0.05896	-5.51416	5.49023	0.06983
H	4.90760	-5.81365	2.10789	-5.94721	-4.79158	2.04974	-4.80574	5.93479	2.06043
H	5.85420	-4.92082	-1.99630	-4.80846	-5.96548	-1.93335	-5.98881	4.81256	-1.92451
H	6.26763	-6.24956	0.06836	-6.25932	-6.26599	0.06785	-6.28584	6.25461	0.08369
C	3.50170	3.49921	0.02870	3.50580	-3.50405	0.03475	-3.51293	-3.50837	0.03294
C	3.74098	4.25492	1.18675	4.32964	-3.68216	1.15775	-3.68731	-4.33081	1.15855
C	4.27558	3.75030	-1.11472	3.67843	-4.34993	-1.07329	-4.35751	-3.69365	-1.07438
C	4.73222	5.23985	1.20204	5.30685	-4.68076	1.17162	-4.68124	-5.31232	1.17735
H	3.14704	4.06276	2.07574	4.19441	-3.03721	2.02106	-3.04144	-4.19092	2.02059
C	5.26594	4.73620	-1.10188	4.66168	-5.34139	-1.06347	-5.34847	-4.67821	-1.05858
H	4.09364	3.16939	-2.01441	3.04015	-4.22045	-1.94225	-4.22789	-3.06293	-1.94917
C	5.49735	5.48368	0.05714	5.47784	-5.51126	0.06001	-5.51429	-5.49015	0.06807
H	4.90758	5.81376	2.10770	5.93200	-4.80981	2.05068	-4.80632	-5.93513	2.05873
H	5.85409	4.92086	-1.99650	4.78982	-5.98093	-1.93225	-5.98849	-4.81208	-1.92624
H	6.26755	6.24964	0.06811	6.23963	-6.28558	0.06909	-6.28601	-6.25450	0.08161
C	-3.50175	3.49916	-0.02870	3.51682	3.49298	-0.03478	3.51293	-3.50837	-0.03294
C	-4.27556	3.75031	1.11476	3.69222	4.33822	1.07334	4.35760	-3.69356	1.07432
C	-3.74112	4.25479	-1.18679	4.34110	3.66863	-1.15785	3.68721	-4.33091	-1.15849
C	-5.26593	4.73620	1.10192	4.67859	5.32657	1.06351	5.34857	-4.67812	1.05853
H	-4.09355	3.16946	2.01448	3.05364	4.21064	1.94235	4.22806	-3.06275	1.94907
C	-4.73238	5.23970	-1.20208	5.32145	4.66415	-1.17171	4.68114	-5.31242	-1.17729
H	-3.14724	4.06257	-2.07580	4.20377	3.02419	-2.02120	3.04127	-4.19110	-2.02049
C	-5.49743	5.48359	-0.05714	5.49517	5.49399	-0.06003	5.51429	-5.49015	-0.06807
H	-5.85402	4.92091	1.99656	4.80883	5.96561	1.93235	5.98866	-4.81191	1.92614
H	-4.90780	5.81355	-2.10776	5.94693	4.79131	-2.05081	4.80615	-5.93530	-2.05863
H	-6.26764	6.24955	-0.06812	6.25939	6.26590	-0.06910	6.28601	-6.25450	-0.08161
Cu	0.00000	0.00000	0.00000	-0.00001	0.00000	0.00000	0.00000	-0.00001	0.00000

CuTPP, total charge 1

		Singlet			Triplet			Quintet	
N	0.29146	2.00304	-0.07502	-2.03117	0.00000	-0.04820	2.03160	-0.00014	-0.03804
N	2.00304	-0.29146	0.07502	0.00000	2.03168	0.00001	-0.00013	-2.02994	-0.00009
N	-0.29146	-2.00304	-0.07502	2.03117	0.00001	0.04818	-2.03157	0.00015	0.03813
N	-2.00304	0.29146	0.07502	0.00001	-2.03168	0.00001	0.00014	2.02996	-0.00009
C	-0.68327	2.93918	0.21744	-2.85946	-1.09806	0.00577	2.86194	1.10301	0.00828
C	-0.08720	4.14521	0.72358	-4.23402	-0.68195	0.11185	4.25756	0.67410	0.10177
C	1.26338	3.94864	0.72513	-4.23403	0.68194	0.11182	4.25747	-0.67465	0.10185
C	1.49209	2.62267	0.21970	-2.85947	1.09806	0.00572	2.86179	-1.10338	0.00840
C	2.76195	2.06047	0.00204	-2.44589	2.44630	0.01270	2.46648	-2.43857	0.01719
C	2.93918	0.68327	-0.21744	-1.09828	2.86160	0.00765	1.09699	-2.86212	0.00889
C	4.14521	0.08720	-0.72358	-0.68190	4.24002	-0.00530	0.68543	-4.23645	-0.00426
C	3.94865	-1.26338	-0.72513	0.68189	4.24002	0.00546	-0.68601	-4.23635	0.00323
C	2.62267	-1.49209	-0.21970	1.09828	2.86160	-0.00759	-1.09739	-2.86198	-0.00934

C	2.06048	-2.76195	-0.00204	2.44588	2.44632	-0.01270	-2.46681	-2.43822	-0.01723
C	0.68327	-2.93918	0.21744	2.85946	1.09806	-0.00579	-2.86193	-1.10300	-0.00810
C	0.08720	-4.14521	0.72359	4.23402	0.68196	-0.11197	-4.25759	-0.67408	-0.10105
C	-1.26338	-3.94864	0.72514	4.23402	-0.68193	-0.11200	-4.25749	0.67467	-0.10096
C	-1.49209	-2.62267	0.21970	2.85947	-1.09805	-0.00583	-2.86177	1.10339	-0.00798
C	-2.76196	-2.06048	0.00204	2.44589	-2.44630	-0.01278	-2.46647	2.43857	-0.01702
C	-2.93918	-0.68327	-0.21744	1.09828	-2.86159	-0.00763	-1.09698	2.86213	-0.00924
C	-4.14521	-0.08720	-0.72359	0.68190	-4.24002	0.00542	-0.68542	4.23646	0.00329
C	-3.94864	1.26338	-0.72513	-0.68189	-4.24002	-0.00527	0.68602	4.23636	-0.00436
C	-2.62267	1.49209	-0.21970	-1.09827	-2.86160	0.00769	1.09740	2.86199	0.00876
C	-2.06047	2.76195	-0.00204	-2.44588	-2.44631	0.01277	2.46682	2.43824	0.01697
H	-0.63516	5.01200	1.06219	-5.08186	-1.34299	0.20485	5.10221	1.34054	0.18781
H	2.03489	4.62342	1.06527	-5.08186	1.34299	0.20479	5.10203	-1.34120	0.18798
H	5.01201	0.63516	-1.06218	-1.34218	5.09321	-0.02337	1.34755	-5.08807	-0.01928
H	4.62342	-2.03489	-1.06527	1.34216	5.09321	0.02359	-1.34825	-5.08790	0.01792
H	0.63516	-5.01200	1.06219	5.08184	1.34300	-0.20499	-5.10227	-1.34051	-0.18688
H	-2.03489	-4.62341	1.06529	5.08185	-1.34297	-0.20505	-5.10208	1.34123	-0.18671
H	-5.01200	-0.63516	-1.06219	1.34218	-5.09320	0.02352	-1.34754	5.08810	0.01805
H	-4.62342	2.03489	-1.06527	-1.34216	-5.09321	-0.02332	1.34825	5.08791	-0.01946
C	2.94569	-3.94910	-0.00363	3.50188	3.49570	-0.03563	-3.51731	-3.49336	-0.03658
C	2.64589	-5.06342	-0.81090	4.38713	3.63411	1.04755	-4.38298	-3.65393	1.05862
C	4.10025	-3.98138	0.80210	3.62963	4.35558	-1.14034	-3.65779	-4.33990	-1.14995
C	3.48672	-6.17600	-0.81957	5.37291	4.62211	1.02988	-5.36840	-4.64360	1.04115
H	1.76668	-5.04024	-1.44723	4.28863	2.97671	1.90630	-4.27147	-3.01065	1.92678
C	4.92645	-5.10491	0.80771	4.62944	5.32922	-1.16308	-4.65236	-5.31917	-1.17036
H	4.32987	-3.13332	1.43969	2.95575	4.24580	-1.98480	-2.99643	-4.21722	-2.00277
C	4.62510	-6.20183	-0.00670	5.49938	5.46822	-0.07665	-5.50736	-5.47554	-0.07399
H	3.25522	-7.02104	-1.46064	6.04125	4.73021	1.87867	-6.02450	-4.76489	1.89774
H	5.80323	-5.12547	1.44763	4.72891	5.97766	-2.02820	-4.76065	-5.95786	-2.04173
H	5.27404	-7.07232	-0.00789	6.27168	6.23112	-0.09250	-6.27655	-6.24160	-0.08900
C	3.94910	2.94568	0.00363	-3.50189	3.49569	0.03563	3.51683	-3.49385	0.03660
C	5.06342	2.64588	0.81090	-3.62971	4.35550	1.14039	3.65672	-4.34083	1.14972
C	3.98139	4.10025	-0.80210	-4.38707	3.63416	-1.04760	4.38296	-3.65413	-1.05828
C	6.17600	3.48671	0.81957	-4.62952	5.32913	1.16312	4.65114	-5.32024	1.17019
H	5.04025	1.76667	1.44723	-2.95589	4.24567	1.98489	2.99501	-4.21838	2.00229
C	5.10491	4.92644	-0.80771	-5.37285	4.62216	-1.02993	5.36823	-4.64396	-1.04076
H	3.13332	4.32987	-1.43969	-4.28851	2.97682	-1.90638	4.27190	-3.01053	-1.92626
C	6.20184	4.62509	0.00670	-5.49939	5.46821	0.07664	5.50660	-5.47632	0.07413
H	7.02105	3.25520	1.46064	-4.72905	5.97753	2.02827	4.75897	-5.95926	2.04138
H	5.12548	5.80323	-1.44763	-6.04113	4.73032	-1.87876	6.02468	-4.76502	-1.89712
H	7.07233	5.27403	0.00789	-6.27170	6.23111	0.09249	6.27567	-6.24249	0.08919
C	-2.94569	3.94910	-0.00363	-3.50188	-3.49570	0.03576	3.51732	3.49337	0.03621
C	-4.10025	3.98139	0.80210	-3.62965	-4.35548	1.14055	3.65745	4.34040	1.14926
C	-2.64589	5.06342	-0.81090	-4.38709	-3.63421	-1.04743	4.38337	3.65345	-1.05877
C	-4.92645	5.10491	0.80771	-4.62946	-5.32912	1.16334	4.65203	5.31966	1.16957
H	-4.32987	3.13332	1.43969	-2.95580	-4.24562	1.98503	2.99581	4.21811	2.00191
C	-3.48672	6.17600	-0.81957	-5.37286	-4.62222	-1.02970	5.36880	4.64312	-1.04140
H	-1.76668	5.04024	-1.44723	-4.28857	-2.97690	-1.90623	4.27213	3.00980	-1.92668
C	-4.62510	6.20183	-0.00671	-5.49936	-5.46823	0.07690	5.50740	5.47554	0.07342
H	-5.80323	5.12548	1.44763	-4.72894	-5.97749	2.02852	4.76005	5.95872	2.04070
H	-3.25522	7.02104	-1.46064	-6.04117	-4.73040	-1.87850	6.02518	4.76402	-1.89783
H	-5.27404	7.07233	-0.00789	-6.27166	-6.23114	0.09280	6.27660	6.24158	0.08835
C	-3.94910	-2.94569	0.00363	3.50189	-3.49569	-0.03576	-3.51684	3.49384	-0.03619
C	-3.98141	-4.10023	-0.80213	4.38717	-3.63413	1.04738	-4.38240	3.65441	1.05909
C	-5.06341	-2.64590	0.81092	3.62960	-4.35554	-1.14051	-3.65732	4.34050	-1.14948
C	-5.10493	-4.92642	-0.80774	5.37294	-4.62213	1.02965	-5.36771	4.64421	1.04180
H	-3.13335	-4.32983	-1.43974	4.28870	-2.97676	1.90615	-4.27089	3.01105	1.92718
C	-6.17599	-3.48673	0.81959	4.62940	-5.32918	-1.16330	-4.65177	5.31989	-1.16971
H	-5.04022	-1.76671	1.44728	2.95569	-4.24574	-1.98495	-2.99605	4.21782	-2.00236
C	-6.20184	-4.62509	0.00670	5.49937	-5.46822	-0.07690	-5.50667	5.47627	-0.07325
H	-5.12551	-5.80319	-1.44768	6.04130	-4.73026	1.87842	-6.02372	4.76549	1.89846
H	-7.02103	-3.25524	1.46068	4.72884	-5.97760	-2.02844	-4.76007	5.95867	-2.04101
H	-7.07234	-5.27402	0.00789	6.27168	-6.23112	-0.09280	-6.27576	6.24242	-0.08813
Cu	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00001	-0.00002

H-CuTPP, total charge 0

		Singlet			Triplet			Quintet	
N	0.00009	2.12723	-0.11661	2.01274	0.25096	-0.03832	0.01358	2.04177	-0.05823
N	1.96667	-0.00013	0.02902	0.25084	-2.01377	-0.02641	2.04974	-0.01226	-0.02455
N	-0.00009	-2.12666	-0.11399	-2.01080	-0.25091	-0.01944	-0.01351	-2.03729	0.00571

N	-1.96667	0.00003	0.02903	-0.24934	2.01406	-0.04456	-2.04961	0.01494	-0.02462
C	-1.09650	2.93230	-0.19755	2.69649	1.44653	-0.04354	-1.08148	2.87904	-0.00575
C	-0.68230	4.31150	-0.40900	4.11983	1.19767	-0.09024	-0.66543	4.23220	0.07917
C	0.68266	4.31144	-0.40905	4.28725	-0.15387	-0.08839	0.72172	4.22300	0.07843
C	1.09674	2.93221	-0.19754	2.96744	-0.74173	-0.05469	1.11967	2.86443	-0.00683
C	2.41434	2.46411	-0.03005	2.72395	-2.12050	-0.02550	2.48091	2.42276	-0.00272
C	2.78647	1.11459	0.14773	1.44730	-2.69551	-0.00164	2.88441	1.08746	-0.01403
C	4.14128	0.68218	0.39916	1.20166	-4.11940	0.02572	4.26618	0.65374	-0.03377
C	4.14144	-0.68180	0.39953	-0.14965	-4.28895	0.03048	4.25803	-0.70547	-0.02975
C	2.78673	-1.11451	0.14825	-0.74036	-2.96996	-0.00857	2.87090	-1.12233	-0.03360
C	2.41442	-2.46402	-0.02922	-2.11972	-2.72594	-0.03321	2.44904	-2.45208	-0.03455
C	1.09666	-2.93162	-0.19674	-2.69249	-1.44707	-0.05902	1.08163	-2.87391	-0.04541
C	0.68232	-4.31025	-0.41044	-4.11312	-1.19912	-0.15495	0.66561	-4.22565	-0.15309
C	-0.68268	-4.31018	-0.41047	-4.28153	0.15229	-0.15510	-0.72140	-4.21645	-0.15388
C	-1.09690	-2.93153	-0.19673	-2.96521	0.74144	-0.05837	-1.11956	-2.85932	-0.04662
C	-2.41463	-2.46383	-0.02921	-2.72320	2.12155	-0.02509	-2.48129	-2.41936	-0.03665
C	-2.78682	-1.11428	0.14826	-1.44531	2.69604	0.00301	-2.88544	-1.08414	-0.03475
C	-4.14150	-0.68146	0.39952	-1.19706	4.11698	0.09424	-4.26691	-0.64890	-0.03036
C	-4.14123	0.68252	0.39916	0.15447	4.28488	0.09698	-4.25701	0.71030	-0.03282
C	-2.78638	1.11481	0.14772	0.74312	2.96796	0.00780	-2.86960	1.12560	-0.01290
C	-2.41414	2.46431	-0.03006	2.12299	2.72452	-0.00984	-2.44842	2.45545	-0.00078
H	-1.34345	5.15604	-0.54138	4.88240	1.96170	-0.12204	-1.31755	5.08959	0.14787
H	1.34387	5.15591	-0.54147	5.21295	-0.70990	-0.11007	1.38523	5.07167	0.14646
H	4.98434	1.33906	0.55473	1.96801	-4.88041	0.03850	5.12281	1.31064	-0.05242
H	4.98460	-1.33845	0.55548	-0.70288	-5.21607	0.05612	5.10711	-1.37225	-0.02701
H	1.34345	-5.15453	-0.54443	-4.87242	-1.96354	-0.22889	1.31854	-5.08072	-0.24143
H	-1.34388	-5.15441	-0.54449	-5.20531	0.70665	-0.22980	-1.38550	-5.06280	-0.24296
H	-4.98472	-1.33804	0.55547	-1.96091	4.87751	0.16058	-5.12475	-1.30436	-0.02825
H	-4.98423	1.33947	0.55472	0.70910	5.20903	0.16538	-5.10485	1.37855	-0.05058
C	3.50526	-3.48771	-0.02468	-3.04214	-3.90460	-0.03751	3.48753	-3.52246	-0.04185
C	3.58550	-4.44011	1.00365	-3.80847	-4.21335	1.09697	3.64311	-4.36852	1.06876
C	4.45894	-3.52254	-1.05470	-3.15850	-4.71818	-1.17512	4.31988	-3.70900	-1.15731
C	4.59878	-5.40213	1.00532	-4.67078	-5.31294	1.09543	4.61832	-5.36785	1.06901
H	2.85167	-4.41734	1.80400	-3.72080	-3.58774	1.98062	2.99804	-4.23254	1.93166
C	5.46784	-4.48867	-1.05808	-4.02275	-5.81625	-1.17922	5.28895	-4.71554	-1.16106
H	4.39977	-2.79049	-1.85486	-2.57025	-4.48169	-2.05716	4.19696	-3.06496	-2.02314
C	5.54202	-5.43026	-0.02658	-4.78083	-6.11726	-0.04326	5.44325	-5.54579	-0.04681
H	4.65119	-6.12766	1.81224	-5.25410	-5.54137	1.98304	4.73337	-6.00729	1.93968
H	6.19387	-4.50638	-1.86605	-4.10491	-6.43383	-2.06924	5.92058	-4.85120	-2.03448
H	6.32814	-6.17995	-0.02734	-5.45195	-6.97143	-0.04548	6.19876	-6.32628	-0.04805
C	3.50545	3.48757	-0.02503	3.90579	-3.04069	-0.01747	3.53670	3.47595	0.02321
C	3.58672	4.43866	1.00441	4.30477	-3.67651	1.16767	4.35855	3.63874	1.15012
C	4.45834	3.52341	-1.05573	4.63083	-3.28132	-1.19406	3.72249	4.32606	-1.07955
C	4.60024	5.40043	1.00648	5.40712	-4.53561	1.17685	5.34608	4.62687	1.17314
H	2.85349	4.41510	1.80529	3.74726	-3.49130	2.08143	4.21323	2.99022	2.00907
C	5.46749	4.48929	-1.05870	5.73274	-4.14104	-1.18667	4.71608	5.30702	-1.06048
H	4.39838	2.79233	-1.85672	4.32396	-2.79282	-2.11457	3.08679	4.20759	-1.95197
C	5.54269	5.42960	-0.02611	6.12397	-4.77036	-0.00071	5.52975	5.46195	0.06694
H	4.65345	6.12497	1.81424	5.70582	-5.01900	2.10282	5.96940	4.74430	2.05511
H	6.19292	4.50779	-1.86720	6.28298	-4.31976	-2.10625	4.85440	5.94983	-1.92528
H	6.32900	6.17909	-0.02656	6.98055	-5.43838	0.00576	6.29960	6.22812	0.08318
C	-3.50516	3.48786	-0.02503	3.04263	3.90512	0.01651	-3.49019	3.52248	0.02672
C	-4.45806	3.52377	-1.05573	3.79254	4.19993	1.16560	-4.30889	3.69529	1.15441
C	-3.58633	4.43897	1.00440	3.16896	4.73733	-1.10642	-3.66561	4.37579	-1.07528
C	-5.46713	4.48974	-1.05869	4.64953	5.30333	1.19214	-5.28319	4.69643	1.17899
H	-4.39817	2.79268	-1.85671	3.69603	3.56070	2.03850	-4.17146	3.04427	2.01277
C	-4.59977	5.40083	1.00648	4.02793	5.83932	-1.08241	-4.64607	5.36984	-1.05465
H	-2.85309	4.41535	1.80527	2.59232	4.51253	-1.99913	-3.03224	4.24956	-1.94830
C	-5.54223	5.43007	-0.02610	4.77023	6.12585	0.06759	-5.45667	5.53471	0.07358
H	-6.19257	4.50830	-1.86717	5.22007	5.52075	2.09075	-5.90417	4.82146	2.06157
H	-4.65290	6.12538	1.81423	4.11800	6.47150	-1.96137	-4.77656	6.01509	-1.91885
H	-6.32847	6.17963	-0.02655	5.43720	6.98305	0.08731	-6.21625	6.31104	0.09104
C	-3.50555	-3.48742	-0.02468	-3.90502	3.03928	-0.01744	-3.53399	-3.47575	-0.04551
C	-3.58589	-4.43980	1.00366	-4.73653	3.12243	1.11030	-3.70174	-4.32054	1.06430
C	-4.45922	-3.52218	-1.05471	-4.20217	3.83175	-1.13715	-4.36811	-3.65006	-1.16164
C	-4.59925	-5.40173	1.00534	-5.83959	3.98011	1.11948	-4.69042	-5.30655	1.06311
H	-2.85206	-4.41708	1.80402	-4.50954	2.51344	1.98061	-3.05548	-4.19399	1.92774
C	-5.46820	-4.48823	-1.05809	-5.30705	4.68716	-1.13078	-5.35075	-4.64334	-1.16682
H	-4.39997	-2.79015	-1.85488	-3.56377	3.76922	-2.01376	-4.23597	-3.00697	-2.02681
C	-5.54247	-5.42980	-0.02658	-6.12855	4.76447	-0.00168	-5.51700	-5.47235	-0.05336

H	-4.65174	-6.12725	1.81226	-6.47064	4.03667	2.00202	-4.81471	-5.94505	1.93320
H	-6.19422	-4.50589	-1.86607	-5.52642	5.29041	-2.00729	-5.98364	-4.76967	-2.04073
H	-6.32866	-6.17942	-0.02734	-6.98676	5.43038	0.00443	-6.28305	-6.24249	-0.05569
Cu	0.00000	-0.00206	0.20304	0.00125	0.00037	0.11037	0.00006	0.00268	0.08085
H	0.00001	0.01560	1.65427	0.01465	0.01600	1.89510	0.00035	0.04221	1.90001

FeTPP, total charge 0

	Singlet			Triplet			Quintet		
N	-2.00584	0.10927	0.01123	2.00627	0.00002	-0.01137	2.05484	0.00198	-0.03612
N	0.10928	2.00586	-0.01131	0.00002	-2.00658	0.00000	0.00203	-2.07964	-0.00001
N	2.00585	-0.10928	0.01117	-2.00626	-0.00001	0.01138	-2.05484	-0.00198	0.03612
N	-0.10929	-2.00586	-0.01140	-0.00002	2.00659	0.00000	-0.00203	2.07964	0.00001
C	-2.89846	-0.94458	0.06089	2.84217	1.10058	0.01500	2.87077	1.11470	0.00711
C	-4.24981	-0.44985	0.17939	4.22067	0.68098	0.07042	4.24777	0.68760	0.08603
C	-4.17585	0.90891	0.17866	4.22068	-0.68089	0.07051	4.24910	-0.67937	0.08603
C	-2.77875	1.25387	0.06012	2.84219	-1.10053	0.01513	2.87294	-1.10915	0.00710
C	-2.30285	2.56819	-0.00068	2.43972	-2.43980	0.01440	2.44894	-2.45561	0.00923
C	-0.94457	2.89847	-0.06095	1.10065	-2.84290	0.00629	1.11037	-2.89376	0.00434
C	-0.44984	4.24984	-0.17934	0.68098	-4.22241	-0.00117	0.68561	-4.28136	-0.00259
C	0.90892	4.17588	-0.17855	-0.68091	-4.22242	0.00108	-0.67731	-4.28267	0.00260
C	1.25387	2.77877	-0.06009	-1.10061	-2.84291	-0.00632	-1.10475	-2.89589	-0.00435
C	2.56819	2.30286	0.00067	-2.43968	-2.43984	-0.01440	-2.44416	-2.46033	-0.00925
C	2.89846	0.94457	0.06086	-2.84217	-1.10057	-0.01509	-2.87077	-1.11470	-0.00711
C	4.24982	0.44984	0.17930	-4.22067	-0.68096	-0.07041	-4.24777	-0.68760	-0.08603
C	4.17586	-0.90893	0.17853	-4.22068	0.68091	-0.07032	-4.24910	0.67937	-0.08603
C	2.77875	-1.25388	0.06001	-2.84219	1.10054	-0.01497	-2.87294	1.10915	-0.00710
C	2.30285	-2.56820	-0.00081	-2.43972	2.43981	-0.01417	-2.44894	2.45561	-0.00923
C	0.94457	-2.89846	-0.06109	-1.10066	2.84291	-0.00619	-1.11037	2.89376	-0.00434
C	0.44984	-4.24982	-0.17955	-0.68098	4.22242	0.00117	-0.68561	4.28136	0.00260
C	-0.90893	-4.17587	-0.17874	0.68091	4.22243	-0.00126	0.67731	4.28267	-0.00260
C	-1.25387	-2.77877	-0.06020	1.10061	2.84292	0.00616	1.10475	2.89589	0.00435
C	-2.56819	-2.30286	0.00061	2.43968	2.43985	0.01417	2.44416	2.46033	0.00925
H	-5.13115	-1.06830	0.26263	5.06966	1.34677	0.11737	5.10164	1.34592	0.15165
H	-4.98484	1.61949	0.26118	5.06968	-1.34666	0.11754	5.10425	-1.33603	0.15165
H	-1.06830	5.13118	-0.26249	1.34647	-5.07288	-0.00647	1.34607	-5.13605	-0.01119
H	1.61951	4.98488	-0.26097	-1.34639	-5.07290	0.00634	-1.33613	-5.13863	0.01122
H	5.13116	1.06829	0.26251	-5.06967	-1.34675	-0.11741	-5.10164	-1.34592	-0.15165
H	4.98487	-1.61950	0.26098	-5.06969	1.34669	-0.11724	-5.10425	1.33603	-0.15165
H	1.06831	-5.13115	-0.26277	-1.34647	5.07289	0.00651	-1.34607	5.13605	0.01119
H	-1.61952	-4.98486	-0.26119	1.34639	5.07291	-0.00664	1.33613	5.13863	-0.01122
C	3.68224	3.30178	0.00160	-3.49925	-3.49703	-0.02838	-3.50902	-3.51326	-0.02920
C	3.90224	4.12623	1.11605	-4.26162	-3.75785	1.12050	-4.31761	-3.73313	1.09694
C	4.52698	3.43172	-1.11177	-3.74933	-4.24292	-1.19041	-3.71864	-4.29792	-1.17406
C	4.94357	5.05804	1.11877	-5.25177	-4.74402	1.10900	-5.31126	-4.71549	1.08033
H	3.25331	4.02895	1.98171	-4.07091	-3.18442	2.02319	-4.15930	-3.13074	1.98690
C	5.56686	4.36515	-1.11226	-4.74031	-5.22819	-1.20423	-4.71326	-5.27923	-1.19341
H	4.36066	2.79792	-1.97811	-3.16411	-4.04291	-2.08345	-3.09871	-4.13058	-2.05019
C	5.77869	5.18078	0.00379	-5.49414	-5.48184	-0.05397	-5.51242	-5.49140	-0.06559
H	5.10304	5.68540	1.99134	-5.83119	-4.93641	2.00767	-5.92549	-4.87552	1.96210
H	6.20892	4.45611	-1.98397	-4.92425	-5.79471	-2.11284	-4.86491	-5.87497	-2.08922
H	6.58761	5.90583	0.00461	-6.26413	-6.24803	-0.06385	-6.28525	-6.25465	-0.07961
C	-3.30180	3.68222	-0.00158	3.49931	-3.49698	0.02838	3.51585	-3.50646	0.02918
C	-3.43174	4.52695	1.11181	3.74932	-4.24294	1.19038	3.72700	-4.29071	1.17405
C	-4.12629	3.90221	-1.11600	4.26175	-3.75771	-1.12046	4.32488	-3.72474	-1.09695
C	-4.36519	5.56680	1.11233	4.74031	-5.22820	1.20420	4.72356	-5.27004	1.19341
H	-2.79794	4.36063	1.97815	3.16403	-4.04301	2.08339	3.10673	-4.12458	2.05017
C	-5.05811	4.94352	-1.11869	5.25192	-4.74387	-1.10897	5.32047	-4.70514	-1.08032
H	-4.02906	3.25328	-1.98166	4.07110	-3.18422	-2.02313	4.16540	-3.12266	-1.98691
C	-5.18085	5.77864	-0.00370	5.49422	-5.48176	0.05397	5.52315	-5.48064	0.06560
H	-4.45615	6.20884	1.98406	4.92420	-5.79477	2.11278	4.87637	-5.86548	2.08923
H	-5.68550	5.10299	-1.99124	5.83141	-4.93618	-2.00761	5.93503	-4.86395	-1.96208
H	-5.90590	6.58756	-0.00450	6.26423	-6.24793	0.06385	6.29749	-6.24236	0.07964
C	-3.68224	-3.30179	0.00154	3.49926	3.49703	0.02798	3.50902	3.51326	0.02920
C	-3.90224	-4.12615	1.11605	3.74938	4.24309	1.18991	3.71864	4.29792	1.17407
C	-4.52698	-3.43182	-1.11183	4.26161	3.75768	-1.12094	4.31760	3.73313	-1.09694
C	-4.94358	-5.05794	1.11885	4.74037	5.22835	1.20357	4.71327	5.27922	1.19341
H	-3.25330	-4.02883	1.98169	3.16417	4.04322	2.08299	3.09871	4.13058	2.05020
C	-5.56686	-4.36524	-1.11223	5.25177	4.74384	-1.10961	5.31126	4.71549	-1.08033
H	-4.36064	-2.79813	-1.97824	4.07087	3.18412	-2.02355	4.15929	3.13075	-1.98690

C	-5.77872	-5.18077	0.00389	5.49418	5.48182	0.05325	5.51242	5.49140	0.06559
H	-5.10306	-5.68524	1.99147	4.92434	5.79499	2.11209	4.86491	5.87496	2.08923
H	-6.20891	-4.45627	-1.98394	5.83118	4.93609	-2.00832	5.92548	4.87553	-1.96210
H	-6.58766	-5.90579	0.00478	6.26418	6.24800	0.06300	6.28525	6.25465	0.07961
C	3.30179	-3.68223	-0.00163	-3.49931	3.49698	-0.02798	-3.51585	3.50646	-0.02919
C	3.43164	-4.52690	1.11182	-4.26159	3.75768	1.12098	-4.32488	3.72474	1.09695
C	4.12637	-3.90227	-1.11597	-3.74952	4.24295	-1.18994	-3.72700	4.29071	-1.17405
C	4.36511	-5.56674	1.11247	-5.25177	4.74383	1.10964	-5.32048	4.70513	1.08032
H	2.79778	-4.36054	1.97810	-4.07079	3.18419	2.02361	-4.16540	3.12266	1.98691
C	5.05822	-4.94356	-1.11852	-4.74053	5.22820	-1.20360	-4.72356	5.27004	-1.19341
H	4.02918	-3.25337	-1.98166	-3.16437	4.04303	-2.08305	-3.10673	4.12459	-2.05017
C	5.18087	-5.77861	-0.00348	-5.49426	5.48173	-0.05325	-5.52315	5.48064	-0.06560
H	4.45600	-6.20873	1.98424	-5.83112	4.93613	2.00838	-5.93503	4.86395	1.96208
H	5.68569	-5.10306	-1.99101	-4.92456	5.79478	-2.11214	-4.87637	5.86548	-2.08923
H	5.90594	-6.58752	-0.00417	-6.26428	6.24790	-0.06300	-6.29749	6.24236	-0.07964
Fe	0.00000	0.00000	-0.00006	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

FeTPP, total charge 1

		Doublet			**Quartet**			**Sextet**	
N	2.01257	0.00001	-0.03666	1.97516	-0.00004	-0.00616	2.07221	0.00001	-0.07635
N	0.00000	-2.01327	-0.00003	0.00000	-1.97557	-0.00015	0.00001	-2.07283	0.00000
N	-2.01256	0.00001	0.03670	-1.97516	-0.00004	0.00645	-2.07221	-0.00001	0.07634
N	0.00000	2.01330	-0.00003	0.00000	1.97544	-0.00015	-0.00001	2.07283	0.00000
C	2.84999	1.09620	0.01125	2.82760	1.10703	0.01962	2.88873	1.10458	-0.00386
C	4.22243	0.68209	0.11119	4.19189	0.68223	0.07281	4.26133	0.68375	0.12782
C	4.22243	-0.68203	0.11141	4.19190	-0.68243	0.07147	4.26133	-0.68372	0.12782
C	2.84999	-1.09618	0.01156	2.82760	-1.10714	0.01773	2.88874	-1.10456	-0.00386
C	2.44374	-2.44413	0.01584	2.44438	-2.44458	0.01241	2.45584	-2.45655	0.00512
C	1.09639	-2.85205	0.00808	1.10716	-2.82837	0.00270	1.10493	-2.89209	0.00286
C	0.68202	-4.22787	-0.00558	0.68231	-4.19366	-0.00476	0.68369	-4.27071	-0.00837
C	-0.68202	-4.22787	0.00525	-0.68231	-4.19366	0.00345	-0.68366	-4.27072	0.00835
C	-1.09639	-2.85205	-0.00823	-1.10715	-2.82837	-0.00328	-1.10491	-2.89210	-0.00287
C	-2.44373	-2.44412	-0.01584	-2.44438	-2.44457	-0.01242	-2.45582	-2.45656	-0.00513
C	-2.84999	-1.09618	-0.01142	-2.82760	-1.10714	-0.01715	-2.88873	-1.10458	0.00387
C	-4.22244	-0.68203	-0.11108	-4.19194	-0.68244	-0.07017	-4.26133	-0.68375	-0.12780
C	-4.22244	0.68209	-0.11086	-4.19193	0.68222	-0.07151	-4.26133	0.68372	-0.12780
C	-2.84999	1.09620	-0.01111	-2.82761	1.10702	-0.01905	-2.88874	1.10456	0.00387
C	-2.44374	2.44415	-0.01529	-2.44437	2.44445	-0.01576	-2.45584	2.45654	-0.00513
C	-1.09639	2.85208	-0.00792	-1.10715	2.82824	-0.00518	-1.10494	2.89209	-0.00287
C	-0.68202	4.22790	0.00546	-0.68233	4.19353	0.00212	-0.68369	4.27071	0.00835
C	0.68202	4.22790	-0.00580	0.68231	4.19353	-0.00342	0.68366	4.27072	-0.00836
C	1.09639	2.85208	0.00777	1.10715	2.82824	0.00460	1.10491	2.89210	0.00286
C	2.44374	2.44416	0.01529	2.44437	2.44446	0.01576	2.45582	2.45656	0.00512
H	5.07007	1.34393	0.19965	5.03908	1.34998	0.11765	5.11137	1.33939	0.23980
H	5.07007	-1.34384	0.20008	5.03909	-1.35027	0.11502	5.11139	-1.33935	0.23980
H	1.34312	-5.08038	-0.02307	1.34983	-5.04215	-0.01248	1.33816	-5.12854	-0.03052
H	-1.34312	-5.08039	0.02262	-1.34984	-5.04215	0.01076	-1.33812	-5.12855	0.03050
H	-5.07010	-1.34384	-0.19964	-5.03914	-1.35029	-0.11330	-5.11138	-1.33939	-0.23977
H	-5.07010	1.34392	-0.19921	-5.03914	1.34998	-0.11593	-5.11139	1.33935	-0.23977
H	-1.34311	5.08042	0.02305	-1.34988	5.04201	0.00814	-1.33816	5.12854	0.03050
H	1.34310	5.08042	-0.02350	1.34986	5.04201	-0.00986	1.33812	5.12855	-0.03052
C	-3.49946	-3.49366	-0.03665	-3.50315	-3.50097	-0.02303	-3.51286	-3.50456	-0.03329
C	-4.37792	-3.63687	1.05126	-4.24023	-3.77546	1.13869	-4.41913	-3.62586	1.03507
C	-3.63314	-4.34878	-1.14421	-3.77044	-4.22517	-1.19453	-3.62312	-4.38046	-1.12783
C	-5.36349	-4.62518	1.03518	-5.22883	-4.76288	1.12899	-5.40631	-4.61214	1.01373
H	-4.27450	-2.98301	1.91215	-4.03338	-3.21897	2.04858	-4.33453	-2.95698	1.88635
C	-4.63255	-5.32295	-1.16499	-4.76264	-5.20894	-1.20374	-4.62471	-5.35192	-1.15508
H	-2.96414	-4.23515	-1.99207	-3.20485	-4.01182	-2.09727	-2.93503	-4.28323	-1.96224
C	-5.49604	-5.46678	-0.07406	-5.49230	-5.48014	-0.04208	-5.51454	-5.47382	-0.08273
H	-6.02685	-4.73706	1.88739	-5.79044	-4.97158	2.03458	-6.09001	-4.70698	1.85181
H	-4.73670	-5.96800	-2.03210	-4.96562	-5.76050	-2.11676	-4.71049	-6.01185	-2.01296
H	-6.26808	-6.22997	-0.08853	-6.26189	-6.24596	-0.04946	-6.28819	-6.23528	-0.10183
C	3.49946	-3.49366	0.03665	3.50316	-3.50097	0.02303	3.51289	-3.50453	0.03329
C	3.63299	-4.34893	1.14411	3.76967	-4.22597	1.19421	3.62314	-4.38044	1.12782
C	4.37808	-3.63672	-1.05116	4.24103	-3.77466	-1.13837	4.41917	-3.62582	-1.03507
C	4.63240	-5.32310	1.16489	4.76187	-5.20972	1.20343	4.62474	-5.35190	1.15507
H	2.96388	-4.23542	1.99190	3.20346	-4.01324	2.09672	2.93505	-4.28322	1.96223
C	5.36365	-4.62503	-1.03508	5.22964	-4.76209	-1.12868	5.40636	-4.61209	-1.01372
H	4.27477	-2.98274	-1.91197	4.03479	-3.21756	-2.04802	4.33457	-2.95693	-1.88634
C	5.49604	-5.46678	0.07407	5.49232	-5.48013	0.04209	5.51458	-5.47378	0.08273

H	4.73644	-5.96827	2.03193	4.96424	-5.76190	2.11623	4.71051	-6.01183	2.01294
H	6.02712	-4.73679	-1.88721	5.79185	-4.97016	-2.03403	6.09006	-4.70691	-1.85180
H	6.26808	-6.22997	0.08853	6.26191	-6.24595	0.04946	6.28824	-6.23524	0.10183
C	3.49949	3.49367	0.03566	3.50303	3.50094	0.02880	3.51286	3.50456	0.03329
C	3.63331	4.34915	1.14292	3.76795	4.22468	1.20112	3.62311	4.38047	1.12782
C	4.37787	3.63647	-1.05237	4.24227	3.77609	-1.13139	4.41914	3.62585	-1.03506
C	4.63277	5.32329	1.16328	4.75996	5.20860	1.21268	4.62470	5.35193	1.15508
H	2.96440	4.23584	1.99089	3.20064	4.01085	2.10269	2.93502	4.28324	1.96223
C	5.36348	4.62474	-1.03672	5.23068	4.76368	-1.11936	5.40632	4.61213	-1.01372
H	4.27434	2.98231	-1.91302	4.03722	3.22000	-2.04193	4.33454	2.95697	-1.88634
C	5.49616	5.46671	0.07223	5.49180	5.48044	0.05254	5.51454	5.47382	0.08273
H	4.73703	5.96862	2.03016	4.96110	5.75979	2.12634	4.71047	6.01186	2.01295
H	6.02677	4.73630	-1.88902	5.79396	4.97289	-2.02379	6.09002	4.70696	-1.85180
H	6.26824	6.22987	0.08636	6.26125	6.24639	0.06173	6.28819	6.23528	0.10183
C	-3.49949	3.49367	-0.03566	-3.50304	3.50093	-0.02880	-3.51289	3.50453	-0.03329
C	-4.37772	3.63662	1.05247	-4.24148	3.77687	1.13170	-4.41916	3.62583	1.03507
C	-3.63346	4.34900	-1.14302	-3.76874	4.22387	-1.20144	-3.62315	4.38043	-1.12783
C	-5.36333	4.62488	1.03682	-5.22989	4.76446	1.11967	-5.40635	4.61211	1.01372
H	-4.27408	2.98257	1.91320	-4.03582	3.22140	2.04248	-4.33455	2.95696	1.88635
C	-4.63292	5.32313	-1.16337	-4.76075	5.20780	-1.21298	-4.62475	5.35188	-1.15509
H	-2.96466	4.23556	-1.99106	-3.20205	4.00943	-2.10324	-2.93507	4.28320	-1.96225
C	-5.49616	5.46671	-0.07222	-5.49180	5.48043	-0.05254	-5.51458	5.47378	-0.08273
H	-6.02651	4.73656	1.88920	-5.79256	4.97428	2.02434	-6.09004	4.70693	1.85181
H	-4.73730	5.96835	-2.03033	-4.96250	5.75838	-2.12688	-4.71053	6.01181	-2.01296
H	-6.26824	6.22987	-0.08635	-6.26124	6.24638	-0.06172	-6.28824	6.23524	-0.10183
Fe	0.00000	0.00001	0.00000	0.00000	-0.00005	0.00000	0.00000	0.00000	0.00002

FeTPP, total charge -1

		Doublet			**Quartet**			**Sextet**	
N	-2.00173	0.00000	-0.02356	0.00015	-2.02150	0.00001	-0.00125	2.08044	-0.03550
N	0.00001	2.02466	0.00004	-2.01774	-0.00014	-0.04236	2.07553	0.00124	0.00001
N	2.00174	-0.00001	0.02351	-0.00015	2.02153	0.00002	0.00125	-2.08044	0.03550
N	0.00000	-2.02467	0.00004	2.01774	0.00015	0.04236	-2.07553	-0.00124	-0.00001
C	-2.84374	-1.10804	0.00213	1.10405	-2.86113	-0.00178	-1.11360	2.89828	0.02375
C	-4.22807	-0.67799	0.06340	0.69123	-4.22356	0.00544	-0.69537	4.25918	0.12996
C	-4.22806	0.67800	0.06345	-0.69063	-4.22366	-0.00524	0.69027	4.26001	0.12996
C	-2.84374	1.10805	0.00219	-1.10364	-2.86128	0.00186	1.11013	2.89961	0.02375
C	-2.45419	2.43738	0.00922	-2.45832	-2.43846	0.00223	2.46978	2.45153	0.01897
C	-1.10216	2.86352	0.00586	-2.85314	-1.10824	-0.00997	2.89155	1.11881	0.01192
C	-0.69044	4.22693	-0.00204	-4.23584	-0.67929	0.05685	4.27867	0.68327	0.00027
C	0.69046	4.22692	0.00255	-4.23593	0.67872	0.05664	4.27948	-0.67815	-0.00022
C	1.10218	2.86352	-0.00564	-2.85329	1.10785	-0.01027	2.89289	-1.11534	-0.01190
C	2.45421	2.43737	-0.00920	-2.45867	2.43814	0.00171	2.47272	-2.44857	-0.01896
C	2.84374	1.10804	-0.00236	-1.10405	2.86115	0.00156	1.11360	-2.89828	-0.02376
C	4.22806	0.67798	-0.06388	-0.69123	4.22359	-0.00546	0.69537	-4.25918	-0.12998
C	4.22805	-0.67801	-0.06384	0.69063	4.22368	0.00563	-0.69027	-4.26001	-0.12998
C	2.84374	-1.10806	-0.00229	1.10364	2.86131	-0.00148	-1.11013	-2.89961	-0.02376
C	2.45420	-2.43739	-0.00909	2.45832	2.43848	-0.00170	-2.46978	-2.45153	-0.01897
C	1.10216	-2.86353	-0.00557	2.85313	1.10826	0.01022	-2.89155	-1.11881	-0.01192
C	0.69043	-4.22693	0.00259	4.23583	0.67933	-0.05679	-4.27867	-0.68327	-0.00025
C	-0.69046	-4.22693	-0.00208	4.23593	-0.67868	-0.05700	-4.27948	0.67815	0.00024
C	-1.10218	-2.86352	0.00580	2.85330	-1.10783	0.00992	-2.89289	1.11534	0.01190
C	-2.45421	-2.43737	0.00911	2.45868	-2.43812	-0.00222	-2.47272	2.44857	0.01896
H	-5.07967	-1.34070	0.11973	1.35071	-5.07894	0.02001	-1.34953	5.11498	0.21654
H	-5.07967	1.34071	0.11982	-1.34999	-5.07913	-0.01973	1.34340	5.11659	0.21654
H	-1.35083	5.08183	-0.01223	-5.08773	-1.34110	0.11872	5.13829	1.33825	-0.00792
H	1.35086	5.08182	0.01292	-5.08792	1.34043	0.11831	5.13989	-1.33210	0.00798
H	5.07965	1.34068	-0.12041	-1.35070	5.07897	-0.02015	1.34953	-5.11498	-0.21657
H	5.07965	-1.34072	-0.12032	1.34998	5.07916	0.02037	-1.34340	-5.11659	-0.21657
H	1.35083	-5.08183	0.01300	5.08772	1.34116	-0.11851	-5.13829	-1.33825	0.00794
H	-1.35086	-5.08183	-0.01232	5.08792	-1.34036	-0.11893	-5.13989	1.33210	-0.00796
C	3.51259	3.49204	-0.03014	-3.51451	3.49421	0.02835	3.52507	-3.50942	-0.03617
C	4.33512	3.71379	1.08692	-3.69744	4.30336	1.16331	3.69055	-4.37685	1.05815
C	3.71178	4.29081	-1.16915	-4.35395	3.70728	-1.07826	4.37268	-3.67647	-1.14496
C	5.33213	4.69389	1.06503	-4.69064	5.28521	1.19593	4.67496	-5.36785	1.05088
H	4.18413	3.10528	1.97399	-3.05071	4.14928	2.02221	3.03628	-4.26119	1.91735
C	4.70497	5.27320	-1.19505	-5.35156	4.68673	-1.04932	5.36147	-4.66498	-1.15575
H	3.07766	4.12925	-2.03605	-4.21551	3.09243	-1.96299	4.24617	-3.01987	-2.00094
C	5.52143	5.47866	-0.07691	-5.52444	5.48087	0.08856	5.51762	-5.51594	-0.05715
H	5.95748	4.84662	1.94137	-4.81749	5.89428	2.08772	4.78757	-6.02197	1.91217

H	4.84461	5.87532	-2.08962	-5.98983	4.83185	-1.91763	6.00514	-4.77359	-2.02540
H	6.29527	6.24196	-0.09589	-6.29854	6.24375	0.11291	6.28470	-6.28622	-0.06406
C	-3.51257	3.49206	0.03013	-3.51398	-3.49470	0.02926	3.52087	3.51363	0.03618
C	-3.71202	4.29058	1.16927	-3.69657	-4.30365	1.16441	4.36827	3.68170	1.14497
C	-4.33483	3.71405	-1.08707	-4.35356	-3.70816	-1.07717	3.68532	4.38125	-1.05816
C	-4.70521	5.27297	1.19515	-4.68958	-5.28568	1.19740	5.35588	4.67139	1.15574
H	-3.07810	4.12882	2.03628	-3.04972	-4.14928	2.02317	4.24254	3.02497	2.00095
C	-5.33184	4.69416	-1.06521	-5.35098	-4.68778	-1.04787	4.66855	5.37342	-1.05090
H	-4.18364	3.10573	-1.97424	-4.21537	-3.09346	-1.96205	3.03118	4.26480	-1.91736
C	-5.52140	5.47868	0.07686	-5.52353	-5.48172	0.09021	5.51103	5.52252	0.05714
H	-4.84506	5.87491	2.08981	-4.81617	-5.89459	2.08933	5.99942	4.78078	2.02540
H	-5.95698	4.84707	-1.94166	-5.98936	-4.83320	-1.91604	4.78038	6.02766	-1.91220
H	-6.29524	6.24198	0.09581	-6.29749	-6.24474	0.11484	6.27719	6.29371	0.06404
C	-3.51259	-3.49204	0.02994	3.51449	-3.49421	-0.02926	-3.52507	3.50942	0.03617
C	-3.71210	-4.29060	1.16904	4.35423	-3.70741	1.07710	-4.37266	3.67648	1.14497
C	-4.33481	-3.71397	-1.08731	3.69706	-4.30326	-1.16434	-3.69057	4.37684	-1.05816
C	-4.70530	-5.27298	1.19484	5.35180	-4.68689	1.04778	-5.36145	4.66499	1.15576
H	-3.07822	-4.12888	2.03609	4.21606	-3.09264	1.96193	-4.24614	3.01989	2.00095
C	-5.33184	-4.69407	-1.06552	4.69021	-5.28514	-1.19734	-4.67498	5.36784	-1.05088
H	-4.18357	-3.10562	-1.97444	3.05008	-4.14908	-2.02304	-3.03631	4.26117	-1.91737
C	-5.52145	-5.47863	0.07651	5.52433	-5.48093	-0.09023	-5.51762	5.51593	0.05716
H	-4.84520	-5.87495	2.08948	5.99031	-4.83212	1.91589	-6.00511	4.77361	2.02543
H	-5.95694	-4.84695	-1.94201	4.81678	-5.89413	-2.08922	-4.78760	6.02195	-1.91218
H	-6.29530	-6.24193	0.09540	6.29839	-6.24384	-0.11487	-6.28470	6.28621	0.06407
C	3.51258	-3.49206	-0.02994	3.51400	3.49472	-0.02836	-3.52087	-3.51363	-0.03618
C	4.33506	-3.71376	1.08715	3.69675	4.30393	-1.16330	-3.68530	-4.38126	1.05815
C	3.71182	-4.29087	-1.16892	4.35347	3.70786	1.07822	-4.36828	-3.68169	-1.14496
C	5.33207	-4.69387	1.06534	4.68981	5.28593	-1.19593	-4.66853	-5.37343	1.05089
H	4.18403	-3.10522	1.97420	3.05000	4.14979	-2.02217	-3.03116	-4.26483	1.91734
C	4.70501	-5.27326	-1.19474	5.35093	4.68746	1.04927	-5.35590	-4.67138	-1.15573
H	3.07773	-4.12934	-2.03585	4.21516	3.09295	1.96293	-4.24256	-3.02495	-2.00094
C	5.52142	-5.47867	-0.07656	5.52364	5.48167	-0.08860	-5.51103	-5.52252	-0.05713
H	5.95738	-4.84656	1.94172	4.81653	5.89505	-2.08770	-4.78036	-6.02768	1.91218
H	4.84469	-5.87541	-2.08929	5.98922	4.83264	1.91755	-5.99945	-4.78076	-2.02538
H	6.29527	-6.24198	-0.09547	6.29763	6.24466	-0.11295	-6.27719	-6.29371	-0.06403
Fe	0.00000	0.00000	0.00001	0.00000	0.00001	0.00000	0.00000	0.00000	0.00000

H-FeTPP, total charge 0

		Doublet			Quartet			Sextet	
N	-1.73013	0.99461	-0.02727	2.00758	-0.00012	-0.04164	2.04757	-0.00001	-0.02047
N	1.00321	1.71927	-0.01877	0.00163	-2.00548	-0.02970	0.00239	-2.04559	0.00740
N	1.72653	-0.99984	-0.02938	-2.00267	0.00013	-0.01768	-2.04290	0.00001	0.03473
N	-1.01169	-1.72970	-0.03959	0.00186	2.00550	-0.02970	0.00242	2.04559	0.00740
C	-3.00998	0.46746	-0.07316	2.84210	1.10045	-0.02168	2.87103	1.10617	-0.01264
C	-3.99144	1.52053	-0.00248	4.22018	0.68072	0.01372	4.25187	0.68209	0.00959
C	-3.30676	2.69223	0.10079	4.22010	-0.68121	0.01383	4.25186	-0.68214	0.00959
C	-1.90273	2.36310	0.07379	2.84197	-1.10078	-0.02152	2.87101	-1.10620	-0.01265
C	-0.88330	3.31624	0.12983	2.44118	-2.43930	-0.01451	2.45031	-2.44719	-0.01110
C	0.47411	2.99366	0.06397	1.10262	-2.83968	-0.02795	1.10918	-2.86768	-0.01587
C	1.52706	3.97925	0.02915	0.68347	-4.21818	-0.05171	0.68597	-4.24784	-0.06895
C	2.70234	3.30095	-0.07339	-0.67846	-4.21876	-0.05043	-0.67828	-4.24897	-0.06518
C	2.37437	1.89735	-0.09720	-1.09874	-2.84036	-0.04122	-1.10338	-2.86883	-0.02600
C	3.32864	0.88136	-0.16219	-2.43724	-2.43939	-0.04215	-2.44408	-2.44753	-0.03225
C	3.00338	-0.47595	-0.11908	-2.83665	-1.10046	-0.04799	-2.86352	-1.10613	-0.02869
C	3.98153	-1.53482	-0.14779	-4.21353	-0.68069	-0.11717	-4.23992	-0.68209	-0.14121
C	3.29696	-2.70675	-0.04583	-4.21345	0.68122	-0.11706	-4.23991	0.68214	-0.14121
C	1.89623	-2.36980	0.03031	-2.83652	1.10081	-0.04783	-2.86351	1.10617	-0.02870
C	0.87721	-3.32353	0.08973	-2.43695	2.43970	-0.04188	-2.44405	2.44756	-0.03226
C	-0.48108	-3.00362	0.03360	-1.09840	2.84051	-0.04107	-1.10334	2.86884	-0.02600
C	-1.53475	-3.98944	0.00947	-0.67796	4.21885	-0.05032	-0.67823	4.24897	-0.06518
C	-2.70975	-3.31088	-0.09290	0.68397	4.21811	-0.05182	0.68602	4.24784	-0.06895
C	-2.38152	-1.90647	-0.10157	1.10296	2.83955	-0.02811	1.10921	2.86767	-0.01586
C	-3.33628	-0.88804	-0.13393	2.44148	2.43902	-0.01478	2.45034	2.44717	-0.01109
H	-5.06087	1.37068	-0.01216	5.06915	1.34725	0.04669	5.10539	1.34348	0.03348
H	-3.70620	3.69145	0.19157	5.06899	-1.34784	0.04691	5.10538	-1.34354	0.03348
H	1.37507	5.04770	0.07025	1.35046	-5.06730	-0.06752	1.34811	-5.10018	-0.10967
H	3.70329	3.70309	-0.12398	-1.34451	-5.06868	-0.05699	-1.33881	-5.10300	-0.09170
H	5.04758	-1.39027	-0.24143	-5.06104	-1.34761	-0.17336	-5.08860	-1.34416	-0.23084
H	3.69186	-3.71199	-0.04236	-5.06088	1.34825	-0.17314	-5.08859	1.34422	-0.23085

H	-1.38446	-5.05779	0.05636	-1.34391	5.06885	-0.05678	-1.33875	5.10302	-0.09170
H	-3.70997	-3.71359	-0.15122	1.35106	5.06715	-0.06774	1.34817	5.10016	-0.10966
C	4.77170	1.26706	-0.25737	-3.49833	-3.49468	-0.04659	-3.50671	-3.50159	-0.06808
C	5.61853	1.14738	0.85491	-4.24723	-3.75306	1.11160	-4.30220	-3.74668	1.06186
C	5.29890	1.75831	-1.46115	-3.76398	-4.23871	-1.20622	-3.73008	-4.25616	-1.23016
C	6.96486	1.51128	0.76595	-5.24018	-4.73644	1.11115	-5.29764	-4.72698	1.03194
H	5.21391	0.77035	1.78987	-4.04329	-3.18065	2.01199	-4.13253	-3.16616	1.96416
C	6.64556	2.12088	-1.55230	-4.75795	-5.22109	-1.20852	-4.72678	-5.23504	-1.26225
H	4.64732	1.85192	-2.32531	-3.18936	-4.03960	-2.10636	-3.12074	-4.06691	-2.10930
C	7.48220	1.99865	-0.43847	-5.49843	-5.47297	-0.04923	-5.51293	-5.47383	-0.13057
H	7.60753	1.41599	1.63670	-5.80932	-4.92768	2.01656	-5.90238	-4.90772	1.91619
H	7.04009	2.49666	-2.49222	-4.95459	-5.78658	-2.11508	-4.89024	-5.80787	-2.17080
H	8.52879	2.28112	-0.50836	-6.27064	-6.23697	-0.05021	-6.28730	-6.23526	-0.15466
C	-1.26196	4.76019	0.23986	3.49859	-3.49811	0.00893	3.50785	-3.50694	-0.01103
C	-1.08933	5.44932	1.44981	3.74746	-4.22851	1.18095	3.73801	-4.28296	1.13553
C	-1.78958	5.44894	-0.86288	4.25725	-3.77670	-1.13806	4.28518	-3.74252	-1.15551
C	-1.43874	6.79831	1.55620	4.73514	-5.21683	1.20600	4.72478	-5.27238	1.13840
H	-0.68191	4.92015	2.30656	3.16455	-4.01354	2.07198	3.14116	-4.10244	2.02497
C	-2.13759	6.79841	-0.75876	5.24402	-4.76610	-1.11484	5.27067	-4.73327	-1.15478
H	-1.92191	4.92064	-1.80281	4.06644	-3.21543	-2.04838	4.10889	-3.14694	-2.04671
C	-1.96363	7.47673	0.45177	5.48588	-5.48858	0.05782	5.49369	-5.50066	-0.00717
H	-1.30232	7.31737	2.50081	4.91891	-5.77155	2.12184	4.89376	-5.86188	2.03517
H	-2.54184	7.31895	-1.62247	5.82103	-4.97294	-2.01183	5.86131	-4.90638	-2.05006
H	-2.23457	8.52550	0.53358	6.25328	-6.25717	0.07676	6.26027	-6.27031	-0.00565
C	-4.78319	-1.26538	-0.20196	3.49903	3.49769	0.00845	3.50789	3.50690	-0.01102
C	-5.44199	-1.78199	0.92402	3.74811	4.22818	1.18037	3.73806	4.28292	1.13555
C	-5.50516	-1.10037	-1.39349	4.25760	3.77607	-1.13865	4.28523	3.74247	-1.15550
C	-6.79452	-2.12758	0.86007	4.73593	5.21636	1.20522	4.72484	5.27232	1.13842
H	-4.88801	-1.90749	1.84995	3.16528	4.01337	2.07149	3.14120	4.10240	2.02498
C	-6.85741	-1.44739	-1.45967	5.24451	4.76533	-1.11563	5.27073	4.73320	-1.15477
H	-4.99948	-0.70045	-2.26783	4.06662	3.21473	-2.04889	4.10893	3.14689	-2.04669
C	-7.50586	-1.96176	-0.33257	5.48659	5.48790	0.05694	5.49375	5.50060	-0.00715
H	-7.29181	-2.52330	1.74122	4.91988	5.77114	2.12099	4.89382	5.86182	2.03519
H	-7.40242	-1.31690	-2.39041	5.82146	4.97200	-2.01269	5.86138	4.90631	-2.05004
H	-8.55711	-2.23075	-0.38295	6.25410	6.25638	0.07572	6.26034	6.27023	-0.00563
C	1.26864	-4.76542	0.18339	-3.49792	3.49510	-0.04610	-3.50667	3.50164	-0.06809
C	1.75474	-5.29036	1.39023	-4.24667	3.75345	1.11219	-4.30217	3.74673	1.06184
C	1.16593	-5.61139	-0.93130	-3.76362	4.23927	-1.20564	-3.73002	4.25620	-1.23017
C	2.12734	-6.63422	1.48241	-5.23952	4.73694	1.11194	-5.29759	4.72705	1.03192
H	1.83653	-4.63883	2.25559	-4.04270	3.18093	2.01250	-4.13250	3.16621	1.96414
C	1.54009	-6.95485	-0.84138	-4.75748	5.22175	-1.20774	-4.72671	5.23510	-1.26226
H	0.79478	-5.20833	-1.86931	-3.18912	4.04019	-2.10586	-3.12068	4.06695	-2.10931
C	2.02124	-7.47017	0.36643	-5.49782	5.47361	-0.04835	-5.51287	5.47390	-0.13059
H	2.49885	-7.02702	2.42475	-5.80855	4.92815	2.01742	-5.90234	4.90779	1.91616
H	1.45805	-7.59668	-1.71413	-4.95417	5.78735	-2.11422	-4.89016	5.80793	-2.17082
H	2.31166	-8.51453	0.43709	-6.26994	6.23768	-0.04917	-6.28723	6.23533	-0.15469
Fe	-0.00406	0.00105	0.08273	0.00283	0.00000	0.20509	0.00666	-0.00001	0.46846
H	0.02757	-0.17590	1.53755	0.01990	0.00000	1.91996	0.04174	-0.00001	2.13702

H-FeTPP, total charge 1

		Singlet			Triplet			Quintet	
N	-0.86780	1.78650	-0.06706	1.95136	-0.00451	-0.12528	2.04011	-0.00002	-0.05769
N	1.75699	0.82956	-0.01494	-0.00462	-1.96442	0.02988	0.00002	-2.04134	-0.01215
N	0.85393	-1.81070	-0.02218	-1.95146	0.00453	-0.12503	-2.04146	0.00003	0.03207
N	-1.71261	-0.82899	0.06073	0.00458	1.96447	0.02975	0.00007	2.04133	-0.01214
C	-2.19097	2.07886	0.05030	2.79984	1.09921	-0.23529	2.87082	1.10453	-0.01522
C	-2.45835	3.45200	-0.30480	4.13344	0.67283	-0.52831	4.24417	0.68252	0.06752
C	-1.26166	4.00694	-0.63647	4.13023	-0.69197	-0.52857	4.24415	-0.68264	0.06751
C	-0.25791	2.98993	-0.42658	2.79465	-1.11218	-0.23563	2.87078	-1.10461	-0.01523
C	1.11049	3.20833	-0.42211	2.42668	-2.44009	-0.02518	2.45026	-2.45022	-0.01552
C	2.03275	2.18343	-0.07442	1.09863	-2.80645	0.18076	1.10503	-2.87254	-0.01492
C	3.37267	2.44157	0.31017	0.67286	-4.13524	0.49753	0.68286	-4.24803	-0.04113
C	3.93939	1.21996	0.62125	-0.69207	-4.13208	0.49765	-0.68222	-4.24817	-0.02995
C	2.95269	0.23068	0.36518	-1.11172	-2.80131	0.18097	-1.10461	-2.87254	-0.02518
C	3.20008	-1.16009	0.38654	-2.43812	-2.42877	-0.02458	-2.44954	-2.45031	-0.03663
C	2.20496	-2.09241	0.08347	-2.79993	-1.09919	-0.23507	-2.87042	-1.10457	-0.02687
C	2.45823	-3.46626	-0.26545	-4.13358	-0.67282	-0.52793	-4.24140	-0.68249	-0.14217
C	1.25434	-4.01968	-0.58972	-4.13038	0.69199	-0.52809	-4.24139	0.68261	-0.14218
C	0.26588	-2.99542	-0.38682	-2.79476	1.11218	-0.23530	-2.87039	1.10466	-0.02689
C	-1.12806	-3.20233	-0.41173	-2.42674	2.44011	-0.02514	-2.44947	2.45038	-0.03665

C	-2.02581	-2.19256	-0.08275	-1.09866	2.80650	0.18052	-1.10453	2.87257	-0.02519
C	-3.40404	-2.42310	0.25173	-0.67289	4.13535	0.49713	-0.68210	4.24819	-0.02996
C	-3.95391	-1.22741	0.59172	0.69203	4.13216	0.49738	0.68299	4.24801	-0.04112
C	-2.94833	-0.22035	0.40469	1.11169	2.80136	0.18084	1.10511	2.87251	-0.01490
C	-3.19185	1.14103	0.39941	2.43807	2.42879	-0.02470	2.45033	2.45015	-0.01550
H	-3.43723	3.90688	-0.32651	4.96452	1.33746	-0.70981	5.09532	1.34218	0.14129
H	-1.06643	5.01016	-0.98344	4.95819	-1.36040	-0.71034	5.09528	-1.34233	0.14128
H	3.82859	3.41803	0.37552	1.33773	-4.96289	0.69394	1.34151	-5.10255	-0.06769
H	4.93358	1.03261	0.99801	-1.36075	-4.95662	0.69419	-1.34115	-5.10292	-0.02559
H	3.43383	-3.92742	-0.30081	-4.96467	-1.33743	-0.70940	-5.09037	-1.34185	-0.23894
H	1.05282	-5.02309	-0.93215	-4.95837	1.36042	-0.70972	-5.09034	1.34199	-0.23896
H	-3.87569	-3.39436	0.25738	-1.33779	4.96302	0.69337	-1.34100	5.10296	-0.02560
H	-4.96253	-1.03338	0.92330	1.36069	4.95672	0.69390	1.34165	5.10251	-0.06767
C	4.57056	-1.65621	0.66514	-3.49825	-3.47778	-0.00917	-3.50751	-3.50049	-0.07031
C	4.78157	-2.56366	1.72014	-4.48697	-3.47577	0.98827	-4.37754	-3.66210	1.02092
C	5.66754	-1.25460	-0.11983	-3.51792	-4.48098	-0.99185	-3.64938	-4.33410	-1.19222
C	6.06321	-3.04087	1.99561	-5.47455	-4.46299	1.00478	-5.36530	-4.64841	0.99330
H	3.93993	-2.87407	2.33188	-4.47148	-2.70673	1.75521	-4.26807	-3.02335	1.89248
C	6.94462	-1.74919	0.14665	-4.51326	-5.46045	-0.98026	-4.64951	-5.30770	-1.22343
H	5.50891	-0.57941	-0.95507	-2.75967	-4.48258	-1.76960	-2.98564	-4.20605	-2.04228
C	7.14677	-2.63739	1.20828	-5.49131	-5.45507	0.01930	-5.50591	-5.47004	-0.12967
H	6.21585	-3.72643	2.82354	-6.22802	-4.45795	1.78658	-6.02374	-4.77416	1.84739
H	7.78003	-1.44564	-0.47685	-4.52530	-6.22503	-1.75111	-4.75950	-5.93767	-2.10086
H	8.14246	-3.01586	1.41839	-6.26210	-6.21963	0.03020	-6.27892	-6.23204	-0.15266
C	1.65522	4.56223	-0.70215	3.48191	-3.49403	-0.01009	3.50671	-3.50241	-0.00370
C	1.29124	5.67055	0.08312	4.47088	-3.49671	0.98711	3.65699	-4.34574	1.10991
C	2.56800	4.74226	-1.75757	3.49663	-4.49730	-0.99280	4.36556	-3.65741	-1.10458
C	1.82532	6.93162	-0.18576	5.45380	-4.48857	1.00336	4.65455	-5.32239	1.12329
H	0.61017	5.53390	0.91749	4.45915	-2.72762	1.75407	3.00142	-4.22338	1.96713
C	3.08557	6.00796	-2.03534	4.48735	-5.48144	-0.98147	5.35076	-4.64662	-1.09473
H	2.85309	3.89076	-2.36833	2.73819	-4.49535	-1.77037	4.24897	-3.01158	-1.96997
C	2.71777	7.10458	-1.24873	5.46565	-5.48069	0.01785	5.50003	-5.47781	0.02008
H	1.54837	7.77694	0.43680	6.20746	-4.48710	1.78499	4.77112	-5.96003	1.99430
H	3.77536	6.13767	-2.86369	4.49561	-6.24604	-1.75235	6.00049	-4.76718	-1.95622
H	3.12750	8.08749	-1.46034	6.23285	-6.24887	0.02855	6.27099	-6.24218	0.02921
C	-4.55999	1.65678	0.68172	3.49828	3.47772	-0.00916	3.50681	3.50231	-0.00365
C	-5.64558	1.33163	-0.14846	3.51810	4.48100	-0.99176	3.65710	4.34564	1.10996
C	-4.76741	2.50871	1.77977	4.48695	3.47552	0.98833	4.36568	3.65730	-1.10452
C	-6.91579	1.84635	0.11807	4.51353	5.46038	-0.98001	4.65468	5.32226	1.12336
H	-5.48725	0.69126	-1.01120	2.75990	4.48275	-1.76955	3.00151	4.22329	1.96717
C	-6.04172	3.00899	2.05320	5.47462	4.46264	1.00498	5.35091	4.64647	-1.09465
H	-3.93072	2.76651	2.42269	4.47135	2.70640	1.75519	4.24908	3.01147	-1.96991
C	-7.11759	2.68101	1.22191	5.49152	5.45481	0.01959	5.50018	5.47765	0.02017
H	-7.74530	1.59834	-0.53717	4.52569	6.22502	-1.75080	4.77126	5.95989	1.99438
H	-6.19348	3.65484	2.91268	6.22805	4.45746	1.78682	6.00066	4.76702	-1.95613
H	-8.10689	3.07632	1.43119	6.26239	6.21930	0.03061	6.27117	6.24200	0.02931
C	-1.66455	-4.55928	-0.70102	-3.48195	3.49408	-0.01008	-3.50741	3.50060	-0.07036
C	-1.34372	-5.65674	0.11645	-4.47067	3.49705	0.98735	-4.37745	3.66224	1.02086
C	-2.52218	-4.75009	-1.79839	-3.49686	4.49709	-0.99305	-3.64923	4.33420	-1.19227
C	-1.87144	-6.91922	-0.15966	-5.45357	4.48893	1.00357	-5.36518	4.64857	0.99322
H	-0.69811	-5.51287	0.97758	-4.45879	2.72816	1.75451	-4.26802	3.02349	1.89242
C	-3.03426	-6.01715	-2.08199	-4.48755	5.48126	-0.98175	-4.64933	5.30783	-1.22351
H	-2.77226	-3.90554	-2.43391	-2.73859	4.49492	-1.77079	-2.98548	4.20613	-2.04232
C	-2.71260	-7.10346	-1.26180	-5.46563	5.48079	0.01779	-5.50574	5.47021	-0.12976
H	-1.62803	-7.75704	0.48663	-6.20706	4.48768	1.78536	-6.02364	4.77435	1.84730
H	-3.68332	-6.15559	-2.94130	-4.49597	6.24566	-1.75282	-4.75929	5.93780	-2.10094
H	-3.11680	-8.08745	-1.47898	-6.23280	6.24899	0.02846	-6.27873	6.23223	-0.15277
Fe	-0.02285	-0.02686	0.09306	-0.00001	0.00001	0.06247	0.00567	-0.00002	0.37286
H	-0.21282	0.13258	1.52364	0.00100	0.00022	1.56214	0.06969	-0.00002	1.99435

H-FeTPP, total charge -1

		Singlet			Triplet			Quintet	
N	0.00008	-2.00474	0.01391	-1.05680	1.74579	-0.11682	1.98293	0.31478	-0.05019
N	-1.99733	-0.00007	-0.03257	1.69839	1.03150	0.00720	0.31842	-1.99245	-0.04649
N	-0.00008	2.00475	0.01390	1.05603	-1.74091	-0.09262	-1.97753	-0.32307	-0.01119
N	1.99733	0.00008	-0.03257	-1.69664	-1.02681	0.05718	-0.31163	1.97382	-0.01645
C	1.09742	-2.84262	0.06113	-2.42841	1.88303	-0.19529	2.63760	1.52506	0.08479
C	0.68077	-4.22310	0.18638	-2.77992	3.25114	-0.38245	4.07035	1.31333	0.12164
C	-0.68045	-4.22315	0.18636	-1.59644	3.96652	-0.40090	4.28339	-0.02355	-0.02104
C	-1.09720	-2.84270	0.06112	-0.54464	3.02512	-0.20595	2.99049	-0.65123	-0.11657

C	-2.43303	-2.43454	-0.01231	0.82594	3.35802	-0.04898	2.80233	-2.02205	-0.19123
C	-2.83550	-1.09784	-0.09468	1.83392	2.41533	0.09051	1.54513	-2.65058	-0.14110
C	-4.21297	-0.68055	-0.25120	3.22333	2.75243	0.31406	1.35364	-4.06136	-0.11997
C	-4.21303	0.68024	-0.25116	3.92727	1.59074	0.32430	0.00188	-4.27876	0.02537
C	-2.83558	1.09763	-0.09468	2.98763	0.51263	0.10374	-0.62748	-2.99254	0.05638
C	-2.43322	2.43436	-0.01231	3.35702	-0.81746	-0.03307	-2.02674	-2.79523	0.14987
C	-1.09742	2.84263	0.06112	2.42594	-1.87487	-0.20617	-2.62753	-1.53680	0.07091
C	-0.68077	4.22311	0.18637	2.76988	-3.23208	-0.46770	-4.06011	-1.34162	-0.03158
C	0.68044	4.22316	0.18637	1.58625	-3.94814	-0.47726	-4.27412	-0.00490	-0.17365
C	1.09720	2.84271	0.06111	0.54076	-3.01529	-0.21934	-2.98370	0.63612	-0.13974
C	2.43302	2.43455	-0.01233	-0.82940	-3.35195	-0.06340	-2.79401	2.00714	-0.20973
C	2.83549	1.09785	-0.09469	-1.83757	-2.41105	0.08945	-1.53711	2.63373	-0.13103
C	4.21298	0.68057	-0.25115	-3.23598	-2.75038	0.24694	-1.34381	4.04371	-0.11529
C	4.21302	-0.68022	-0.25121	-3.93808	-1.58762	0.25822	0.00968	4.26069	0.01744
C	2.83558	-1.09762	-0.09468	-2.98611	-0.50616	0.12495	0.63457	2.97418	0.08157
C	2.43321	-2.43435	-0.01231	-3.35347	0.82286	-0.01746	2.03495	2.78074	0.17224
H	1.34495	-5.07112	0.27248	-3.78625	3.63441	-0.47092	4.80918	2.09048	0.25132
H	-1.34456	-5.07123	0.27244	-1.46984	5.03236	-0.52469	5.22841	-0.54780	-0.03430
H	-5.05811	-1.34509	-0.36038	3.60070	3.75526	0.45262	2.13839	-4.80028	-0.19352
H	-5.05823	1.34471	-0.36030	4.98973	1.46324	0.47313	-0.50854	-5.22734	0.10157
H	-1.34495	5.07113	0.27247	3.77083	-3.60547	-0.62977	-4.79464	-2.13387	-0.02755
H	1.34455	5.07124	0.27246	1.45457	-5.00741	-0.64503	-5.21760	0.50677	-0.29956
H	5.05812	1.34511	-0.36029	-3.62235	-3.75635	0.32290	-2.12921	4.78214	-0.18850
H	5.05821	-1.34470	-0.36039	-5.00870	-1.46121	0.33160	0.52732	5.20809	0.05125
C	-3.49408	3.48834	-0.00945	4.80547	-1.17336	0.00166	-2.90950	-3.99110	0.27302
C	-3.64275	4.36793	-1.09452	5.31954	-1.98796	1.02647	-3.67358	-4.20390	1.43458
C	-4.36981	3.62319	1.08065	5.69274	-0.71685	-0.98850	-3.01927	-4.93217	-0.76698
C	-4.63499	5.35228	-1.09199	6.67440	-2.32417	1.06787	-4.51931	-5.31048	1.55256
H	-2.96993	4.26993	-1.94154	4.64065	-2.35060	1.79258	-3.59630	-3.48540	2.24573
C	-5.36327	4.60615	1.08763	7.04993	-1.05061	-0.95047	-3.85908	-6.04259	-0.65206
H	-4.26061	2.94693	1.92346	5.30402	-0.09676	-1.79108	-2.43877	-4.77791	-1.67198
C	-5.50030	5.47575	0.00030	7.54761	-1.85574	0.07881	-4.61538	-6.23760	0.50955
H	-4.73391	6.02039	-1.94408	7.05007	-2.94845	1.87494	-5.09913	-5.45101	2.46177
H	-6.02803	4.69459	1.94345	7.71638	-0.68596	-1.72841	-3.92932	-6.75219	-1.47316
H	-6.27255	6.24086	0.00412	8.60239	-2.11696	0.10992	-5.27072	-7.10027	0.59977
C	-3.49380	-3.48861	-0.00947	1.18682	4.80612	-0.01802	4.01532	-2.89307	-0.27970
C	-4.36951	-3.62356	1.08063	0.74069	5.63606	1.02575	4.44398	-3.64481	0.82594
C	-3.64239	-4.36820	-1.09455	1.97510	5.38042	-1.02997	4.75688	-2.96958	-1.46878
C	-5.36290	-4.60660	1.08760	1.07938	6.99060	1.06304	5.58524	-4.44777	0.74769
H	-4.26038	-2.94730	1.92345	0.12709	5.20210	1.80967	3.87295	-3.58917	1.74811
C	-4.63455	-5.35263	-1.09203	2.31721	6.73570	-0.99608	5.89956	-3.77180	-1.55151
H	-2.96958	-4.27012	-1.94157	2.31724	4.74964	-1.84541	4.42881	-2.39083	-2.32748
C	-5.49985	-5.47619	0.00025	1.87099	7.54740	0.05147	6.31808	-4.51413	-0.44273
H	-6.02764	-4.69512	1.94342	0.72939	7.61095	1.88453	5.90424	-5.01804	1.61663
H	-4.73341	-6.02074	-1.94413	2.92809	7.15736	-1.79066	6.46064	-3.81738	-2.48167
H	-6.27203	-6.24138	0.00406	2.13532	8.60149	0.07961	7.20632	-5.13783	-0.50478
C	3.49407	-3.48833	-0.00945	-4.80666	1.17017	0.00936	2.89555	3.98865	0.32603
C	4.36978	-3.62322	1.08066	-5.53324	1.13740	1.21087	2.83100	4.77358	1.49194
C	3.64275	-4.36791	-1.09454	-5.48036	1.54232	-1.16581	3.78666	4.38854	-0.68614
C	5.36324	-4.60619	1.08764	-6.89478	1.45455	1.23686	3.63012	5.90894	1.64505
H	4.26057	-2.94698	1.92349	-5.01674	0.85883	2.12502	2.14289	4.47873	2.27905
C	4.63499	-5.35226	-1.09201	-6.83996	1.86492	-1.14373	4.59230	5.52084	-0.53571
H	2.96995	-4.26988	-1.94156	-4.92476	1.57257	-2.09878	3.83893	3.79837	-1.59662
C	5.50028	-5.47576	0.00030	-7.55408	1.82044	0.05896	4.51812	6.28810	0.63151
H	6.02797	-4.69466	1.94347	-7.43849	1.42016	2.17782	3.56398	6.49508	2.55863
H	4.73392	-6.02035	-1.94411	-7.34278	2.14585	-2.06597	5.27269	5.80775	-1.33411
H	6.27252	-6.24088	0.00411	-8.61219	2.06910	0.07747	5.14223	7.17034	0.74966
C	3.49381	3.48861	-0.00947	-1.18663	-4.80122	-0.07464	-3.99593	2.88604	-0.34994
C	3.64240	4.36821	-1.09454	-0.74344	-5.65654	0.94968	-4.88060	3.07638	0.72319
C	4.36953	3.62352	1.08062	-1.96070	-5.35348	-1.10963	-4.26122	3.54592	-1.56048
C	4.63458	5.35263	-1.09201	-1.07293	-7.01388	0.94736	-6.00548	3.89621	0.58893
H	2.96958	4.27016	-1.94156	-0.13868	-5.24014	1.74989	-4.67654	2.57323	1.66387
C	5.36293	4.60656	1.08760	-2.29390	-6.71140	-1.11534	-5.38412	4.36661	-1.69889
H	4.26039	2.94725	1.92343	-2.29829	-4.70376	-1.91197	-3.57688	3.40641	-2.39234
C	5.49988	5.47616	0.00027	-1.85188	-7.54821	-0.08591	-6.26177	4.54438	-0.62355
H	4.73344	6.02075	-1.94410	-0.72522	-7.65418	1.75441	-6.67873	4.03048	1.43200
H	6.02768	4.69505	1.94342	-2.89393	-7.11556	-1.92709	-5.57491	4.86461	-2.64632
H	6.27207	6.24134	0.00409	-2.10918	-8.60441	-0.08878	-7.13568	5.18221	-0.72968
Fe	0.00000	0.00001	0.09284	0.00255	0.00470	0.24184	0.00837	-0.00327	0.08944
H	0.00001	0.00001	1.57345	0.01238	0.03196	1.92458	-0.07476	-0.13948	1.55030

	H_2TPP, total charge 0			H_2TPP, total charge 1			H-H_2TPP, total charge 0		
	Singlet			Doublet			Doublet		
N	0.00135	2.10727	-0.06220	-2.10492	0.00049	-0.12532	0.00812	2.13289	-0.02771
N	2.04307	-0.00128	0.00000	0.00048	2.05736	-0.00001	2.02709	0.00037	-0.12836
N	-0.00135	-2.10727	0.06220	2.10492	-0.00049	0.12532	0.00903	-2.13291	-0.02773
N	-2.04307	0.00128	0.00000	-0.00048	-2.05737	0.00001	-2.13143	-0.00042	0.09419
C	-1.13031	2.89006	-0.01337	-2.88657	-1.12580	-0.02922	-1.13192	2.90151	0.15920
C	-0.68325	4.25190	0.06430	-4.23626	-0.68725	0.12951	-0.65902	4.22035	0.51301
C	0.68864	4.25104	0.06431	-4.23593	0.68920	0.12956	0.70774	4.21876	0.47996
C	1.13398	2.88864	-0.01337	-2.88604	1.12714	-0.02914	1.15537	2.90047	0.11553
C	2.46410	2.43865	-0.00168	-2.43808	2.47258	-0.01172	2.46112	2.45389	-0.06400
C	2.87039	1.08786	0.00018	-1.08730	2.88944	-0.00426	2.84713	1.09312	-0.26831
C	4.27263	0.67587	-0.00473	-0.67732	4.28840	-0.01214	4.20007	0.68534	-0.57465
C	4.27177	-0.68129	0.00465	0.67931	4.28809	0.01204	4.20033	-0.68361	-0.57469
C	2.86900	-1.09149	-0.00020	1.08865	2.88894	0.00422	2.84753	-1.09192	-0.26835
C	2.46099	-2.44176	0.00167	2.43923	2.47145	0.01171	2.46211	-2.45300	-0.06417
C	1.13031	-2.89006	0.01337	2.88657	1.12580	0.02916	1.15657	-2.90005	0.11529
C	0.68325	-4.25190	-0.06431	4.23626	0.68722	-0.12952	0.70942	-4.21865	0.47952
C	-0.68864	-4.25104	-0.06431	4.23594	-0.68922	-0.12947	-0.65728	-4.22075	0.51271
C	-1.13398	-2.88864	0.01337	2.88604	-1.12714	0.02924	-1.13074	-2.90198	0.15917
C	-2.46410	-2.43865	0.00168	2.43808	-2.47259	0.01185	-2.45547	-2.49484	0.01933
C	-2.87039	-1.08786	-0.00018	1.08730	-2.88945	0.00431	-2.87690	-1.14252	-0.20324
C	-4.27263	-0.67587	0.00474	0.67731	-4.28841	0.01214	-4.08569	-0.70132	-0.76409
C	-4.27177	0.68129	-0.00465	-0.67931	-4.28810	-0.01214	-4.08600	0.69956	-0.76415
C	-2.86900	1.09149	0.00020	-1.08865	-2.88895	-0.00431	-2.87736	1.14134	-0.20337
C	-2.46099	2.44176	-0.00167	-2.43923	-2.47146	-0.01184	-2.45655	2.49383	0.01915
H	-1.33886	5.10699	0.13062	-5.08477	-1.34018	0.26223	-1.30600	5.04284	0.77820
H	1.34532	5.10530	0.13062	-5.08414	1.34251	0.26234	1.36776	5.04171	0.71082
H	5.12586	1.33846	-0.01628	-1.33653	5.14268	-0.03770	5.03241	1.34615	-0.76921
H	5.12415	-1.34497	0.01615	1.33893	5.14206	0.03757	5.03292	-1.34407	-0.76934
H	1.33886	-5.10699	-0.13062	5.08478	1.34014	-0.26227	1.36978	-5.04138	0.71019
H	-1.34532	-5.10530	-0.13063	5.08414	-1.34254	-0.26218	-1.30395	-5.04352	0.77782
H	-5.12586	-1.33846	0.01628	1.33653	-5.14269	0.03773	-4.85270	-1.35409	-1.15377
H	-5.12415	1.34497	-0.01615	-1.33892	-5.14207	-0.03774	-4.85327	1.35195	-1.15392
C	3.51884	-3.50153	-0.02655	3.50180	3.51411	-0.02635	3.53891	-3.48695	-0.01098
C	3.75061	-4.31028	1.09703	4.41336	3.63802	1.03711	4.53742	-3.43149	0.97666
C	4.29299	-3.70845	-1.17913	3.61258	4.38016	-1.12848	3.57218	-4.53947	-0.94086
C	4.73575	-5.30112	1.07093	5.40603	4.61867	1.00423	5.53681	-4.40469	1.03644
H	3.15738	-4.15292	1.99333	4.32806	2.97734	1.89481	4.51918	-2.62105	1.69909
C	5.27710	-4.69994	-1.20754	4.61903	5.34608	-1.16692	4.57429	-5.51192	-0.88507
H	4.11619	-3.08787	-2.05285	2.91923	4.28109	-1.95822	2.81115	-4.58394	-1.71454
C	5.50177	-5.49914	-0.08207	5.51409	5.47129	-0.09916	5.55934	-5.44840	0.10486
H	4.90605	-5.91490	1.95107	6.09351	4.71644	1.83887	6.29633	-4.34951	1.81138
H	5.86553	-4.84899	-2.10858	4.70436	5.99954	-2.02977	4.58743	-6.31460	-1.61721
H	6.26745	-6.26940	-0.10335	6.29147	6.22867	-0.12716	6.33856	-6.20399	0.14973
C	3.52329	3.49708	0.02655	-3.50016	3.51574	0.02635	3.53746	3.48836	-0.01068
C	4.29779	3.70293	1.17909	-3.61049	4.38187	1.12846	4.53573	3.43343	0.97722
C	3.75602	4.30562	-1.09699	-4.41170	3.64005	-1.03708	3.57044	4.54079	-0.94066
C	5.28317	4.69316	1.20750	-4.61649	5.34826	1.16692	5.53467	4.40710	1.03714
H	4.12027	3.08251	2.05277	-2.91715	4.28250	1.95817	4.51767	2.62304	1.69971
C	4.74242	5.29520	-1.07089	-5.40391	4.62117	-1.00419	4.57213	5.51366	-0.88476
H	3.16253	4.14908	-1.99326	-4.32674	2.97931	-1.89476	2.80953	4.58485	-1.71448
C	5.50878	5.49215	0.08208	-5.51153	5.47386	0.09919	5.55697	5.45068	0.10542
H	5.87186	4.84140	2.10851	-4.70148	6.00178	2.02975	6.29402	4.35236	1.81228
H	4.91345	5.90882	-1.95100	-6.09137	4.71924	-1.83880	4.58513	6.31626	-1.61699
H	6.27544	6.26143	0.10335	-6.28855	6.23161	0.12720	6.33583	6.20662	0.15039
C	-3.51884	3.50153	0.02655	-3.50181	-3.51411	0.02610	-3.52980	3.52575	0.03733
C	-4.29299	3.70846	1.17914	-3.61265	-4.38025	1.12816	-4.62652	3.40268	0.91072
C	-3.75062	4.31028	-1.09704	-4.41332	-3.63793	-1.03741	-3.48726	4.63534	-0.82627
C	-5.27710	4.69994	1.20755	-4.61911	-5.34615	1.16648	-5.63712	4.36458	0.93187
H	-4.11618	3.08788	2.05285	-2.91934	-4.28124	1.95794	-4.67524	2.54757	1.57834
C	-4.73575	5.30112	-1.07093	-5.40600	-4.61858	-1.00465	-4.49869	5.59866	-0.80659
H	-3.15739	4.15292	-1.99334	-4.32798	-2.97719	-1.89505	-2.65951	4.73035	-1.52269
C	-5.50177	5.49914	0.08208	-5.51413	-5.47127	0.09867	-5.57695	5.46849	0.07369
H	-5.86552	4.84900	2.10859	-4.70449	-5.99967	2.02928	-6.46981	4.25524	1.62118
H	-4.90605	5.91490	-1.95107	-6.09345	-4.71627	-1.83932	-4.44832	6.44517	-1.48584
H	-6.26745	6.26940	0.10335	-6.29152	-6.22865	0.12658	-6.36450	6.21645	0.08870

C	-3.52329	-3.49708	-0.02655	3.50017	-3.51574	-0.02610	-3.52837	-3.52716	0.03771
C	-3.75602	-4.30562	1.09699	4.41161	-3.64000	1.03742	-4.62487	-3.40454	0.91143
C	-4.29780	-3.70293	-1.17909	3.61061	-4.38191	-1.12817	-3.48568	-4.63664	-0.82599
C	-4.74242	-5.29520	1.07088	5.40383	-4.62112	1.00465	-5.63513	-4.36679	0.93280
H	-3.16252	-4.14909	1.99326	4.32656	-2.97924	1.89507	-4.67370	-2.54949	1.57913
C	-5.28318	-4.69315	-1.20750	4.61662	-5.34829	-1.16650	-4.49679	-5.60032	-0.80612
H	-4.12027	-3.08250	-2.05277	2.91735	-4.28256	-1.95795	-2.65808	-4.73131	-1.52265
C	-5.50879	-5.49215	-0.08208	5.51157	-5.47384	-0.09869	-5.57483	-5.47059	0.07448
H	-4.91344	-5.90883	1.95099	6.09123	-4.71915	1.83933	-6.46766	-4.25781	1.62236
H	-5.87186	-4.84139	-2.10851	4.70170	-6.00183	-2.02931	-4.44632	-6.44674	-1.48547
H	-6.27545	-6.26143	-0.10335	6.28860	-6.23158	-0.12660	-6.36211	-6.21882	0.08964
H	-0.00072	-1.09336	0.09242	1.09392	-0.00024	0.20753	0.06643	-1.18187	-0.36429
H	0.00072	1.09336	-0.09242	-1.09393	0.00026	-0.20754	0.06588	1.18196	-0.36450
H							-1.40739	-0.00024	0.80142

	MgTPP, total charge 0			**MgTPP, total charge 1**			**H-MgTPP, total charge 0**		
	Singlet			**Doublet**			**Doublet**		
N	-2.06503	0.00000	-0.03095	-1.46840	-1.46140	-0.01057	-2.06539	-0.00003	-0.05011
N	0.00000	2.06537	0.00000	-1.46276	1.46705	0.01061	0.00192	2.06759	-0.01491
N	2.06503	0.00000	0.03095	1.46589	1.46217	0.05694	2.06979	0.00003	0.02867
N	0.00000	-2.06537	0.00000	1.46024	-1.46780	-0.05690	0.00197	-2.06760	-0.01491
C	-2.88267	-1.10790	0.00861	-1.27311	-2.82244	-0.03872	-2.88281	-1.10911	-0.00493
C	-4.26448	-0.68268	0.08272	-2.54658	-3.49613	-0.11826	-4.26399	-0.68279	0.07510
C	-4.26448	0.68268	0.08272	-3.51088	-2.52695	-0.10526	-4.26401	0.68268	0.07512
C	-2.88267	1.10790	0.00861	-2.82857	-1.25734	-0.04853	-2.88284	1.10904	-0.00493
C	-2.45195	2.45216	0.01096	-3.47322	0.00669	-0.00003	-2.44971	2.45111	-0.00595
C	-1.10804	2.88383	0.00481	-2.82372	1.26823	0.04852	-1.10517	2.88449	-0.01028
C	-0.68269	4.26753	-0.00228	-3.50113	2.54045	0.10527	-0.68104	4.26930	-0.01511
C	0.68269	4.26753	0.00228	-2.53311	3.50592	0.11834	0.68415	4.27003	-0.00766
C	1.10805	2.88383	-0.00481	-1.26225	2.82733	0.03882	1.10964	2.88576	-0.01584
C	2.45195	2.45215	-0.01096	0.00254	3.47329	-0.00661	2.45284	2.45201	-0.02014
C	2.88267	1.10790	-0.00861	1.26428	2.81955	-0.04092	2.88596	1.10702	-0.01594
C	4.26448	0.68268	-0.08272	2.52775	3.48785	-0.23318	4.26791	0.68281	-0.09752
C	4.26448	-0.68268	-0.08272	3.49352	2.51945	-0.23607	4.26792	-0.68271	-0.09754
C	2.88267	-1.10790	-0.00861	2.82237	1.25745	-0.04470	2.88599	-1.10695	-0.01594
C	2.45195	-2.45216	-0.01096	3.47123	-0.00668	-0.00004	2.45290	-2.45195	-0.02014
C	1.10804	-2.88383	-0.00481	2.81751	-1.26829	0.04467	1.10971	-2.88574	-0.01584
C	0.68269	-4.26753	0.00228	3.48381	-2.53286	0.23604	0.68425	-4.27002	-0.00765
C	-0.68269	-4.26753	-0.00228	2.51432	-3.49754	0.23322	-0.68093	-4.26931	-0.01511
C	-1.10805	-2.88383	0.00481	1.25342	-2.82439	0.04101	-1.10510	-2.88452	-0.01027
C	-2.45195	-2.45215	0.01096	-0.01083	-3.47326	0.00674	-2.44965	-2.45117	-0.00595
H	-5.11840	-1.34133	0.14507	-2.69181	-4.56376	-0.18033	-5.11803	-1.34109	0.13990
H	-5.11840	1.34133	0.14507	-4.58095	-2.66586	-0.13020	-5.11806	1.34096	0.13993
H	-1.34087	5.12398	-0.01022	-4.57066	2.68348	0.13017	-1.33957	5.12543	-0.02305
H	1.34087	5.12397	0.01021	-2.67424	4.57409	0.18043	1.34171	5.12686	0.00344
H	5.11840	1.34133	-0.14506	2.66257	4.54870	-0.37978	5.12146	1.34127	-0.16579
H	5.11840	-1.34133	-0.14506	4.55403	2.65199	-0.38696	5.12149	-1.34115	-0.16581
H	1.34087	-5.12398	0.01022	4.54381	-2.66948	0.38688	1.34184	-5.12683	0.00345
H	-1.34087	-5.12397	-0.01023	2.64507	-4.55889	0.37985	-1.33945	-5.12547	-0.02306
C	3.51275	3.50920	-0.03023	0.01097	4.96111	-0.03285	3.51390	3.50829	-0.03818
C	4.32196	3.73002	1.09540	0.63049	5.68592	1.00128	4.32865	3.72030	1.08519
C	3.71984	4.29611	-1.17417	-0.59364	5.66242	-1.09168	3.71546	4.30273	-1.17788
C	5.31313	4.71491	1.07929	0.63261	7.08126	0.98234	5.31988	4.70502	1.07102
H	4.16633	3.12589	1.98466	1.09241	5.15125	1.82584	4.17698	3.11007	1.97092
C	4.71184	5.28007	-1.19307	-0.57091	7.05743	-1.11826	4.70840	5.28568	-1.19487
H	3.09992	4.12838	-2.05025	-1.06198	5.10976	-1.90056	3.09117	4.14138	-2.05202
C	5.51138	5.49294	-0.06565	0.03673	7.77006	-0.07923	5.51322	5.49046	-0.06972
H	5.92774	4.87521	1.96077	1.09920	7.62956	1.79506	5.93855	4.85921	1.95070
H	4.86128	5.87723	-2.08833	-1.02630	7.58696	-1.94956	4.85424	5.88856	-2.08685
H	6.28227	6.25817	-0.07932	0.04639	8.85558	-0.09710	6.28452	6.25529	-0.08189
C	-3.51275	3.50920	0.03023	-4.96486	0.00956	-0.00008	-3.51009	3.50839	0.01702
C	-3.71983	4.29612	1.17417	-5.67487	0.43398	1.13570	-3.71512	4.29105	1.16417
C	-4.32196	3.73002	-1.09540	-5.67641	-0.41213	-1.13592	-4.32072	3.73205	-1.10683
C	-4.71183	5.28008	1.19307	-7.07102	0.42793	1.13690	-4.70754	5.27438	1.18772
H	-3.09991	4.12840	2.05025	-5.13014	0.75408	2.01907	-3.09374	4.12040	2.03863
C	-5.31313	4.71491	-1.07929	-7.07252	-0.40069	-1.13723	-5.31176	4.71699	-1.08600
H	-4.16633	3.12588	-1.98466	-5.13285	-0.73433	-2.01925	-4.16637	3.13060	-1.99813
C	-5.51138	5.49294	0.06565	-7.77269	0.01497	-0.00020	-5.50852	5.49089	0.06199
H	-4.86127	5.87724	2.08832	-7.60919	0.74536	2.02489	-4.85608	5.86833	2.08523

H	-5.92774	4.87520	-1.96076	-7.61185	-0.71603	-2.02528	-5.92761	4.88028	-1.96604
H	-6.28226	6.25818	0.07932	-8.85837	0.01707	-0.00024	-6.27952	6.25593	0.07929
C	-3.51275	-3.50920	0.03023	-0.00814	-4.96110	0.03303	-3.51001	-3.50847	0.01702
C	-3.71984	-4.29612	1.17417	-0.61544	-5.66003	1.09189	-3.71502	-4.29114	1.16417
C	-4.32196	-3.73001	-1.09540	0.60852	-5.68835	-1.00111	-4.32063	-3.73214	-1.10683
C	-4.71183	-5.28008	1.19306	-0.59814	-7.05512	1.11851	-4.70742	-5.27450	1.18772
H	-3.09991	-4.12840	2.05025	-1.08160	-5.10553	1.90078	-3.09365	-4.12048	2.03863
C	-5.31314	-4.71491	-1.07929	0.60520	-7.08368	-0.98214	-5.31165	-4.71711	-1.08601
H	-4.16634	-3.12588	-1.98466	1.07246	-5.15551	-1.82571	-4.16629	-3.13069	-1.99813
C	-5.51138	-5.49294	0.06565	0.00668	-7.77013	0.07947	-5.50839	-5.49102	0.06198
H	-4.86127	-5.87724	2.08832	-1.05557	-7.58285	1.94983	-4.85595	-5.86845	2.08522
H	-5.92775	-4.87520	-1.96076	1.06961	-7.63382	-1.79486	-5.92750	-4.88040	-1.96604
H	-6.28227	-6.25817	0.07931	0.01210	-8.85568	0.09737	-6.27938	-6.25607	0.07928
C	3.51275	-3.50920	-0.03023	4.95762	-0.00954	-0.00009	3.51399	-3.50820	-0.03817
C	4.32195	-3.73002	1.09540	5.67310	0.64775	1.01796	4.32874	-3.72020	1.08519
C	3.71984	-4.29612	-1.17417	5.67046	-0.66962	-1.01819	3.71557	-4.30263	-1.17788
C	5.31313	-4.71491	1.07930	7.06819	0.63442	1.02247	5.31999	-4.70490	1.07102
H	4.16632	-3.12589	1.98466	5.13053	1.14891	1.81381	4.17705	-3.10998	1.97092
C	4.71183	-5.28007	-1.19307	7.06560	-0.66172	-1.02279	4.70853	-5.28556	-1.19487
H	3.09992	-4.12839	-2.05025	5.12589	-1.16868	-1.81399	3.09128	-4.14130	-2.05202
C	5.51138	-5.49294	-0.06565	7.76767	-0.01502	-0.00019	5.51335	-5.49033	-0.06972
H	5.92773	-4.87521	1.96077	7.60836	1.12983	1.82345	5.93865	-4.85909	1.95071
H	4.86128	-5.87723	-2.08832	7.60378	-1.15924	-1.82381	4.85439	-5.88844	-2.08685
H	6.28226	-6.25818	-0.07931	8.85339	-0.01713	-0.00022	6.28467	-6.25514	-0.08189
Mg	0.00000	0.00000	0.00000	-0.00118	0.00001	0.00003	0.00228	0.00000	0.06983
H							-0.67500	-0.00003	2.18779

MnTPP, total charge 0

	Doublet			Quartet			Sextet		
N	2.02479	0.00000	-0.01387	2.02743	-0.00003	-0.01533	2.09105	0.00000	-0.05660
N	0.00000	-2.02508	0.00000	-0.00003	-2.02770	0.00000	0.00000	-2.09106	0.00000
N	-2.02479	0.00000	0.01386	-2.02743	0.00002	0.01532	-2.09105	0.00000	0.05660
N	0.00000	2.02508	0.00000	0.00003	2.02769	0.00000	0.00000	2.09106	0.00000
C	2.85603	1.10354	0.01463	2.85760	1.10373	0.01364	2.89828	1.11272	-0.00144
C	4.23516	0.68165	0.07410	4.23689	0.68162	0.07345	4.27913	0.68340	0.09323
C	4.23516	-0.68163	0.07411	4.23688	-0.68175	0.07336	4.27913	-0.68340	0.09323
C	2.85604	-1.10353	0.01463	2.85757	-1.10381	0.01353	2.89828	-1.11272	-0.00144
C	2.44405	-2.44418	0.01448	2.44439	-2.44465	0.01380	2.45768	-2.45786	0.00392
C	1.10363	-2.85681	0.00651	1.10383	-2.85841	0.00612	1.11296	-2.89980	0.00137
C	0.68165	-4.23713	-0.00103	0.68161	-4.23893	-0.00148	0.68344	-4.28368	-0.00414
C	-0.68163	-4.23714	0.00127	-0.68172	-4.23892	0.00162	-0.68344	-4.28368	0.00415
C	-1.10362	-2.85681	-0.00643	-1.10390	-2.85838	-0.00607	-1.11297	-2.89980	-0.00137
C	-2.44404	-2.44419	-0.01448	-2.44446	-2.44459	-0.01380	-2.45768	-2.45786	-0.00393
C	-2.85603	-1.10354	-0.01472	-2.85760	-1.10374	-0.01358	-2.89828	-1.11272	0.00144
C	-4.23515	-0.68164	-0.07435	-4.23689	-0.68164	-0.07351	-4.27913	-0.68340	-0.09324
C	-4.23516	0.68163	-0.07434	-4.23687	0.68173	-0.07359	-4.27913	0.68340	-0.09324
C	-2.85604	1.10353	-0.01471	-2.85757	1.10380	-0.01370	-2.89828	1.11272	0.00144
C	-2.44405	2.44419	-0.01446	-2.44439	2.44464	-0.01400	-2.45768	2.45786	-0.00392
C	-1.10363	2.85681	-0.00642	-1.10383	2.85840	-0.00619	-1.11296	2.89980	-0.00137
C	-0.68165	4.23713	0.00127	-0.68161	4.23892	0.00154	-0.68344	4.28368	0.00415
C	0.68164	4.23713	-0.00104	0.68172	4.23891	-0.00140	0.68344	4.28368	-0.00414
C	1.10362	2.85681	0.00650	1.10390	2.85837	0.00624	1.11297	2.89980	0.00137
C	2.44404	2.44419	0.01446	2.44446	2.44458	0.01400	2.45768	2.45786	0.00392
H	5.08634	1.34458	0.12461	5.08823	1.34439	0.12415	5.13422	1.33907	0.17145
H	5.08634	-1.34456	0.12462	5.08819	-1.34454	0.12398	5.13422	-1.33907	0.17145
H	1.34425	-5.08999	-0.00676	1.34398	-5.09201	-0.00781	1.33840	-5.14270	-0.01557
H	-1.34422	-5.09000	0.00710	-1.34410	-5.09198	0.00801	-1.33840	-5.14270	0.01558
H	-5.08633	-1.34457	-0.12496	-5.08822	-1.34441	-0.12418	-5.13422	-1.33907	-0.17146
H	-5.08633	1.34456	-0.12495	-5.08819	1.34452	-0.12434	-5.13422	1.33907	-0.17146
H	-1.34423	5.09000	0.00711	-1.34397	5.09201	0.00785	-1.33840	5.14270	0.01558
H	1.34423	5.09000	-0.00677	1.34411	5.09197	-0.00765	1.33840	5.14270	-0.01557
C	-3.50399	-3.50147	-0.02946	-3.50445	-3.50190	-0.02929	-3.51911	-3.51414	-0.02857
C	-4.28241	-3.74788	1.11200	-4.28485	-3.74703	1.11111	-4.34805	-3.71976	1.08572
C	-3.73924	-4.26237	-1.18503	-3.73781	-4.26418	-1.18436	-3.70839	-4.31488	-1.16618
C	-5.27282	-4.73373	1.09973	-5.27519	-4.73292	1.09834	-5.34037	-4.70332	1.06494
H	-4.10385	-3.16318	2.00992	-4.10783	-3.16128	2.00866	-4.20626	-3.10516	1.97006
C	-4.73039	-5.24739	-1.19984	-4.72891	-5.24922	-1.19972	-4.70171	-5.29728	-1.18980
H	-3.14205	-4.07407	-2.07267	-3.13914	-4.07689	-2.07124	-3.07403	-4.15837	-2.03391

C	-5.49993	-5.48629	-0.05685	-5.50034	-5.48685	-0.05773	-5.52058	-5.49510	-0.07354
H	-5.86432	-4.91449	1.99295	-5.86820	-4.91268	1.99077	-5.96994	-4.85189	1.93786
H	-4.90237	-5.82516	-2.10371	-4.89936	-5.82807	-2.10319	-4.83735	-5.90480	-2.08026
H	-6.27011	-6.25227	-0.06743	-6.27049	-6.25287	-0.06871	-6.29249	-6.25922	-0.09090
C	3.50400	-3.50146	0.02946	3.50437	-3.50199	0.02929	3.51911	-3.51414	0.02857
C	3.73945	-4.26214	1.18512	3.73781	-4.26415	1.18442	3.70839	-4.31487	1.16618
C	4.28221	-3.74807	-1.11209	4.28464	-3.74725	-1.11116	4.34804	-3.71977	-1.08572
C	4.73060	-5.24717	1.19994	4.72889	-5.24922	1.19977	4.70172	-5.29727	1.18980
H	3.14241	-4.07369	2.07284	3.13925	-4.07676	2.07133	3.07404	-4.15836	2.03392
C	5.27263	-4.73392	-1.09982	5.27496	-4.73317	-1.09839	5.34036	-4.70333	-1.06495
H	4.10350	-3.16352	-2.01008	4.10754	-3.16159	-2.00876	4.20624	-3.10518	-1.97007
C	5.49994	-5.48627	0.05685	5.50020	-5.48698	0.05774	5.52058	-5.49510	0.07354
H	4.90273	-5.82478	2.10387	4.89942	-5.82798	2.10329	4.83736	-5.90479	2.08027
H	5.86398	-4.91484	-1.99311	5.86787	-4.91303	-1.99086	5.96992	-4.85190	-1.93786
H	6.27013	-6.25225	0.06744	6.27033	-6.25302	0.06872	6.29248	-6.25922	0.09090
C	3.50399	3.50147	0.02943	3.50444	3.50189	0.02965	3.51911	3.51414	0.02857
C	3.73945	4.26216	1.18509	3.73780	4.26397	1.18485	3.70840	4.31487	1.16618
C	4.28220	3.74808	-1.11212	4.28481	3.74724	-1.11072	4.34804	3.71977	-1.08572
C	4.73060	5.24719	1.19989	4.72888	5.24903	1.20037	4.70172	5.29727	1.18980
H	3.14242	4.07371	2.07281	3.13915	4.07652	2.07170	3.07404	4.15836	2.03392
C	5.27261	4.73392	-1.09986	5.27514	4.73315	-1.09779	5.34036	4.70332	-1.06495
H	4.10348	3.16352	-2.01011	4.10779	3.16165	-2.00837	4.20624	3.10518	-1.97007
C	5.49993	5.48628	0.05681	5.50030	5.48687	0.05841	5.52058	5.49510	0.07354
H	4.90273	5.82481	2.10383	4.89934	5.82772	2.10394	4.83736	5.90478	2.08027
H	5.86396	4.91484	-1.99315	5.86814	4.91307	-1.99020	5.96992	4.85190	-1.93786
H	6.27011	6.25226	0.06738	6.27043	6.25290	0.06952	6.29249	6.25922	0.09090
C	-3.50400	3.50146	-0.02943	-3.50436	3.50198	-0.02965	-3.51911	3.51414	-0.02857
C	-4.28241	3.74786	1.11203	-4.28484	3.74723	1.11066	-4.34805	3.71976	1.08572
C	-3.73926	4.26236	-1.18499	-3.73758	4.26419	-1.18480	-3.70839	4.31488	-1.16618
C	-5.27283	4.73371	1.09977	-5.27514	4.73316	1.09774	-5.34037	4.70332	1.06494
H	-4.10385	3.16315	2.00995	-4.10791	3.16154	2.00828	-4.20626	3.10517	1.97006
C	-4.73041	5.24738	-1.19980	-4.72864	5.24927	-1.20031	-4.70171	5.29728	-1.18980
H	-3.14207	4.07407	-2.07264	-3.13885	4.07681	-2.07161	-3.07402	4.15837	-2.03391
C	-5.49995	5.48627	-0.05680	-5.50016	5.48701	-0.05841	-5.52058	5.49510	-0.07354
H	-5.86433	4.91446	1.99299	-5.86822	4.91301	1.99011	-5.96994	4.85189	1.93786
H	-4.90240	5.82516	-2.10366	-4.89900	5.82806	-2.10384	-4.83735	5.90480	-2.08026
H	-6.27014	6.25225	-0.06737	-6.27028	6.25306	-0.06951	-6.29248	6.25922	-0.09090
Mn	0.00000	0.00000	0.00000	0.00000	-0.00001	0.00000	0.00000	0.00000	0.00000

MnTPP, total charge 1

	Singlet			Triplet			Quintet		
N	-1.96781	-0.00001	-0.00463	2.03383	0.00000	-0.04431	-1.99924	0.00007	-0.01067
N	-0.00001	1.96828	-0.00021	0.00000	-2.03438	0.00000	0.00001	1.99968	0.00000
N	1.96781	0.00000	0.00503	-2.03383	0.00000	0.04432	1.99924	0.00006	0.01067
N	0.00000	-1.96829	-0.00021	0.00000	2.03438	0.00000	-0.00001	-1.99946	0.00000
C	-2.82923	-1.10763	0.02157	2.86526	1.09927	0.00759	-2.84253	-1.11070	0.01931
C	-4.18947	-0.68462	0.08081	4.23841	0.68275	0.11325	-4.20785	-0.68205	0.07658
C	-4.18947	0.68460	0.08083	4.23841	-0.68275	0.11327	-4.20785	0.68246	0.07425
C	-2.82923	1.10762	0.02160	2.86526	-1.09927	0.00762	-2.84252	1.11092	0.01596
C	-2.44603	2.44619	0.01426	2.44834	-2.44883	0.01322	-2.44907	2.44934	0.01115
C	-1.10773	2.83013	0.00251	1.09949	-2.86743	0.00659	-1.11089	2.84344	0.00206
C	-0.68459	4.19160	-0.00558	0.68268	-4.24445	-0.00650	-0.68222	4.20992	-0.00489
C	0.68458	4.19160	0.00365	-0.68268	-4.24445	0.00647	0.68225	4.20992	0.00479
C	1.10771	2.83013	-0.00337	-1.09950	-2.86743	-0.00660	1.11091	2.84343	-0.00210
C	2.44602	2.44618	-0.01427	-2.44835	-2.44882	-0.01322	2.44908	2.44933	-0.01115
C	2.82924	1.10763	-0.02075	-2.86526	-1.09927	-0.00761	2.84253	1.11090	-0.01592
C	4.18953	0.68461	-0.07891	-4.23842	-0.68274	-0.11325	4.20786	0.68243	-0.07415
C	4.18954	-0.68460	-0.07889	-4.23842	0.68276	-0.11322	4.20785	-0.68208	-0.07648
C	2.82924	-1.10762	-0.02072	-2.86526	1.09928	-0.00758	2.84252	-1.11072	-0.01927
C	2.44603	-2.44617	-0.01421	-2.44834	2.44883	-0.01315	2.44904	-2.44913	-0.01695
C	1.10772	-2.83013	-0.00334	-1.09949	2.86743	-0.00656	1.11088	-2.84321	-0.00545
C	0.68460	-4.19160	0.00367	-0.68267	4.24445	0.00650	0.68224	-4.20969	0.00246
C	-0.68457	-4.19161	-0.00560	0.68268	4.24445	-0.00653	-0.68226	-4.20969	-0.00257
C	-1.10772	-2.83014	0.00248	1.09950	2.86743	0.00655	-1.11089	-2.84320	0.00541
C	-2.44602	-2.44620	0.01421	2.44835	2.44883	0.01315	-2.44906	-2.44912	0.01695
H	-5.03908	-1.34933	0.12953	5.08789	1.34191	0.20572	-5.05608	-1.34815	0.12552
H	-5.03909	1.34930	0.12957	5.08788	-1.34191	0.20577	-5.05608	1.34873	0.12096
H	-1.34896	5.04278	-0.01428	1.34104	-5.09921	-0.02540	-1.34808	5.05967	-0.01334
H	1.34896	5.04278	0.01172	-1.34104	-5.09921	0.02536	1.34811	5.05966	0.01320
H	5.03917	1.34933	-0.12703	-5.08789	-1.34190	-0.20573	5.05609	1.34870	-0.12082

H	5.03918	-1.34931	-0.12699	-5.08789	1.34192	-0.20568	5.05607	-1.34818	-0.12537
H	1.34898	-5.04278	0.01177	-1.34103	5.09921	0.02541	1.34814	-5.05943	0.00865
H	-1.34893	-5.04279	-0.01433	1.34104	5.09921	-0.02545	-1.34817	-5.05942	-0.00880
C	3.50496	3.50234	-0.02563	-3.50446	-3.49833	-0.03582	3.50818	3.50570	-0.02244
C	4.24719	3.77269	1.13395	-4.39130	-3.63526	1.04627	4.26291	3.76323	1.13194
C	3.76791	4.23063	-1.19577	-3.63104	-4.36012	-1.13920	3.75853	4.24684	-1.18719
C	5.23615	4.75979	1.12355	-5.37718	-4.62318	1.02892	5.25166	4.75041	1.12179
H	4.04340	3.21357	2.04295	-4.29401	-2.97652	1.90414	4.06923	3.19391	2.03673
C	4.76044	5.21407	-1.20570	-4.63072	-5.33393	-1.16171	4.75107	5.23016	-1.19703
H	3.19902	4.02000	-2.09713	-2.95609	-4.25179	-1.98300	3.17970	4.04655	-2.08448
C	5.49502	5.48102	-0.04613	-5.50218	-5.47120	-0.07630	5.49809	5.48440	-0.04260
H	5.80146	4.96531	2.02757	-6.04669	-4.72982	1.87699	5.82658	4.94600	2.02193
H	4.96007	5.76853	-2.11772	-4.72896	-5.98383	-2.02590	4.94094	5.79449	-2.10506
H	6.26488	6.24658	-0.05405	-6.27447	-6.23412	-0.09195	6.26790	6.24999	-0.05040
C	-3.50498	3.50233	0.02563	3.50446	-3.49834	0.03582	-3.50816	3.50573	0.02244
C	-3.76674	4.23183	1.19529	3.63102	-4.36014	1.13919	-3.75842	4.24695	1.18716
C	-4.24843	3.77147	-1.13346	4.39131	-3.63525	-1.04626	-4.26297	3.76318	-1.13190
C	-4.75929	5.21525	1.20522	4.63070	-5.33395	1.16170	-4.75095	5.23028	1.19700
H	-3.19692	4.02215	2.09628	2.95606	-4.25181	1.98299	-3.17953	4.04672	2.08442
C	-5.23738	4.75856	-1.12306	5.37718	-4.62317	-1.02891	-5.25171	4.75036	-1.12175
H	-4.04556	3.21141	-2.04209	4.29403	-2.97650	-1.90412	-4.06936	3.19379	-2.03667
C	-5.49507	5.48099	0.04614	5.50217	-5.47120	0.07630	-5.49806	5.48444	0.04260
H	-4.95800	5.77064	2.11689	4.72892	-5.98386	2.02588	-4.94076	5.79467	2.10500
H	-5.80362	4.96315	-2.02671	6.04671	-4.72981	-1.87697	-5.82669	4.94589	-2.02187
H	-6.26493	6.24654	0.05407	6.27446	-6.23413	0.09195	-6.26786	6.25003	0.05040
C	-3.50496	-3.50235	0.02553	3.50447	3.49833	0.03570	-3.50796	-3.50563	0.03232
C	-3.76675	-4.23187	1.19517	3.63107	4.36016	1.13905	-3.75554	-4.24476	1.19894
C	-4.24839	-3.77146	-1.13358	4.39129	3.63521	-1.04641	-4.26506	-3.76553	-1.11997
C	-4.75930	-5.21529	1.20507	4.63075	5.33396	1.16150	-4.74775	-5.22837	1.21272
H	-3.19695	-4.02220	2.09617	2.95614	4.25186	1.98287	-3.17480	-4.04270	2.09461
C	-5.23734	-4.75856	-1.12322	5.37717	4.62313	-1.02911	-5.25348	-4.75299	-1.10589
H	-4.04550	-3.21139	-2.04220	4.29398	2.97644	-1.90425	-4.07347	-3.19784	-2.02623
C	-5.49505	-5.48101	0.04596	5.50220	5.47119	0.07607	-5.49719	-5.48493	0.06037
H	-4.95803	-5.77070	2.11671	4.72901	5.98389	2.02567	-4.93548	-5.79112	2.12217
H	-5.80356	-4.96313	-2.02689	6.04667	4.72974	-1.87720	-5.83026	-4.95042	-2.00445
H	-6.26491	-6.24656	0.05386	6.27449	6.23410	0.09168	-6.26675	-6.25074	0.07122
C	3.50498	-3.50233	-0.02553	-3.50446	3.49834	-0.03570	3.50794	-3.50566	-0.03232
C	4.24719	-3.77265	1.13407	-4.39127	3.63523	1.04642	4.26496	-3.76564	1.12000
C	3.76796	-4.23064	-1.19566	-3.63108	4.36015	-1.13906	3.75560	-4.24470	-1.19898
C	5.23615	-4.75974	1.12371	-5.37715	4.62315	1.02912	5.25337	-4.75311	1.10593
H	4.04337	-3.21351	2.04306	-4.29395	2.97647	1.90426	4.07330	-3.19801	2.02629
C	4.76050	-5.21407	-1.20554	-4.63076	5.33396	-1.16151	4.74780	-5.22832	-1.21275
H	3.19909	-4.02003	-2.09703	-2.95615	4.25184	-1.98288	3.17492	-4.04258	-2.09467
C	5.49506	-5.48099	-0.04595	-5.50219	5.47120	-0.07607	5.49715	-5.48497	-0.06037
H	5.80145	-4.96524	2.02774	-6.04664	4.72977	1.87721	5.83008	-4.95060	2.00451
H	4.96015	-5.76854	-2.11755	-4.72902	5.98388	-2.02568	4.93558	-5.79100	-2.12223
H	6.26491	-6.24655	-0.05384	-6.27448	6.23411	-0.09168	6.26670	-6.25078	-0.07122
Mn	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00009	0.00000

H-MnTPP, total charge 0

		Singlet			**Triplet**			**Quintet**	
N	0.00297	1.97922	-0.02098	-0.00019	2.01515	-0.02610	-0.48327	-2.03686	-0.13110
N	2.03504	-0.00291	0.05970	2.01285	0.00019	-0.03039	-1.97261	0.46453	0.05031
N	-0.00280	-1.97921	-0.02094	0.00019	-2.01514	-0.02610	0.48076	2.03882	-0.08291
N	-2.02952	0.00293	-0.03708	-2.01285	-0.00019	-0.03039	1.97115	-0.46291	0.07171
C	-1.10443	2.82253	0.05055	-1.10245	2.84843	0.02649	0.40443	-3.08278	-0.09756
C	-0.67944	4.18399	0.19591	-0.68177	4.22367	0.13553	-0.32407	-4.33565	-0.05893
C	0.68681	4.18094	0.19975	0.68098	4.22379	0.13558	-1.65239	-4.02218	-0.05383
C	1.10907	2.81790	0.04974	1.10192	2.84864	0.02649	-1.74427	-2.57581	-0.08913
C	2.45623	2.42794	-0.00122	2.44085	2.44172	-0.02156	-2.94102	-1.83467	-0.01572
C	2.86868	1.09661	-0.03812	2.84608	1.10237	-0.07832	-3.02965	-0.42907	0.04182
C	4.24110	0.67327	-0.21087	4.22034	0.68177	-0.19982	-4.27128	0.30817	0.03098
C	4.23912	-0.68566	-0.21046	4.22046	-0.68098	-0.19992	-3.95653	1.63658	0.03528
C	2.86548	-1.10491	-0.03741	2.84629	-1.10184	-0.07832	-2.51669	1.73733	0.03231
C	2.44915	-2.43501	0.00005	2.44130	-2.44127	-0.02156	-1.80891	2.95355	-0.02890
C	1.10084	-2.82106	0.05051	1.10245	-2.84843	0.02650	-0.40847	3.08322	-0.08720
C	0.67455	-4.18288	0.20031	0.68177	-4.22366	0.13553	0.31659	4.33728	-0.13323
C	-0.69170	-4.18199	0.19555	-0.68098	-4.22379	0.13558	1.64593	4.02708	-0.12497
C	-1.11266	-2.81932	0.04990	-1.10192	-2.84864	0.02650	1.74124	2.58047	-0.09128
C	-2.45207	-2.42503	-0.02855	-2.44085	-2.44172	-0.02156	2.93731	1.83936	-0.03286

C	-2.86037	-1.09016	-0.10970	-2.84608	-1.10237	-0.07832	3.02539	0.43250	0.02317
C	-4.23823	-0.67298	-0.27691	-4.22034	-0.68177	-0.19983	4.26536	-0.30186	-0.05812
C	-4.23626	0.68541	-0.27642	-4.22046	0.68098	-0.19991	3.95223	-1.63059	-0.06378
C	-2.85719	1.09847	-0.10898	-2.84629	1.10184	-0.07832	2.51466	-1.73472	0.01534
C	-2.44500	2.43212	-0.02733	-2.44130	2.44127	-0.02157	1.80648	-2.95340	-0.04037
H	-1.33947	5.03231	0.30010	-1.34550	5.07201	0.21359	0.12165	-5.31859	-0.01262
H	1.34976	5.02606	0.31123	1.34455	5.07226	0.21368	-2.49045	-4.70205	-0.00378
H	5.08253	1.33798	-0.33910	5.06749	1.34584	-0.28750	-5.25629	-0.13370	0.00327
H	5.07861	-1.35290	-0.33827	5.06773	-1.34488	-0.28768	-4.63756	2.47484	0.02246
H	1.33500	-5.02989	0.31230	1.34550	-5.07201	0.21359	-0.13342	5.31932	-0.15732
H	-1.35424	-5.02840	0.29931	-1.34455	-5.07225	0.21368	2.48281	4.71014	-0.13176
H	-5.07913	-1.33997	-0.39641	-5.06749	-1.34584	-0.28753	5.24638	0.14264	-0.13758
H	-5.07522	1.35493	-0.39545	-5.06773	1.34488	-0.28766	4.63196	-2.46530	-0.14974
C	3.49276	-3.50542	-0.01809	3.50122	-3.49723	-0.01262	-2.61223	4.21878	-0.03807
C	3.62029	-4.36457	-1.12125	3.68530	-4.33606	-1.12285	-2.70141	5.01289	1.11507
C	4.36744	-3.66703	1.06816	4.33038	-3.66609	1.10729	-3.28046	4.63358	-1.19994
C	4.59989	-5.36057	-1.13927	4.67687	-5.32059	-1.11492	-3.44474	6.19645	1.10790
H	2.94920	-4.24234	-1.96659	3.04850	-4.20817	-1.99353	-2.18625	4.69574	2.01736
C	5.34515	-4.66511	1.05342	5.32006	-4.65245	1.11822	-4.02303	5.81748	-1.20924
H	4.27182	-3.00734	1.92577	4.19065	-3.02141	1.97027	-3.21187	4.02379	-2.09639
C	5.46479	-5.51453	-0.05103	5.49669	-5.48221	0.00646	-4.10762	6.60202	-0.05466
H	4.68881	-6.01338	-2.00314	4.80970	-5.95862	-1.98418	-3.50655	6.79930	2.00960
H	6.01052	-4.78011	1.90452	5.95041	-4.77352	1.99476	-4.53260	6.12682	-2.11754
H	6.22567	-6.28973	-0.06379	6.26678	-6.24832	0.01383	-4.68498	7.52215	-0.06108
C	3.50291	3.49533	-0.02023	3.50059	3.49786	-0.01259	-4.22275	-2.60686	0.00897
C	4.37853	3.65491	1.06557	4.32973	3.66682	1.10732	-5.01426	-2.64297	1.16794
C	3.63240	4.35365	-1.12381	3.68453	4.33675	-1.12280	-4.65177	-3.31537	-1.12440
C	5.35907	4.65018	1.04997	5.31925	4.65334	1.11827	-6.20692	-3.37024	1.19352
H	4.28139	2.99587	1.92350	4.19011	3.02208	1.97027	-4.68525	-2.10083	2.04984
C	4.61483	5.34684	-1.14269	4.67595	5.32143	-1.11485	-5.84585	-4.04069	-1.10132
H	2.96060	4.23297	-1.96880	3.04775	4.20878	-1.99348	-4.04504	-3.28964	-2.02504
C	5.48065	5.49879	-0.05490	5.49574	5.48316	0.00653	-6.62686	-4.07081	0.05829
H	6.02514	4.76365	1.90073	5.94959	4.77448	1.99481	-6.80526	-3.39173	2.10007
H	4.70524	5.99902	-2.00688	4.80867	5.95951	-1.98409	-6.16607	-4.57943	-1.98878
H	6.24374	6.27181	-0.06832	6.26572	6.24939	0.01392	-7.55457	-4.63560	0.07731
C	-3.49497	3.49720	-0.02078	-3.50122	3.49723	-0.01262	2.61086	-4.21486	-0.04064
C	-4.35851	3.63881	1.07679	-4.33039	3.66608	1.10729	3.34733	-4.59355	1.09328
C	-3.63870	4.36905	-1.11150	-3.68530	4.33607	-1.12285	2.63896	-5.04539	-1.17226
C	-5.34164	4.63160	1.08546	-5.32006	4.65244	1.11822	4.09332	-5.77476	1.09651
H	-4.25068	2.96766	1.92396	-4.19065	3.02139	1.97026	3.32624	-3.95765	1.97362
C	-4.62441	5.35934	-1.10623	-4.67687	5.32059	-1.11491	3.38767	-6.22506	-1.17186
H	-2.97595	4.26145	-1.96536	-3.04850	4.20818	-1.99353	2.07433	-4.75656	-2.05407
C	-5.47807	5.49428	-0.00675	-5.49669	5.48221	0.00646	4.11656	-6.59387	-0.03682
H	-5.99872	4.73161	1.94484	-5.95041	4.77350	1.99476	4.65310	-6.05581	1.98418
H	-4.72649	6.02255	-1.96066	-4.80970	5.95863	-1.98417	3.40320	-6.85340	-2.05802
H	-6.24352	6.26504	-0.00136	-6.26679	6.24832	0.01384	4.69753	-7.51174	-0.03538
C	-3.50507	-3.48711	-0.02293	-3.50059	-3.49786	-0.01259	4.22246	2.60620	-0.04560
C	-3.65071	-4.35811	-1.11408	-3.68453	-4.33675	-1.12280	4.63231	3.29895	-1.19568
C	-4.36955	-3.62675	1.07416	-4.32973	-3.66682	1.10732	5.03968	2.64746	1.09515
C	-4.63922	-5.34561	-1.10971	-4.67595	-5.32143	-1.11485	5.83169	4.01576	-1.20591
H	-2.98723	-4.25202	-1.96756	-3.04776	-4.20877	-1.99349	4.00687	3.26713	-2.08322
C	-5.35548	-4.61678	1.08193	-5.31924	-4.65334	1.11827	6.23779	3.36619	1.08739
H	-4.26024	-2.95627	1.92167	-4.19010	-3.02209	1.97028	4.72681	2.11547	1.98904
C	-5.49379	-5.47861	-0.01071	-5.49574	-5.48316	0.00653	6.63778	4.05223	-0.06377
H	-4.74273	-6.00818	-1.96447	-4.80867	-5.95951	-1.98410	6.13673	4.54235	-2.10591
H	-6.01326	-4.71529	1.94094	-5.94958	-4.77449	1.99481	6.85631	3.39182	1.98019
H	-6.26142	-6.24721	-0.00603	-6.26571	-6.24939	0.01392	7.56973	4.61028	-0.07078
Mn	0.03878	-0.00004	0.20114	0.00000	0.00000	0.12702	-0.00295	-0.00106	0.33624
H	-0.44265	0.00109	1.62312	0.00000	0.00000	1.64943	-0.02510	-0.03864	1.91890

NiTPP, total charge 0

		Singlet			Triplet			Quintet	
N	1.96544	-0.07716	0.00685	2.03664	0.00000	-0.02059	0.00059	2.04764	-0.03226
N	-0.06586	-1.96980	-0.00839	0.00000	-2.03692	0.00000	2.05675	-0.00059	-0.00001
N	-1.94908	0.06541	0.01149	-2.03664	0.00000	0.02059	-0.00059	-2.04764	0.03226
N	0.07549	1.95153	-0.00615	0.00000	2.03692	0.00000	-2.05676	0.00059	0.00002
C	2.83954	0.95956	0.27665	2.86126	1.10402	0.01197	-1.10043	2.87811	0.02069
C	4.19869	0.47758	0.30313	4.24265	0.68133	0.07611	-0.69204	4.23426	0.11949

C	4.15412	-0.84418	-0.01473	4.24265	-0.68135	0.07610	0.69449	4.23385	0.11951
C	2.76318	-1.18783	-0.17897	2.86126	-1.10403	0.01196	1.10209	2.87747	0.02071
C	2.31777	-2.49430	-0.38371	2.44452	-2.44468	0.01281	2.46722	2.43871	0.01672
C	0.97482	-2.84575	-0.25186	1.10412	-2.86213	0.00599	2.88549	1.10502	0.00981
C	0.50133	-4.20815	-0.23262	0.68134	-4.24490	-0.00128	4.27054	0.67860	-0.00182
C	-0.81912	-4.16168	0.09039	-0.68136	-4.24490	0.00127	4.27014	-0.68109	0.00172
C	-1.17390	-2.76830	0.19887	-1.10413	-2.86212	-0.00599	2.88485	-1.10669	-0.00985
C	-2.47623	-2.31588	0.40665	-2.44453	-2.44467	-0.01281	2.46581	-2.44013	-0.01673
C	-2.82297	-0.97263	0.26827	-2.86126	-1.10402	-0.01195	1.10043	-2.87811	-0.02072
C	-4.18674	-0.50505	0.23499	-4.24265	-0.68133	-0.07608	0.69203	-4.23426	-0.11952
C	-4.14165	0.81599	-0.08652	-4.24265	0.68135	-0.07609	-0.69450	-4.23385	-0.11951
C	-2.74858	1.16914	-0.20876	-2.86126	1.10403	-0.01196	-1.10210	-2.87747	-0.02069
C	-2.30176	2.47316	-0.42432	-2.44452	2.44468	-0.01281	-2.46722	-2.43871	-0.01668
C	-0.95962	2.82494	-0.28376	-1.10412	2.86213	-0.00600	-2.88550	-1.10502	-0.00979
C	-0.47804	4.18394	-0.30847	-0.68134	4.24490	0.00126	-4.27054	-0.67860	0.00184
C	0.84211	4.14001	0.01704	0.68136	4.24490	-0.00128	-4.27015	0.68109	-0.00173
C	1.18480	2.74961	0.18589	1.10413	2.86212	0.00599	-2.88485	1.10669	0.00984
C	2.48909	2.30308	0.40399	2.44453	2.44467	0.01281	-2.46581	2.44013	0.01670
H	5.06530	1.08228	0.52450	5.09374	1.34409	0.13017	-1.34850	5.08749	0.19979
H	4.97465	-1.54151	-0.09771	5.09374	-1.34411	0.13016	1.35146	5.08669	0.19982
H	1.11314	-5.07842	-0.41701	1.34373	-5.09792	-0.00763	5.12510	1.33843	-0.01234
H	-1.50444	-4.98570	0.22203	-1.34375	-5.09792	0.00760	5.12431	-1.34143	0.01220
H	-5.05429	-1.12407	0.41030	-5.09375	-1.34409	-0.13013	1.34849	-5.08748	-0.19983
H	-4.96458	1.50427	-0.21080	-5.09374	1.34411	-0.13014	-1.35146	-5.08669	-0.19981
H	-1.08183	5.05005	-0.53435	-1.34373	5.09792	0.00760	-5.12510	-1.33843	0.01238
H	1.53865	4.96091	0.10277	1.34375	5.09792	-0.00763	-5.12431	1.34143	-0.01221
C	-3.56033	-3.30573	0.69411	-3.50477	-3.50193	-0.02932	3.51306	-3.50246	-0.03442
C	-4.08819	-3.41585	1.98917	-4.28987	-3.74316	1.10869	3.67976	-4.35579	1.06900
C	-4.07947	-4.12314	-0.32147	-3.73381	-4.26779	-1.18290	4.34433	-3.67297	-1.15327
C	-5.11072	-4.32800	2.26521	-5.28048	-4.72876	1.09508	4.66399	-5.34622	1.05900
H	-3.69157	-2.78301	2.77805	-4.11636	-3.15459	2.00507	3.03588	-4.23277	1.93473
C	-5.10198	-5.03521	-0.04720	-4.72532	-5.25239	-1.19915	5.32245	-4.67064	-1.16760
H	-3.67985	-4.03516	-1.32776	-3.13150	-4.08366	-2.06795	4.21400	-3.02272	-2.01334
C	-5.62002	-5.14052	1.24765	-5.50139	-5.48616	-0.05953	5.48737	-5.50820	-0.06038
H	-5.50773	-4.40349	3.27368	-5.87706	-4.90547	1.98573	4.78725	-5.99123	1.92445
H	-5.49552	-5.65949	-0.84456	-4.89243	-5.83388	-2.10154	5.95304	-4.79352	-2.04366
H	-6.41517	-5.84912	1.46134	-6.27181	-6.25189	-0.07119	6.24987	-6.28180	-0.06973
C	3.33486	-3.55541	-0.65736	3.50476	-3.50195	0.02932	3.51504	3.50048	0.03441
C	3.67691	-4.50188	0.32112	3.73378	-4.26782	1.18289	4.34636	3.67058	1.15329
C	3.98294	-3.60379	-1.90118	4.28987	-3.74315	-1.10869	3.68217	4.35374	-1.06899
C	4.64172	-5.47828	0.06026	4.72529	-5.25242	1.19914	5.32498	4.66776	1.16764
H	3.18644	-4.46246	1.28948	3.13146	-4.08370	2.06793	4.21565	3.02043	2.01337
C	4.94643	-4.58128	-2.16447	5.28048	-4.72876	-1.09507	4.66690	5.34367	-1.05897
H	3.72494	-2.87118	-2.66062	4.11638	-3.15458	-2.00505	3.03822	4.23107	-1.93472
C	5.27840	-5.52157	-1.18427	5.50137	-5.48618	0.05953	5.49035	5.50522	0.06042
H	4.89837	-6.20116	0.82964	4.89238	-5.83393	2.10153	5.95560	4.79034	2.04372
H	5.43614	-4.60785	-3.13390	5.87707	-4.90546	-1.98571	4.79049	5.98863	-1.92441
H	6.02825	-6.28077	-1.38763	6.27179	-6.25191	0.07119	6.25324	6.27845	0.06978
C	3.54799	3.31793	0.69160	3.50477	3.50194	0.02933	-3.51306	3.50247	0.03435
C	3.56558	3.98573	1.92598	3.73379	4.26780	1.18291	-4.34434	3.67300	1.15319
C	4.52479	3.63799	-0.26443	4.28989	3.74314	-1.10867	-3.67975	4.35577	-1.06909
C	4.54205	4.94656	2.20199	4.72530	5.25240	1.19916	-5.32245	4.67067	1.16749
H	2.81012	3.74443	2.66829	3.13147	4.08368	2.06795	-4.21401	3.02277	2.01327
C	5.50001	4.60044	0.00899	5.28050	4.72874	-1.09505	-4.66397	5.34620	-1.05912
H	4.50969	3.13231	-1.22559	4.11640	3.15457	-2.00504	-3.03586	4.23273	-1.93481
C	5.51228	5.25664	1.24401	5.50139	5.48616	0.05955	-5.48736	5.50821	0.06026
H	4.54468	5.45115	3.16412	4.89240	5.83391	2.10155	-5.95305	4.79358	2.04354
H	6.24631	4.84002	-0.74334	5.87709	4.90544	-1.98569	-4.78722	5.99119	-1.92458
H	6.27070	6.00455	1.45723	6.27181	6.25189	0.07122	-6.24986	6.28181	0.06958
C	-3.31292	3.53106	-0.72878	-3.50476	3.50195	-0.02933	-3.51504	-3.50048	-0.03434
C	-3.95491	3.55300	-1.97664	-4.28986	3.74317	1.10868	-3.68214	-4.35373	1.06907
C	-3.65323	4.50379	0.22428	-3.73379	4.26780	-1.18292	-4.34638	-3.67060	-1.15320
C	-4.91114	4.52946	-2.26830	-5.28047	4.72878	1.09506	-4.66687	-5.34367	1.05909
H	-3.69763	2.80076	-2.71685	-4.11636	3.15461	2.00506	-3.03818	-4.23105	1.93479
C	-4.61083	5.47926	-0.06501	-4.72530	5.25240	-1.19917	-5.32500	-4.66778	-1.16752
H	-3.16676	4.48575	1.19527	-3.13149	4.08366	-2.06796	-4.21570	-3.02045	-2.01329
C	-5.24175	5.49562	-1.31307	-5.50137	5.48618	-0.05955	-5.49035	-5.50523	-0.06029
H	-5.39605	4.53527	-3.24047	-5.87704	4.90549	1.98571	-4.79044	-5.98862	1.92454
H	-4.86619	6.22268	0.68499	-4.89241	5.83389	-2.10156	-5.95564	-4.79037	-2.04358
H	-5.98596	6.25412	-1.53857	-6.27179	6.25191	-0.07122	-6.25323	-6.27846	-0.06962

Ni	0.00666	-0.00770	0.00088	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

NiTPP, total charge 1

		Doublet			Quartet			Sextet	
N	1.27603	1.52398	-0.19534	2.04309	0.00000	-0.05232	2.04157	-0.00023	-0.04180
N	1.42591	-1.20183	0.03024	0.00000	-2.04364	0.00000	-0.00022	-2.04455	0.00000
N	-1.30158	-1.36160	0.03473	-2.04309	0.00000	0.05232	-2.04157	0.00023	0.04181
N	-1.45044	1.37746	-0.19744	0.00000	2.04364	0.00000	0.00022	2.04456	-0.00001
C	1.05660	2.85062	0.02766	2.86894	1.09954	0.00447	2.86949	1.09815	0.01851
C	2.18617	3.62339	-0.42126	4.24378	0.68240	0.11528	4.23977	0.68579	0.13307
C	3.09564	2.73529	-0.92683	4.24378	-0.68240	0.11527	4.23962	-0.68671	0.13309
C	2.55834	1.41985	-0.71172	2.86894	-1.09954	0.00445	2.86924	-1.09877	0.01853
C	3.25762	0.21274	-0.84478	2.44850	-2.44895	0.01145	2.44033	-2.47036	0.01238
C	2.72200	-1.01335	-0.38206	1.09980	-2.87126	0.00671	1.10459	-2.87372	0.00461
C	3.49076	-2.20510	-0.15124	0.68235	-4.25032	-0.00581	0.67431	-4.27286	-0.00823
C	2.64777	-3.11352	0.42902	-0.68235	-4.25032	0.00585	-0.67525	-4.27271	0.00818
C	1.35725	-2.48673	0.51584	-1.09979	-2.87126	-0.00669	-1.10523	-2.87348	-0.00462
C	0.16577	-3.15166	0.87866	-2.44850	-2.44895	-0.01145	-2.44087	-2.46982	-0.01236
C	-1.09929	-2.61355	0.58446	-2.86894	-1.09954	-0.00447	-2.86949	-1.09815	-0.01849
C	-2.35288	-3.31120	0.67586	-4.24377	-0.68240	-0.11531	-4.23978	-0.68579	-0.13298
C	-3.29714	-2.50580	0.09934	-4.24377	0.68240	-0.11532	-4.23963	0.68672	-0.13296
C	-2.63080	-1.29108	-0.28004	-2.86894	1.09954	-0.00449	-2.86924	1.09877	-0.01847
C	-3.29028	-0.14208	-0.79555	-2.44850	2.44895	-0.01147	-2.44033	2.47036	-0.01233
C	-2.70589	1.12495	-0.73967	-1.09980	2.87126	-0.00671	-1.10459	2.87372	-0.00461
C	-3.35400	2.37290	-1.03768	-0.68235	4.25032	0.00584	-0.67431	4.27286	0.00817
C	-2.54734	3.36499	-0.55195	0.68235	4.25032	-0.00580	0.67525	4.27272	-0.00827
C	-1.36982	2.72369	-0.02530	1.09979	2.87126	0.00673	1.10523	2.87349	0.00457
C	-0.19454	3.38873	0.46880	2.44850	2.44895	0.01147	2.44087	2.46983	0.01233
H	2.23779	4.70157	-0.44357	5.09273	1.34163	0.21183	5.08733	1.34691	0.22732
H	4.04021	2.95681	-1.39994	5.09273	-1.34163	0.21181	5.08704	-1.34801	0.22735
H	4.53957	-2.32222	-0.37905	1.34072	-5.10506	-0.02462	1.33815	-5.12368	-0.02620
H	2.86949	-4.12423	0.73722	-1.34071	-5.10506	0.02468	-1.33928	-5.12339	0.02611
H	-2.49539	-4.28773	1.11244	-5.09273	-1.34163	-0.21187	-5.08734	-1.34690	-0.22720
H	-4.35285	-2.69878	-0.01906	-5.09273	1.34162	-0.21189	-5.08705	1.34802	-0.22718
H	-4.29908	2.48260	-1.54767	-1.34072	5.10506	0.02466	-1.33815	5.12369	0.02612
H	-2.69847	4.43031	-0.63670	1.34071	5.10506	-0.02460	1.33928	5.12339	-0.02626
C	0.27896	-4.50086	1.48888	-3.50487	-3.49819	-0.03529	-3.50297	-3.51350	-0.03285
C	-0.23470	-5.64165	0.84715	-4.39564	-3.63203	1.04405	-4.38283	-3.65123	1.05486
C	0.93806	-4.64780	2.72270	-3.62819	-4.36267	-1.13704	-3.64612	-4.36690	-1.14011
C	-0.09691	-6.90117	1.43224	-5.38175	-4.61965	1.02583	-5.37507	-4.63296	1.04018
H	-0.71417	-5.54131	-0.12169	-4.30103	-2.97123	1.90061	-4.27672	-2.99665	1.91511
C	1.05785	-5.90662	3.31306	-4.62839	-5.33584	-1.16068	-4.64859	-5.33920	-1.15817
H	1.33976	-3.77064	3.22126	-2.95045	-4.25667	-1.97888	-2.98003	-4.25515	-1.99085
C	0.54249	-7.03594	2.66889	-5.50350	-5.47018	-0.07783	-5.51223	-5.47693	-0.06717
H	-0.48387	-7.77693	0.92019	-6.05411	-4.72400	1.87193	-6.03947	-4.73926	1.89237
H	1.55451	-6.00526	4.27349	-4.72418	-5.98761	-2.02374	-4.75570	-5.98554	-2.02404
H	0.64318	-8.01596	3.12517	-6.27611	-6.23276	-0.09426	-6.28836	-6.23599	-0.07987
C	4.63862	0.20894	-1.39107	3.50488	-3.49819	0.03529	3.50220	-3.51426	0.03285
C	4.92921	-0.55879	-2.53338	3.62821	-4.36265	1.13705	3.64512	-4.36776	1.14007
C	5.67144	0.93909	-0.77684	4.39563	-3.63205	-1.04407	4.38208	-3.65213	-1.05483
C	6.22019	-0.57546	-3.06268	4.62841	-5.33582	1.16070	4.64737	-5.34029	1.15811
H	4.13643	-1.12707	-3.01071	2.95049	-4.25663	1.97890	2.97902	-4.25592	1.99078
C	6.96541	0.90586	-1.29898	5.38173	-4.61966	-1.02585	5.37410	-4.63407	-1.04017
H	5.46300	1.50656	0.12494	4.30100	-2.97126	-1.90063	4.27614	-2.99747	-1.91505
C	7.24133	0.15495	-2.44612	5.50350	-5.47018	0.07782	5.51103	-5.47814	0.06714
H	6.42858	-1.15904	-3.95419	4.72421	-5.98757	2.02376	4.75431	-5.98670	2.02394
H	7.75820	1.46123	-0.80708	6.05408	-4.72403	-1.87195	6.03851	-4.74047	-1.89234
H	8.24727	0.13478	-2.85411	6.27612	-6.23276	0.09426	6.28699	-6.23737	0.07982
C	-0.26208	4.56496	1.32920	3.50487	3.49819	0.03534	3.50298	3.51350	0.03277
C	-1.50059	5.13314	1.73761	3.62819	4.36264	1.13711	3.64611	4.36697	1.13998
C	0.91504	5.11374	1.91179	4.39564	3.63207	-1.04401	4.38286	3.65116	-1.05493
C	-1.54809	6.24055	2.57509	4.62839	5.33581	1.16078	4.64858	5.33927	1.15800
H	-2.43457	4.68891	1.42545	2.95046	4.25661	1.97895	2.98000	4.25528	1.99072
C	0.86154	6.22065	2.74977	5.38174	4.61968	-1.02576	5.37510	4.63288	-1.04030
H	1.87465	4.64595	1.73989	4.30102	2.97128	-1.90058	4.27675	2.99653	-1.91515
C	-0.36793	6.80697	3.07148	5.50349	5.47019	0.07792	5.51224	5.47692	0.06701
H	-2.51109	6.65287	2.85968	4.72418	5.98756	2.02385	4.75569	5.98566	2.02383
H	1.78021	6.61423	3.17347	6.05410	4.72405	-1.87186	6.03952	4.73912	-1.89248
H	-0.40869	7.66881	3.73033	6.27610	6.23277	0.09437	6.28838	6.23598	0.07967
C	-4.67353	-0.30895	-1.30552	-3.50487	3.49819	-0.03534	-3.50221	3.51427	-0.03278

C	-4.91803	-1.20563	-2.36224	-4.39566	3.63204	1.04399	-4.38202	3.65216	1.05495
C	-5.75464	0.39058	-0.73942	-3.62818	4.36266	-1.13710	-3.64518	4.36773	-1.14001
C	-6.21052	-1.37660	-2.85842	-5.38176	4.61966	1.02575	-5.37404	4.63410	1.04031
H	-4.08855	-1.75171	-2.80150	-4.30106	2.97125	1.90055	-4.27604	2.99753	1.91518
C	-7.04906	0.20274	-1.22621	-4.62838	5.33583	-1.16077	-4.64744	5.34025	-1.15803
H	-5.58105	1.05426	0.10188	-2.95043	4.25664	-1.97893	-2.97913	4.25587	-1.99076
C	-7.27910	-0.67449	-2.29078	-5.50350	5.47018	-0.07792	-5.51103	5.47814	-0.06701
H	-6.38366	-2.05796	-3.68579	-6.05413	4.72402	1.87183	-6.03841	4.74052	1.89252
H	-7.87772	0.73592	-0.77024	-4.72415	5.98759	-2.02383	-4.75443	5.98664	-2.02387
H	-8.28598	-0.81508	-2.67186	-6.27611	6.23276	-0.09437	-6.28700	6.23737	-0.07967
Ni	-0.01116	0.07733	-0.04836	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

H-NiTPP, total charge 0

		Doublet			Quartet			Sextet	
N	1.68989	-1.12116	-0.05917	-0.31238	-2.03206	-0.00826	1.33267	1.45776	0.03613
N	-1.12243	-1.69247	-0.06588	-1.99041	0.30660	-0.03141	1.53518	-1.38584	-0.23265
N	-1.69141	1.12119	-0.04059	0.31480	2.03235	0.01781	-1.32718	-1.65517	-0.24815
N	1.12071	1.69223	-0.04677	1.99345	-0.30628	-0.05044	-1.51262	1.19405	0.03363
C	2.98816	-0.65927	0.00231	0.65067	-3.01166	0.01299	1.06139	2.73371	0.45643
C	3.90462	-1.77282	0.10976	0.02538	-4.31726	0.06309	2.29638	3.47523	0.58077
C	3.15171	-2.90789	0.11068	-1.32087	-4.11039	0.05962	3.30081	2.64444	0.16390
C	1.76945	-2.49661	0.00449	-1.52530	-2.67719	0.00676	2.69075	1.38229	-0.17477
C	0.68339	-3.38374	-0.01702	-2.78058	-2.05156	-0.02602	3.37259	0.23680	-0.63410
C	-0.66261	-2.99200	-0.05232	-2.97748	-0.66144	-0.05917	2.80023	-1.05012	-0.72387
C	-1.77895	-3.91186	-0.07605	-4.27194	-0.03167	-0.13992	3.42900	-2.22832	-1.21260
C	-2.91364	-3.15848	-0.07231	-4.06370	1.31739	-0.13877	2.56425	-3.28717	-0.96160
C	-2.49873	-1.77307	-0.06077	-2.63972	1.52704	-0.05802	1.42196	-2.74022	-0.32550
C	-3.38288	-0.68598	-0.02777	-2.03310	2.79299	-0.03006	0.26050	-3.46968	0.20472
C	-2.99016	0.65948	-0.00233	-0.64812	3.01247	0.00123	-1.04944	-2.97365	-0.19866
C	-3.91085	1.77378	0.04005	-0.02209	4.31866	-0.00167	-2.18928	-3.74259	-0.61570
C	-3.15880	2.90940	0.04342	1.32400	4.11115	-0.00726	-3.19188	-2.84143	-0.89331
C	-1.77332	2.49752	-0.01127	1.52799	2.67707	0.00761	-2.65614	-1.53308	-0.64470
C	-0.68700	3.38376	-0.03967	2.78340	2.05152	-0.02273	-3.36386	-0.32680	-0.66272
C	0.65919	2.99098	-0.06818	2.98128	0.66149	-0.05065	-2.83748	0.93586	-0.29730
C	1.77331	3.91017	-0.14418	4.27789	0.03113	-0.05960	-3.58844	2.14709	-0.21720
C	2.90875	3.15788	-0.14300	4.06938	-1.31785	-0.06192	-2.72368	3.13516	0.20185
C	2.49660	1.77352	-0.06577	2.64327	-1.52707	-0.03937	-1.43236	2.53234	0.33850
C	3.38237	0.68642	-0.02814	2.03590	-2.79257	-0.00698	-0.23873	3.25006	0.64666
H	4.97864	-1.68949	0.18756	0.55283	-5.25907	0.10235	2.38564	4.49329	0.92931
H	3.49232	-3.92992	0.18853	-2.10653	-4.85068	0.09641	4.35811	2.86099	0.11518
H	-1.69765	-4.98871	-0.09270	-5.21467	-0.55513	-0.20066	4.39740	-2.27289	-1.68936
H	-3.93827	-3.50042	-0.07678	-4.80438	2.10130	-0.19749	2.70880	-4.32978	-1.20719
H	-4.98753	1.69012	0.06258	-0.54872	5.26166	-0.00815	-2.21956	-4.81866	-0.71055
H	-3.50267	3.93268	0.07792	2.10993	4.85179	-0.02784	-4.19788	-3.05458	-1.22502
H	1.68979	4.98530	-0.20468	5.22297	0.55383	-0.05872	-4.63702	2.25185	-0.45355
H	3.93126	3.50040	-0.20329	4.81224	-2.10176	-0.07270	-2.94599	4.17990	0.36155
C	-4.85098	-0.98351	-0.00821	-2.92948	3.99256	-0.04478	0.41289	-4.58784	1.09904
C	-5.58888	-0.85747	1.17827	-3.65915	4.35039	1.09914	-0.71395	-5.20501	1.72427
C	-5.51026	-1.39343	-1.17670	-3.05450	4.77731	-1.20126	1.69614	-5.09110	1.47256
C	-6.95830	-1.13594	1.19682	-4.49511	5.47022	1.08805	-0.56686	-6.27470	2.59747
H	-5.08222	-0.54216	2.08600	-3.56421	3.74708	1.99749	-1.70699	-4.81473	1.54135
C	-6.88000	-1.67059	-1.16017	-3.89191	5.89605	-1.21460	1.83143	-6.16094	2.34812
H	-4.94330	-1.49082	-2.09822	-2.49392	4.50285	-2.09033	2.58885	-4.62113	1.08097
C	-7.60774	-1.54293	0.02713	-4.61415	6.24599	-0.06938	0.70444	-6.77657	2.90987
H	-7.51594	-1.03645	2.12391	-5.05076	5.73666	1.98280	-1.45065	-6.71397	3.05215
H	-7.37738	-1.98418	-2.07375	-3.98092	6.49165	-2.11885	2.82665	-6.51477	2.60340
H	-8.67227	-1.75885	0.04074	-5.26446	7.11606	-0.07886	0.81507	-7.61464	3.59143
C	0.98308	-4.85031	0.01731	-3.99527	-2.92657	-0.02704	4.80438	0.39253	-1.01502
C	0.72375	-5.60655	1.17067	-4.81509	-3.01013	1.10903	5.80909	-0.33784	-0.35712
C	1.53115	-5.49195	-1.10390	-4.33282	-3.67921	-1.16240	5.17519	1.28370	-2.03665
C	1.00667	-6.97461	1.20307	-5.94729	-3.82912	1.11068	7.15063	-0.17718	-0.70912
H	0.30200	-5.11431	2.04231	-4.55648	-2.43207	1.99159	5.53030	-1.01910	0.44079
C	1.81128	-6.86069	-1.07434	-5.46646	-4.49635	-1.16326	6.51588	1.43471	-2.39689
H	1.73297	-4.91137	-1.99954	-3.70303	-3.61637	-2.04523	4.40350	1.84822	-2.55125
C	1.55051	-7.60586	0.07992	-6.27663	-4.57411	-0.02609	7.50802	0.70664	-1.73262
H	0.80402	-7.54548	2.10494	-6.56942	-3.88645	1.99948	7.91619	-0.73973	-0.18229
H	2.23136	-7.34377	-1.95212	-5.71680	-5.06949	-2.05160	6.78466	2.11980	-3.19595
H	1.76939	-8.66960	0.10405	-7.15728	-5.21009	-0.02571	8.55144	0.82797	-2.00922
C	4.84931	0.98312	-0.00883	2.92961	-3.99411	0.01245	-0.39414	4.66068	1.10132
C	5.44773	1.55689	1.12367	3.63786	-4.33789	1.17406	-1.03630	4.94030	2.32004

C	5.65125	0.69136	-1.12314	3.06896	-4.79800	-1.12906	0.07189	5.73507	0.32457
C	6.81769	1.83127	1.14300	4.46794	-5.46189	1.19435	-1.19613	6.25702	2.75677
H	4.83233	1.78266	1.98980	3.53052	-3.72055	2.06141	-1.40337	4.11577	2.92427
C	7.02061	0.96904	-1.10692	3.90055	-5.92107	-1.11099	-0.09317	7.05275	0.75790
H	5.19311	0.24902	-2.00310	2.52378	-4.53535	-2.03120	0.55269	5.53033	-0.62736
C	7.60808	1.53896	0.02698	4.60206	-6.25639	0.05131	-0.72497	7.31820	1.97689
H	7.26663	2.27104	2.02922	5.00688	-5.71726	2.10245	-1.68718	6.45358	3.70572
H	7.62676	0.74175	-1.97942	4.00086	-6.53169	-2.00398	0.26692	7.87119	0.14074
H	8.67289	1.75347	0.04080	5.24778	-7.12979	0.06634	-0.85155	8.34278	2.31479
C	-0.98324	4.85137	-0.03695	3.99655	2.92895	-0.02681	-4.80197	-0.38582	-1.06642
C	-1.52464	5.47244	-1.17296	4.37592	3.62492	1.13121	-5.14943	-0.65040	-2.39991
C	-0.72209	5.63033	1.10074	4.77116	3.07327	-1.18808	-5.82164	-0.19336	-0.12158
C	-1.79757	6.84291	-1.17267	5.50663	4.44613	1.12927	-6.49167	-0.71410	-2.78292
H	-1.72645	4.87457	-2.05714	3.78065	3.51525	2.03322	-4.36240	-0.80045	-3.13307
C	-0.99787	7.00025	1.10387	5.90070	3.89601	-1.19219	-7.16345	-0.26451	-0.50360
H	-0.30416	5.15437	1.98321	4.47988	2.53955	-2.08827	-5.55615	0.00381	0.91285
C	-1.53574	7.61068	-0.03353	6.27210	4.58430	-0.03286	-7.50218	-0.52261	-1.83573
H	-2.21243	7.30978	-2.06163	5.78954	4.97537	2.03491	-6.74637	-0.91339	-3.81997
H	-0.79388	7.58892	1.99393	6.48787	4.00044	-2.10030	-7.94276	-0.12046	0.23938
H	-1.74896	8.67584	-0.03225	7.15055	5.22331	-0.03519	-8.54564	-0.57521	-2.13287
Ni	-0.00094	-0.00067	0.05766	0.00184	0.00000	0.19720	0.00888	-0.11553	0.11339
H	0.00214	-0.01995	1.48111	0.01490	-0.02628	1.99153	0.01838	-0.33397	1.91370

H-NiTPP, total charge 1

		Singlet			Triplet			Quintet	
N	1.26516	1.47368	-0.04015	-0.00508	2.03587	-0.05393	-0.00002	2.06521	-0.01938
N	1.44642	-1.26866	-0.07628	2.03355	0.00507	-0.02284	2.01776	0.00002	-0.02671
N	-1.26516	-1.47368	-0.04015	0.00508	-2.03587	-0.05393	0.00002	-2.06521	-0.01938
N	-1.44642	1.26866	-0.07628	-2.03355	-0.00507	-0.02284	-2.01776	-0.00002	-0.02671
C	1.02231	2.77342	0.40689	-1.10584	2.85607	-0.14743	-1.09710	2.88233	0.08577
C	2.26305	3.46793	0.59595	-0.69315	4.21710	-0.38097	-0.68256	4.24617	0.31136
C	3.25707	2.62702	0.19421	0.67197	4.22051	-0.38101	0.68246	4.24619	0.31137
C	2.63965	1.38474	-0.17385	1.09144	2.86155	-0.14755	1.09703	2.88236	0.08579
C	3.35393	0.24119	-0.53491	2.43702	2.45106	-0.01982	2.43947	2.45628	-0.02084
C	2.76065	-1.01582	-0.46754	2.85082	1.10620	0.10418	2.83924	1.10363	-0.14190
C	3.46898	-2.25446	-0.61765	4.20619	0.69334	0.36375	4.18696	0.68519	-0.39944
C	2.63116	-3.24864	-0.21085	4.20960	-0.67221	0.36379	4.18698	-0.68509	-0.39945
C	1.37627	-2.63794	0.11917	2.85630	-1.09184	0.10428	2.83926	-1.10357	-0.14192
C	0.23618	-3.35891	0.48257	2.44922	-2.43887	-0.01966	2.43953	-2.45623	-0.02088
C	-1.02231	-2.77342	0.40689	1.10584	-2.85607	-0.14743	1.09710	-2.88233	0.08577
C	-2.26305	-3.46793	0.59595	0.69315	-4.21710	-0.38097	0.68256	-4.24617	0.31136
C	-3.25707	-2.62702	0.19421	-0.67197	-4.22051	-0.38101	-0.68246	-4.24619	0.31137
C	-2.63965	-1.38473	-0.17385	-1.09144	-2.86155	-0.14755	-1.09703	-2.88236	0.08579
C	-3.35393	-0.24118	-0.53490	-2.43701	-2.45106	-0.01982	-2.43947	-2.45628	-0.02084
C	-2.76065	1.01582	-0.46754	-2.85082	-1.10620	0.10418	-2.83924	-1.10363	-0.14190
C	-3.46897	2.25446	-0.61765	-4.20618	-0.69334	0.36375	-4.18696	-0.68519	-0.39944
C	-2.63116	3.24864	-0.21085	-4.20960	0.67221	0.36379	-4.18698	0.68509	-0.39945
C	-1.37626	2.63794	0.11918	-2.85630	1.09184	0.10428	-2.83926	1.10357	-0.14192
C	-0.23618	3.35891	0.48257	-2.44922	2.43887	-0.01966	-2.43953	2.45623	-0.02088
H	2.35224	4.47692	0.96904	-1.35507	5.05327	-0.54666	-1.34251	5.08524	0.47041
H	4.32192	2.80602	0.17808	1.32969	5.05998	-0.54677	1.34239	5.08527	0.47043
H	4.48564	-2.34004	-0.96959	5.03988	1.35501	0.54260	5.02290	1.34259	-0.58377
H	2.81972	-4.31118	-0.17452	5.04659	-1.32969	0.54271	5.02293	-1.34246	-0.58380
H	-2.35224	-4.47692	0.96903	1.35507	-5.05327	-0.54665	1.34252	-5.08524	0.47040
H	-4.32192	-2.80602	0.17808	-1.32969	-5.05998	-0.54677	-1.34239	-5.08527	0.47043
H	-4.48563	2.34005	-0.96960	-5.03988	-1.35501	0.54260	-5.02290	-1.34259	-0.58377
H	-2.81972	4.31118	-0.17452	-5.04659	1.32969	0.54271	-5.02293	1.34246	-0.58380
C	0.38652	-4.79019	0.86426	3.50355	-3.48647	-0.00663	3.50302	-3.49399	-0.01224
C	-0.18642	-5.81204	0.08895	3.50205	-4.48874	0.98067	3.52448	-4.50334	-0.99233
C	1.13435	-5.13179	2.00346	4.51748	-3.48873	-0.98203	4.50266	-3.48158	0.97809
C	-0.01751	-7.15009	0.45034	4.49960	-5.46408	0.99727	4.52966	-5.47088	-0.98694
H	-0.74615	-5.55588	-0.80577	2.72968	-4.48577	1.74376	2.76437	-4.51113	-1.76763
C	1.29158	-6.47003	2.36948	5.49994	-4.47935	-0.97595	5.49332	-4.46387	0.99330
H	1.58136	-4.34565	2.60516	4.51801	-2.72488	-1.75368	4.48476	-2.71325	1.74510
C	0.71727	-7.48146	1.59324	5.49689	-5.46536	0.01634	5.51254	-5.45710	0.00844
H	-0.45532	-7.93231	-0.16234	4.49842	-6.22169	1.77495	4.54610	-6.23388	-1.75917
H	1.86173	-6.72178	3.25854	6.26657	-4.48148	-1.74474	6.24853	-4.45438	1.77326
H	0.84427	-8.52217	1.87533	6.26733	-6.23030	0.02517	6.28900	-6.21592	0.01643
C	4.79724	0.38182	-0.87556	3.48604	3.50397	-0.00693	3.50294	3.49406	-0.01217
C	5.79621	-0.17921	-0.06295	4.49987	3.51125	-0.98240	4.50257	3.48166	0.97818

C	5.17089	1.11589	-2.01346	3.47957	4.50630	0.98029	3.52440	4.50343	-0.99225
C	7.14417	-0.01390	-0.38759	5.47735	4.50679	-0.97647	5.49321	4.46396	0.99341
H	5.51456	-0.72779	0.83103	4.50419	2.74734	-1.75399	4.48467	2.71332	1.74517
C	6.51918	1.26924	-2.34267	4.47222	5.48663	0.99674	4.52957	5.47098	-0.98683
H	4.40202	1.55474	-2.64283	2.70730	4.49950	1.74345	2.76431	4.51122	-1.76756
C	7.50802	0.70600	-1.53006	5.46942	5.49285	0.01574	5.51243	5.45720	0.00857
H	7.90857	-0.44293	0.25316	6.24391	4.51271	-1.74531	6.24841	4.45447	1.77339
H	6.79624	1.82816	-3.23133	4.46730	6.24428	1.77437	4.54600	6.23399	-1.75905
H	8.55639	0.83019	-1.78361	6.23599	6.26166	0.02445	6.28888	6.21604	0.01659
C	-0.38652	4.79019	0.86426	-3.50355	3.48647	-0.00663	-3.50302	3.49399	-0.01224
C	-1.13435	5.13179	2.00346	-4.51748	3.48873	-0.98203	-4.50266	3.48158	0.97810
C	0.18641	5.81205	0.08894	-3.50205	4.48874	0.98067	-3.52448	4.50333	-0.99233
C	-1.29158	6.47003	2.36948	-5.49994	4.47935	-0.97595	-5.49332	4.46387	0.99330
H	-1.58135	4.34565	2.60517	-4.51800	2.72488	-1.75368	-4.48475	2.71325	1.74510
C	0.01750	7.15009	0.45033	-4.49961	5.46407	0.99727	-4.52967	5.47087	-0.98694
H	0.74613	5.55588	-0.80577	-2.72968	4.48577	1.74377	-2.76438	4.51113	-1.76763
C	-0.71727	7.48146	1.59324	-5.49690	5.46536	0.01634	-5.51254	5.45709	0.00844
H	-1.86172	6.72178	3.25855	-6.26657	4.48148	-1.74474	-6.24853	4.45438	1.77326
H	0.45530	7.93232	-0.16235	-4.49843	6.22169	1.77495	-4.54610	6.23387	-1.75918
H	-0.84428	8.52218	1.87532	-6.26733	6.23030	0.02517	-6.28901	6.21591	0.01643
C	-4.79724	-0.38182	-0.87556	-3.48604	-3.50397	-0.00693	-3.50294	-3.49406	-0.01217
C	-5.17089	-1.11588	-2.01347	-3.47957	-4.50630	0.98029	-3.52440	-4.50343	-0.99225
C	-5.79622	0.17919	-0.06294	-4.49987	-3.51124	-0.98240	-4.50257	-3.48165	0.97818
C	-6.51917	-1.26924	-2.34267	-4.47221	-5.48663	0.99674	-4.52957	-5.47098	-0.98683
H	-4.40202	-1.55473	-2.64284	-2.70728	-4.49951	1.74344	-2.76431	-4.51122	-1.76756
C	-7.14417	0.01388	-0.38759	-5.47736	-4.50679	-0.97647	-5.49321	-4.46396	0.99341
H	-5.51456	0.72777	0.83104	-4.50420	-2.74733	-1.75398	-4.48467	-2.71332	1.74517
C	-7.50802	-0.70601	-1.53006	-5.46942	-5.49285	0.01574	-5.51243	-5.45720	0.00857
H	-6.79623	-1.82815	-3.23134	-4.46729	-6.24429	1.77436	-4.54600	-6.23399	-1.75905
H	-7.90857	0.44290	0.25317	-6.24392	-4.51270	-1.74530	-6.24841	-4.45447	1.77339
H	-8.55639	-0.83020	-1.78361	-6.23599	-6.26166	0.02445	-6.28888	-6.21604	0.01659
Ni	0.00000	0.00000	0.01342	0.00000	0.00000	0.02528	0.00000	0.00000	0.12022
H	0.00000	0.00000	1.43645	0.00000	0.00000	1.45198	0.00000	-0.00002	1.93428

PbTPP, total charge 0

		Singlet			Triplet			Quintet	
N	-2.08767	-0.00005	0.00965	2.09774	0.00262	-0.03787	-2.09485	0.00006	0.16279
N	0.00646	-2.09011	-0.04099	-0.00568	2.09846	-0.09866	-0.00383	-2.09552	0.10263
N	2.09234	0.00004	-0.09265	-2.09499	-0.00260	-0.15285	2.09389	-0.00006	0.04415
N	0.00637	2.09010	-0.04099	-0.00044	-2.09846	-0.09867	-0.00372	2.09551	0.10263
C	-2.87867	1.10917	-0.16098	2.89709	-1.10473	-0.21222	-2.91533	1.11203	0.18416
C	-4.23716	0.68282	-0.43096	4.22639	-0.68835	-0.50694	-4.29808	0.68491	0.20039
C	-4.23713	-0.68300	-0.43097	4.22466	0.69889	-0.50694	-4.29811	-0.68468	0.20039
C	-2.87862	-1.10929	-0.16098	2.89432	1.11196	-0.21222	-2.91539	-1.11188	0.18415
C	-2.44556	-2.45508	-0.17624	2.43885	2.48098	-0.19810	-2.47372	-2.46673	0.19055
C	-1.10159	-2.89214	-0.16774	1.10478	2.91705	-0.16772	-1.11750	-2.90789	0.18675
C	-0.67189	-4.26419	-0.35337	0.66633	4.30064	-0.24901	-0.69286	-4.28426	0.32327
C	0.69387	-4.25971	-0.36092	-0.69519	4.29424	-0.25866	0.67669	-4.28881	0.30960
C	1.11723	-2.88762	-0.16454	-1.12232	2.90873	-0.15937	1.10724	-2.91253	0.18813
C	2.46301	-2.45360	-0.16939	-2.45636	2.47080	-0.18311	2.46128	-2.46958	0.19748
C	2.89954	-1.10915	-0.16555	-2.91484	1.10421	-0.18902	2.89949	-1.11239	0.18661
C	4.28181	-0.68278	-0.26344	-4.27644	0.68823	-0.24199	4.26224	-0.68490	0.41721
C	4.28179	0.68295	-0.26345	-4.27471	-0.69888	-0.24198	4.26228	0.68468	0.41721
C	2.89949	1.10926	-0.16555	-2.91207	-1.11147	-0.18902	2.89955	1.11223	0.18660
C	2.46291	2.45369	-0.16940	-2.45019	-2.47690	-0.18312	2.46142	2.46944	0.19747
C	1.11711	2.88766	-0.16456	-1.11506	-2.91150	-0.15939	1.10740	2.91247	0.18813
C	0.69370	4.25972	-0.36094	-0.68449	-4.29594	-0.25868	0.67692	4.28876	0.30962
C	-0.67206	4.26415	-0.35339	0.67704	-4.29895	-0.24902	-0.69264	4.28429	0.32330
C	-1.10171	2.89209	-0.16774	1.11206	-2.91428	-0.16774	-1.11735	2.90794	0.18677
C	-2.44565	2.45497	-0.17624	2.44504	-2.47489	-0.19810	-2.47359	2.46686	0.19056
H	-5.06726	1.34228	-0.63943	5.05777	-1.34121	-0.72834	-5.15574	1.34097	0.20717
H	-5.06720	-1.34249	-0.63944	5.05440	1.35383	-0.72835	-5.15581	-1.34069	0.20717
H	-1.32619	-5.11312	-0.48679	1.31725	5.16013	-0.31043	-1.35151	-5.13258	0.43614
H	1.35407	-5.10119	-0.51386	-1.35468	5.14521	-0.34649	1.33046	-5.14381	0.39472
H	5.13713	-1.33909	-0.33095	-5.13774	1.33871	-0.27645	5.09866	-1.34318	0.59987
H	5.13707	1.33929	-0.33095	-5.13439	-1.35150	-0.27644	5.09873	1.34291	0.59986
H	1.35386	5.10123	-0.51389	-1.34186	-5.14855	-0.34652	1.33073	5.14373	0.39475
H	-1.32640	5.11306	-0.48681	1.33010	-5.15682	-0.31044	-1.35124	5.13264	0.43619

C	3.51235	-3.51889	-0.25213	-3.51338	3.52471	-0.23506	3.52558	-3.51112	0.29205
C	4.26540	-3.69914	-1.42336	-4.30339	3.68941	-1.38462	4.42062	-3.71178	-0.77217
C	3.75144	-4.36831	0.83963	-3.73205	4.37192	0.86294	3.66838	-4.29694	1.44794
C	5.23624	-4.70110	-1.50012	-5.28256	4.68372	-1.43738	5.42647	-4.67760	-0.68739
H	4.07943	-3.05171	-2.27546	-4.13924	3.03698	-2.23701	4.32045	-3.10570	-1.66812
C	4.72310	-5.36991	0.76564	-4.71744	5.36144	0.81390	4.67630	-5.26028	1.53588
H	3.17105	-4.23662	1.74839	-3.12670	4.24765	1.75619	2.98816	-4.14102	2.28021
C	5.46901	-5.53918	-0.40497	-5.49433	5.52163	-0.33731	5.55772	-5.45523	0.46758
H	5.80676	-4.82924	-2.41584	-5.87882	4.80452	-2.33746	6.10568	-4.82293	-1.52285
H	4.89760	-6.01567	1.62177	-4.87739	6.00520	1.67428	4.77558	-5.85446	2.44004
H	6.22374	-6.31823	-0.46397	-6.25844	6.29266	-0.37749	6.34078	-6.20502	0.53530
C	-3.51285	-3.49840	-0.30288	3.50684	3.51919	-0.29212	-3.52370	-3.52568	0.23633
C	-3.68925	-4.21043	-1.50000	3.61951	4.34158	-1.42507	-3.70410	-4.40136	-0.84752
C	-4.37302	-3.76636	0.77341	4.43557	3.67500	0.75062	-4.34705	-3.67443	1.36509
C	-4.69695	-5.17132	-1.61632	4.62972	5.30311	-1.50934	-4.68439	-5.39582	-0.80695
H	-3.03497	-3.99986	-2.34106	2.91633	4.21461	-2.24282	-3.07152	-4.29456	-1.72414
C	-5.38040	-4.72833	0.65988	5.43889	4.64272	0.67149	-5.32484	-4.67123	1.40891
H	-4.24568	-3.21588	1.70123	4.36248	3.03365	1.62395	-4.20979	-3.00649	2.21051
C	-5.54503	-5.43436	-0.53577	5.54001	5.45957	-0.45980	-5.49791	-5.53449	0.32218
H	-4.82209	-5.70996	-2.55154	4.70684	5.92609	-2.39602	-4.81355	-6.05989	-1.65710
H	-6.03477	-4.92570	1.50443	6.14237	4.75726	1.49141	-5.94807	-4.77552	2.29272
H	-6.32860	-6.18132	-0.62567	6.32387	6.20885	-0.52385	-6.25907	-6.30876	0.35534
C	-3.51299	3.49825	-0.30287	3.51562	-3.51043	-0.29212	-3.52351	3.52586	0.23636
C	-3.68944	4.21025	-1.49999	3.63035	-4.33252	-1.42507	-3.70386	4.40156	-0.84749
C	-4.37316	3.76619	0.77343	4.44472	-3.66392	0.75064	-4.34686	3.67465	1.36512
C	-4.69718	5.17111	-1.61631	4.64296	-5.29153	-1.50933	-4.68409	5.39608	-0.80692
H	-3.03516	3.99971	-2.34106	2.92687	-4.20730	-2.24283	-3.07128	4.29475	-1.72411
C	-5.38057	4.72812	0.65991	5.45044	-4.62914	0.67152	-5.32459	4.67150	1.40894
H	-4.24578	3.21573	1.70126	4.37001	-3.02276	1.62397	-4.20964	3.00669	2.21053
C	-5.54525	5.43413	-0.53575	5.55361	-5.44573	-0.45977	-5.49761	5.53478	0.32222
H	-4.82236	5.70973	-2.55153	4.72164	-5.91432	-2.39601	-4.81322	6.06017	-1.65706
H	-6.03494	4.92547	1.50447	6.15419	-4.74194	1.49144	-5.94782	4.77582	2.29275
H	-6.32885	6.18106	-0.62565	6.33934	-6.19305	-0.52382	-6.25872	6.30910	0.35539
C	3.51220	3.51902	-0.25215	-3.50457	-3.53344	-0.23507	3.52577	3.51093	0.29203
C	4.26525	3.69930	-1.42337	-4.29417	-3.70012	-1.38463	4.42080	3.71154	-0.77220
C	3.75126	4.36847	0.83960	-3.72111	-4.38121	0.86292	3.66863	4.29674	1.44792
C	5.23606	4.70130	-1.50014	-5.27085	-4.69688	-1.43739	5.42671	4.67730	-0.68744
H	4.07932	3.05185	-2.27547	-4.13165	-3.04727	-2.23701	4.32058	3.10547	-1.66815
C	4.72287	5.37011	0.76561	-4.70403	-5.37318	0.81388	4.67661	5.26001	1.53585
H	3.17086	4.23677	1.74836	-3.11607	-4.25543	1.75617	2.98842	4.14085	2.28020
C	5.46878	5.53940	-0.40500	-5.48053	-5.53531	-0.33733	5.55802	5.45492	0.46753
H	5.80658	4.82945	-2.41585	-5.86681	-4.81915	-2.33747	6.10591	4.82260	-1.52290
H	4.89733	6.01589	1.62173	-4.86237	-6.01735	1.67427	4.77594	5.85418	2.44001
H	6.22348	6.31848	-0.46400	-6.24270	-6.30825	-0.37750	6.34113	6.20466	0.53524
Pb	0.02085	0.00001	1.17335	-0.01560	-0.00004	1.08966	-0.01828	0.00001	-1.09022

PbTPP, total charge 1

		Doublet			Quartet			Sextet	
N	2.09014	-0.00003	0.01047	2.05006	-0.01717	-0.00052	2.16641	0.00043	0.12138
N	-0.00446	2.08865	-0.07251	0.01868	2.04985	0.00056	0.03025	2.08030	0.07678
N	-2.08703	0.00003	-0.15693	-2.04982	0.01750	0.00050	-2.08631	-0.00040	-0.03132
N	-0.00453	-2.08865	-0.07251	-0.01803	-2.04957	-0.00021	0.03105	-2.08029	0.07679
C	2.88661	-1.10595	-0.16255	2.89170	-1.12396	-0.00086	2.98111	-1.14527	0.14885
C	4.23787	-0.68345	-0.44846	4.29642	-0.65606	-0.00039	4.32451	-0.73344	0.05042
C	4.23789	0.68332	-0.44845	4.30618	0.58088	0.00085	4.32423	0.73513	0.05044
C	2.88665	1.10586	-0.16255	2.91031	1.07338	-0.00051	2.98067	1.14644	0.14888
C	2.44946	2.45804	-0.18742	2.47427	2.43185	0.00077	2.50599	2.48227	0.19796
C	1.10052	2.90030	-0.17738	1.12389	2.89125	0.00045	1.12069	2.89143	0.21899
C	0.67466	4.27206	-0.33467	0.65698	4.29544	-0.00018	0.69235	4.25515	0.43828
C	-0.69182	4.26635	-0.35329	-0.58148	4.30627	0.00001	-0.67648	4.25691	0.40365
C	-1.11148	2.89485	-0.17889	-1.07257	2.91073	0.00046	-1.09868	2.89619	0.20056
C	-2.46359	2.45566	-0.18870	-2.43172	2.47550	-0.00049	-2.45267	2.45895	0.18624
C	-2.90421	1.10529	-0.18281	-2.89171	1.12336	0.00048	-2.88708	1.11242	0.13716
C	-4.28660	0.68333	-0.20406	-4.29566	0.65616	-0.00073	-4.25659	0.67854	0.38432
C	-4.28662	-0.68320	-0.20406	-4.30670	-0.58211	0.00001	-4.25632	-0.68017	0.38435
C	-2.90424	-1.10521	-0.18281	-2.91230	-1.07306	-0.00025	-2.88664	-1.11351	0.13719
C	-2.46367	-2.45558	-0.18869	-2.47483	-2.43124	0.00077	-2.45171	-2.45988	0.18630
C	-1.11157	-2.89482	-0.17889	-1.12460	-2.89231	0.00072	-1.09756	-2.89661	0.20059
C	-0.69196	-4.26633	-0.35329	-0.65651	-4.29637	-0.00055	-0.67482	-4.25717	0.40361
C	0.67452	-4.27209	-0.33467	0.58132	-4.30561	-0.00002	0.69401	-4.25488	0.43823

C	1.10043	-2.90033	-0.17738	1.07315	-2.91163	0.00003	1.12182	-2.89101	0.21893
C	2.44938	-2.45812	-0.18742	2.43219	-2.47465	0.00097	2.50696	-2.48129	0.19789
H	5.06481	-1.34057	-0.67197	5.13955	-1.32192	-0.00066	5.18663	-1.37280	-0.07285
H	5.06485	1.34041	-0.67197	5.13753	1.32850	-0.00042	5.18610	1.37483	-0.07281
H	1.32636	5.12625	-0.43670	1.34910	5.13051	-0.00033	1.34674	5.09611	0.61046
H	-1.34893	5.11069	-0.49723	-1.35610	5.12809	-0.00069	-1.33432	5.10309	0.53010
H	-5.14508	1.33770	-0.20859	-5.13913	1.32236	0.00059	-5.08650	1.33999	0.58336
H	-5.14512	-1.33754	-0.20860	-5.13741	-1.32680	-0.00032	-5.08597	-1.34195	0.58342
H	-1.34909	-5.11066	-0.49722	-1.34857	-5.12928	-0.00027	-1.33234	-5.10361	0.53006
H	1.32620	-5.12630	-0.43669	1.35570	-5.12763	-0.00071	1.34872	-5.09560	0.61039
C	-3.51008	3.51481	-0.24975	-3.55108	3.54043	0.00062	-3.51756	3.49766	0.31182
C	-4.36031	3.61849	-1.36433	-4.89069	3.15116	0.00055	-4.39225	3.74176	-0.75944
C	-3.65205	4.43095	0.80691	-3.21767	4.89460	0.00030	-3.67910	4.22279	1.50390
C	-5.32925	4.62160	-1.42123	-5.89810	4.11722	-0.00109	-5.40181	4.70070	-0.64490
H	-4.24595	2.92316	-2.19055	-5.15429	2.08305	-0.00026	-4.27373	3.18406	-1.68425
C	-4.63460	5.42107	0.75550	-4.22575	5.86017	0.00048	-4.69447	5.17485	1.62011
H	-2.99981	4.35516	1.67198	-2.16294	5.20113	-0.00042	-3.01588	4.02783	2.34168
C	-5.47249	5.52118	-0.35983	-5.56562	5.47174	0.00012	-5.55584	5.41812	0.54538
H	-5.97035	4.70106	-2.29391	-6.95337	3.81021	-0.00177	-6.06581	4.88650	-1.48379
H	-4.74445	6.11359	1.58449	-3.96186	6.92855	0.00059	-4.81464	5.72257	2.55002
H	-6.23122	6.29658	-0.40244	-6.35877	6.23304	0.00026	-6.34303	6.16041	0.63575
C	3.51513	3.49383	-0.30598	3.54688	3.54461	0.00074	3.53903	3.55072	0.26459
C	3.62087	4.29313	-1.45716	3.21206	4.89897	-0.00062	3.64652	4.50764	-0.75997
C	4.44514	3.66427	0.73389	4.88739	3.15637	0.00076	4.43007	3.61693	1.35140
C	4.63681	5.24445	-1.56375	4.21767	5.86640	-0.00052	4.62751	5.49942	-0.70354
H	2.91855	4.15185	-2.27323	2.15505	5.20332	-0.00083	2.96305	4.46625	-1.60324
C	5.44861	4.62943	0.63217	5.89324	4.12397	-0.00024	5.40449	4.61588	1.41134
H	4.37085	3.04714	1.62452	5.15174	2.08931	0.00172	4.34055	2.89609	2.15942
C	5.54862	5.41919	-0.51760	5.55731	5.47801	0.00074	5.50787	5.55712	0.38258
H	4.71745	5.84624	-2.46389	3.95235	6.93275	-0.00092	4.70515	6.22588	-1.50687
H	6.15231	4.76206	1.44832	6.94983	3.81921	0.00074	6.07650	4.66248	2.26302
H	6.33426	6.16406	-0.59942	6.34977	6.24053	-0.00029	6.26625	6.33269	0.42793
C	3.51502	-3.49394	-0.30598	3.55150	-3.54030	0.00066	3.54043	-3.54933	0.26449
C	3.62074	-4.29324	-1.45716	3.21823	-4.89308	-0.00032	3.64834	-4.50614	-0.76013
C	4.44503	-3.66441	0.73389	4.89049	-3.15076	-0.00049	4.43147	-3.61524	1.35131
C	4.63665	-5.24459	-1.56376	4.22444	-5.85939	0.00127	4.62973	-5.49752	-0.70373
H	2.91842	-4.15193	-2.27324	2.16255	-5.20117	-0.00026	2.96488	-4.46498	-1.60341
C	5.44847	-4.62960	0.63216	5.89759	-4.11670	-0.00067	5.40628	-4.61380	1.41123
H	4.37076	-3.04728	1.62451	5.15390	-2.08327	-0.00001	4.34163	-2.89449	2.15937
C	5.54846	-5.41937	-0.51761	5.56478	-5.47178	0.00051	5.51007	-5.55494	0.38242
H	4.71727	-5.84638	-2.46390	3.96237	-6.92735	0.00049	4.70769	-6.22391	-1.50710
H	6.15217	-4.76225	1.44831	6.95438	-3.80998	-0.00029	6.07828	-4.66018	2.26293
H	6.33407	-6.16425	-0.59943	6.35875	-6.23272	-0.00099	6.26877	-6.33020	0.42775
C	-3.51019	-3.51471	-0.24974	-3.54663	-3.54378	-0.00065	-3.51620	-3.49900	0.31193
C	-4.36042	-3.61836	-1.36432	-4.88707	-3.15692	-0.00067	-4.39084	-3.74344	-0.75928
C	-3.65219	-4.43083	0.80692	-3.21225	-4.89761	0.00061	-3.67741	-4.22417	1.50403
C	-5.32940	-4.62144	-1.42122	-5.89220	-4.12363	0.00125	-5.40002	-4.70277	-0.64469
H	-4.24603	-2.92304	-2.19055	-5.15156	-2.08860	0.00065	-4.27258	-3.18571	-1.68411
C	-4.63478	-5.42092	0.75551	-4.21800	-5.86575	-0.00012	-4.69241	-5.17663	1.62030
H	-2.99995	-4.35506	1.67199	-2.15668	-5.20296	0.00056	-3.01423	-4.02895	2.34179
C	-5.47266	-5.52101	-0.35982	-5.55819	-5.47761	-0.00032	-5.55373	-5.42024	0.54560
H	-5.97049	-4.70088	-2.29391	-6.94885	-3.81918	0.00167	-6.06399	-4.88883	-1.48354
H	-4.74465	-6.11343	1.58451	-3.95319	-6.93286	-0.00022	-4.81232	-5.72438	2.55022
H	-6.23142	-6.29639	-0.40242	-6.35066	-6.24048	-0.00051	-6.34063	-6.16283	0.63602
Pb	-0.02579	0.00001	1.14890	0.00018	-0.00044	-0.00032	-0.03778	-0.00005	-1.16933

H-PbTPP, total charge 0

		Doublet			Quartet			Sextet	
N	1.00147	-1.80162	-0.07417	1.34728	1.63548	-0.13835	-1.68765	-1.32696	0.15700
N	-1.79103	-1.06047	-0.04692	1.68098	-1.32924	-0.13486	-1.36721	1.63676	0.17437
N	-1.00149	1.80161	-0.07412	-1.27768	-1.66694	-0.43172	1.61612	1.35202	0.33872
N	1.79102	1.06046	-0.04689	-1.60080	1.34831	-0.40398	1.30066	-1.64566	0.36003
C	2.28418	-1.91574	-0.61399	1.01679	2.96002	0.02610	-1.63480	-2.68216	0.20158
C	2.54263	-3.31195	-0.79599	2.21007	3.74545	-0.05100	-2.91587	-3.21637	0.58544
C	1.44069	-4.00990	-0.35887	3.25842	2.88075	-0.27431	-3.75030	-2.14113	0.77026
C	0.46410	-3.05688	0.08933	2.72699	1.55546	-0.31478	-2.98383	-0.95559	0.48483
C	-0.89105	-3.32308	0.49209	3.47629	0.37594	-0.49993	-3.47251	0.36441	0.56744
C	-1.92113	-2.42709	0.00675	2.98656	-0.94304	-0.45265	-2.72980	1.55406	0.40880
C	-3.16013	-2.77289	-0.61909	3.74320	-2.12354	-0.71147	-3.27550	2.88666	0.48352
C	-3.75860	-1.60449	-1.04600	2.90941	-3.20630	-0.51531	-2.23732	3.76090	0.28428

C	-2.91214	-0.51777	-0.67688	1.62863	-2.69498	-0.15511	-1.05253	2.95991	0.09350
C	-3.15896	0.85379	-0.90009	0.40922	-3.46173	0.03620	0.30010	3.43647	-0.03592
C	-2.28420	1.91575	-0.61395	-0.80964	-2.96468	-0.59513	1.33523	2.64773	0.65549
C	-2.54265	3.31196	-0.79591	-1.69403	-3.64605	-1.43804	2.17933	3.08277	1.72493
C	-1.44071	4.00990	-0.35878	-2.73333	-2.75777	-1.76556	3.01732	2.02286	2.02097
C	-0.46411	3.05687	0.08939	-2.48681	-1.54475	-1.10763	2.67963	0.95941	1.11903
C	0.89104	3.32306	0.49215	-3.33203	-0.35474	-1.04623	3.33808	-0.33658	1.00112
C	1.92112	2.42707	0.00679	-2.71367	0.96629	-1.14596	2.45609	-1.49172	1.09808
C	3.16014	2.77289	-0.61900	-3.13879	2.07682	-1.88532	2.62463	-2.63504	1.94264
C	3.75860	1.60450	-1.04594	-2.31165	3.16299	-1.54664	1.58670	-3.50652	1.65601
C	2.91213	0.51777	-0.67686	-1.37772	2.70408	-0.61229	0.79377	-2.87837	0.64956
C	3.15894	-0.85379	-0.90011	-0.33227	3.44981	0.08822	-0.40977	-3.43037	0.00351
H	3.44291	-3.72266	-1.22922	2.24718	4.82425	-0.02455	-3.13164	-4.26126	0.75789
H	1.28253	-5.07666	-0.41386	4.29763	3.13809	-0.41619	-4.77771	-2.15747	1.10409
H	-3.50321	-3.77902	-0.80670	4.77457	-2.14188	-1.03169	-4.30922	3.13188	0.67932
H	-4.68175	-1.50939	-1.59920	3.13881	-4.24976	-0.67365	-2.26510	4.84015	0.32822
H	-3.44293	3.72268	-1.22913	-1.56476	-4.65876	-1.79345	2.13604	4.05194	2.20289
H	-1.28255	5.07665	-0.41374	-3.56435	-2.94852	-2.42915	3.77937	1.97077	2.78592
H	3.50323	3.77903	-0.80656	-3.94630	2.07593	-2.60344	3.41361	-2.75940	2.67093
H	4.68176	1.50941	-1.59912	-2.35218	4.16023	-1.96117	1.38288	-4.47007	2.10272
C	-4.48246	1.20673	-1.50215	0.42675	-4.72214	0.75691	0.63235	4.67124	-0.71719
C	-4.55590	1.73949	-2.79888	-0.73520	-5.53856	0.87196	1.92154	5.26463	-0.61412
C	-5.67178	1.00479	-0.78447	1.57993	-5.16493	1.46918	-0.29384	5.30619	-1.59307
C	-5.79111	2.06495	-3.36498	-0.71774	-6.73667	1.57714	2.23556	6.43954	-1.28892
H	-3.63911	1.89062	-3.36126	-1.66165	-5.21208	0.41892	2.68032	4.79250	-0.00216
C	-6.90696	1.33455	-1.34777	1.58774	-6.36296	2.17447	0.02809	6.48102	-2.26337
H	-5.62053	0.59221	0.21885	2.46669	-4.54471	1.49460	-1.25821	4.84682	-1.77465
C	-6.97019	1.86508	-2.64019	0.44577	-7.17241	2.22341	1.29059	7.06851	-2.10927
H	-5.83178	2.47086	-4.37184	-1.62572	-7.33085	1.63423	3.22871	6.86632	-1.17876
H	-7.81811	1.17835	-0.77713	2.48867	-6.66113	2.70386	-0.70438	6.93307	-2.92660
H	-7.93059	2.11952	-3.07936	0.45496	-8.10821	2.77425	1.53995	7.98527	-2.63514
C	-1.21863	-4.53579	1.25570	4.93712	0.54125	-0.77125	-4.92820	0.51613	0.88043
C	-2.55242	-4.93285	1.53557	5.89150	0.10499	0.16115	-5.33909	1.02984	2.12029
C	-0.20046	-5.31596	1.86695	5.37502	1.13313	-1.96668	-5.90253	0.13863	-0.05623
C	-2.83921	-6.07335	2.28273	7.25586	0.26362	-0.09325	-6.69767	1.16193	2.41774
H	-3.38128	-4.32876	1.19451	5.55673	-0.35261	1.08732	-4.58762	1.31695	2.84983
C	-0.49089	-6.45636	2.61180	6.73953	1.28241	-2.22543	-7.26117	0.27968	0.23742
H	0.83362	-5.00458	1.79248	4.63995	1.46737	-2.69282	-5.58844	-0.26107	-1.01597
C	-1.81384	-6.86229	2.81293	7.68355	0.85067	-1.28826	-7.66238	0.78993	1.47605
H	-3.87786	-6.33778	2.46315	7.98301	-0.07103	0.64110	-7.00129	1.55345	3.38446
H	0.32567	-7.01919	3.05645	7.06401	1.73391	-3.15859	-8.00438	-0.00954	-0.50021
H	-2.04045	-7.75022	3.39550	8.74449	0.97016	-1.48811	-8.71865	0.89567	1.70620
C	4.48245	-1.20672	-1.50217	-0.63337	4.69114	0.80071	-0.38267	-4.70525	-0.67318
C	5.67177	-1.00479	-0.78449	-1.85948	5.38888	0.63773	0.79075	-5.51289	-0.70727
C	4.55589	-1.73946	-2.79890	0.26237	5.20904	1.77753	-1.50668	-5.18154	-1.40989
C	6.90695	-1.33454	-1.34778	-2.12968	6.56072	1.33828	0.81455	-6.72928	-1.37959
H	5.62051	-0.59222	0.21884	-2.61258	4.99931	-0.03223	1.68799	-5.17078	-0.20582
C	5.79110	-2.06492	-3.36500	-0.01587	6.37744	2.47994	-1.47361	-6.40027	-2.07701
H	3.63910	-1.89058	-3.36129	1.16668	4.66392	2.01783	-2.39762	-4.56889	-1.48010
C	6.97019	-1.86505	-2.64021	-1.20718	7.07659	2.25542	-0.31867	-7.19417	-2.06020
H	7.81810	-1.17835	-0.77714	-3.07579	7.06928	1.17462	1.72694	-7.31940	-1.37846
H	5.83177	-2.47081	-4.37187	0.69367	6.73339	3.22188	-2.35004	-6.72855	-2.62919
H	7.93058	-2.11949	-3.07938	-1.42415	7.98856	2.80365	-0.29601	-8.14540	-2.58347
C	1.21864	4.53578	1.25571	-4.76860	-0.47965	-0.85354	4.77549	-0.46367	0.94818
C	0.20049	5.31601	1.86692	-5.40048	-1.74347	-0.64775	5.63155	0.67621	0.91023
C	2.55245	4.93281	1.53556	-5.62565	0.65853	-0.76198	5.41498	-1.73351	0.83799
C	0.49095	6.45643	2.61173	-6.77110	-1.85801	-0.44570	7.01385	0.54922	0.83394
H	-0.83361	5.00466	1.79245	-4.79920	-2.64127	-0.61480	5.19953	1.66974	0.91759
C	2.83927	6.07333	2.28267	-6.99572	0.53493	-0.56150	6.79810	-1.85040	0.76158
H	3.38128	4.32869	1.19451	-5.20232	1.65138	-0.82148	4.81186	-2.63191	0.78568
C	1.81392	6.86233	2.81284	-7.59223	-0.72397	-0.41853	7.61771	-0.71383	0.77422
H	-0.32559	7.01930	3.05635	-7.20155	-2.84450	-0.29403	7.62778	1.44582	0.80930
H	3.87793	6.33775	2.46307	-7.60354	1.43410	-0.50257	7.24253	-2.83885	0.67883
H	2.04055	7.75027	3.39537	-8.66319	-0.81705	-0.26445	8.69782	-0.80915	0.71608
Pb	-0.00001	-0.00001	0.73447	-0.10171	-0.02819	0.47876	0.09458	-0.02624	-0.99603
H	-0.00001	-0.00004	2.44837	-0.13935	-0.03312	2.19576	-0.83722	0.13482	2.51134

PdTPP, total charge 0

	Singlet			Triplet			Quintet		
N	-2.04266	0.00000	-0.01187	0.00020	-2.05723	-0.02317	2.06189	0.00000	-0.04201
N	0.00001	2.04284	0.00009	-2.06164	-0.00020	-0.00001	0.00000	-2.06240	-0.00002
N	2.04268	0.00000	0.01204	-0.00020	2.05722	0.02317	-2.06189	0.00000	0.04198
N	0.00001	-2.04285	0.00009	2.06164	0.00019	0.00000	0.00000	2.06241	-0.00002
C	-2.86046	-1.10739	0.01368	1.10434	-2.87984	0.02010	2.88247	1.10774	0.00741
C	-4.24074	-0.68073	0.06653	0.69297	-4.23662	0.10322	4.25761	0.68427	0.09643
C	-4.24074	0.68074	0.06653	-0.69217	-4.23675	0.10319	4.25761	-0.68426	0.09647
C	-2.86046	1.10740	0.01368	-1.10380	-2.88004	0.02006	2.88247	-1.10774	0.00745
C	-2.44548	2.44560	0.01484	-2.46626	-2.44204	0.01904	2.46109	-2.46149	0.01162
C	-1.10745	2.86103	0.00733	-2.88180	-1.10892	0.01157	1.10793	-2.88422	0.00809
C	-0.68073	4.24225	-0.00029	-4.26522	-0.67997	-0.00068	0.68423	-4.26215	-0.00225
C	0.68075	4.24225	0.00031	-4.26535	0.67917	0.00057	-0.68423	-4.26215	0.00225
C	1.10747	2.86102	-0.00723	-2.88201	1.10838	-0.01162	-1.10793	-2.88422	-0.00810
C	2.44550	2.44559	-0.01476	-2.46672	2.44157	-0.01904	-2.46109	-2.46149	-0.01163
C	2.86047	1.10739	-0.01358	-1.10434	2.87984	-0.02000	-2.88247	-1.10774	-0.00747
C	4.24075	0.68073	-0.06652	-0.69297	4.23663	-0.10305	-4.25761	-0.68426	-0.09647
C	4.24075	-0.68073	-0.06652	0.69217	4.23676	-0.10307	-4.25761	0.68427	-0.09643
C	2.86047	-1.10740	-0.01358	1.10379	2.88005	-0.02004	-2.88247	1.10774	-0.00742
C	2.44550	-2.44560	-0.01476	2.46625	2.44204	-0.01912	-2.46109	2.46149	-0.01154
C	1.10746	-2.86103	-0.00723	2.88179	1.10892	-0.01166	-1.10793	2.88423	-0.00805
C	0.68074	-4.24225	0.00031	4.26522	0.67998	0.00054	-0.68423	4.26216	0.00228
C	-0.68074	-4.24225	-0.00029	4.26535	-0.67916	-0.00065	0.68423	4.26216	-0.00228
C	-1.10746	-2.86103	0.00734	2.88201	-1.10838	0.01162	1.10793	2.88422	0.00804
C	-2.44549	-2.44559	0.01484	2.46672	-2.44157	0.01912	2.46109	2.46149	0.01153
H	-5.09060	-1.34544	0.11170	1.35145	-5.08895	0.17263	5.10598	1.34699	0.17352
H	-5.09060	1.34546	0.11170	-1.35050	-5.08920	0.17258	5.10598	-1.34698	0.17358
H	-1.34519	5.09345	-0.00485	-5.11802	-1.34178	-0.00930	1.34636	-5.11426	-0.01549
H	1.34521	5.09345	0.00479	-5.11828	1.34082	0.00916	-1.34636	-5.11426	0.01551
H	5.09061	1.34545	-0.11176	-1.35146	5.08896	-0.17238	-5.10598	-1.34698	-0.17357
H	5.09061	-1.34545	-0.11176	1.35049	5.08921	-0.17243	-5.10598	1.34699	-0.17351
H	1.34520	-5.09346	0.00479	5.11802	1.34179	0.00910	-1.34636	5.11427	0.01557
H	-1.34520	-5.09346	-0.00485	5.11827	-1.34081	-0.00925	1.34636	5.11427	-0.01555
C	3.50527	3.50329	-0.02941	-3.51603	3.50141	-0.03615	-3.51734	-3.51250	-0.03346
C	4.27402	3.75806	1.11646	-3.69089	4.34679	1.07193	-4.37134	-3.69048	1.06802
C	3.74802	4.25505	-1.18912	-4.34067	3.67598	-1.15911	-3.68250	-4.34182	-1.15557
C	5.26385	4.74449	1.10419	-4.67752	5.33483	1.06199	-5.36241	-4.67476	1.04989
H	4.08865	3.17984	2.01718	-3.05208	4.21936	1.94076	-4.24842	-3.05474	1.94011
C	4.73857	5.24070	-1.20349	-5.32136	4.67114	-1.17275	-4.67658	-5.32302	-1.17647
H	3.15752	4.05947	-2.07964	-4.20318	3.03137	-2.02229	-3.02988	-4.20695	-2.01327
C	5.49906	5.48844	-0.05634	-5.49466	5.50137	-0.06130	-5.51897	-5.49364	-0.07308
H	5.84847	4.93242	2.00042	-4.80773	5.97408	1.93066	-6.00954	-4.80324	1.91306
H	4.91704	5.81202	-2.11016	-5.94724	4.79783	-2.05161	-4.79477	-5.95098	-2.05512
H	6.26878	6.25490	-0.06675	-6.25912	6.27302	-0.07034	-6.29082	-6.25781	-0.08837
C	-3.50526	3.50328	0.02938	-3.51537	-3.50208	0.03615	3.51734	-3.51250	0.03347
C	-3.74811	4.25508	1.18903	-4.34003	-3.67675	1.15908	3.68249	-4.34181	1.15560
C	-4.27394	3.75799	-1.11656	-3.69001	-4.34754	-1.07189	4.37135	-3.69049	-1.06800
C	-4.73867	5.24072	1.20330	-5.32052	-4.67210	1.17272	4.67657	-5.32301	1.17651
H	-3.15767	4.05955	2.07961	-4.20270	-3.03207	2.02223	3.02986	-4.20693	2.01329
C	-5.26378	4.74442	-1.10440	-4.67644	-5.33578	-1.06195	5.36242	-4.67477	-1.04985
H	-4.08850	3.17974	-2.01724	-3.05118	-4.22003	-1.94070	4.24844	-3.05476	-1.94010
C	-5.49909	5.48841	0.05608	-5.49361	-5.50242	0.06130	5.51896	-5.49364	0.07313
H	-4.91722	5.81208	2.10993	-5.94641	-4.79887	2.05156	4.79475	-5.95096	2.05517
H	-5.84834	4.93229	-2.00068	-4.80648	-5.97510	-1.93059	6.00955	-4.80327	-1.91301
H	-6.26881	6.25485	0.06640	-6.25792	-6.27422	0.07035	6.29081	-6.25781	0.08844
C	-3.50527	-3.50328	0.02938	3.51603	-3.50141	0.03629	3.51735	3.51250	0.03331
C	-3.74812	-4.25507	1.18904	4.34071	-3.67587	1.15924	3.68254	4.34185	1.15540
C	-4.27395	-3.75799	-1.11655	3.69086	-4.34688	-1.07172	4.37131	3.69045	-1.06819
C	-4.73869	-5.24070	1.20331	5.32140	-4.67102	1.17293	4.67663	5.32304	1.17625
H	-3.15769	-4.05954	2.07962	4.20325	-3.03119	2.02236	3.02994	4.20700	2.01312
C	-5.26379	-4.74441	-1.10439	4.67749	-5.33492	-1.06172	5.36240	4.67472	-1.05011
H	-4.08851	-3.17974	-2.01723	3.05202	-4.21953	-1.94054	4.24837	3.05469	-1.94027
C	-5.49911	-5.48839	0.05610	5.49467	-5.50135	0.06155	5.51899	5.49363	0.07284
H	-4.91724	-5.81206	2.10995	5.94731	-4.79764	2.05179	4.79484	5.95102	2.05489
H	-5.84836	-4.93228	-2.00067	4.80767	-5.97424	-1.93034	6.00950	4.80319	-1.91330
H	-6.26883	-6.25483	0.06642	6.25914	-6.27300	0.07064	6.29084	6.25779	0.08809
C	3.50527	-3.50329	-0.02942	3.51537	3.50208	-0.03629	-3.51735	3.51250	-0.03329
C	4.27402	-3.75807	1.11645	3.69011	4.34750	1.07177	-4.37130	3.69044	1.06822
C	3.74802	-4.25505	-1.18912	4.33993	3.67677	-1.15928	-3.68255	4.34186	-1.15538

C	5.26385	-4.74450	1.10418	4.67655	5.33574	1.06177	-5.36239	4.67471	1.05015
H	4.08865	-3.17986	2.01717	3.05136	4.21997	1.94063	-4.24835	3.05467	1.94028
C	4.73857	-5.24070	-1.20350	5.32042	4.67211	-1.17298	-4.67664	5.32305	-1.17621
H	3.15752	-4.05947	-2.07965	4.20252	3.03212	-2.02244	-3.02996	4.20702	-2.01311
C	5.49906	-5.48845	-0.05635	5.49362	5.50240	-0.06156	-5.51899	5.49363	-0.07279
H	5.84847	-4.93243	2.00041	4.80667	5.97502	1.93042	-6.00948	4.80316	1.91335
H	4.91704	-5.81202	-2.11018	5.94624	4.79891	-2.05187	-4.79486	5.95104	-2.05484
H	6.26878	-6.25490	-0.06676	6.25794	6.27420	-0.07065	-6.29085	6.25779	-0.08802
Pd	0.00001	0.00000	0.00014	0.00000	0.00000	-0.00002	0.00000	0.00000	-0.00004

PdTPP, total charge 1

		Doublet			**Quartet**			**Sextet**	
N	2.04909	0.00000	-0.04165	-2.05373	-0.00008	-0.05668	2.06881	0.00747	-0.05428
N	0.00001	-2.04946	-0.00005	-0.00007	2.04987	0.00000	0.00008	-2.01854	-0.00011
N	-2.04908	-0.00001	0.04153	2.05373	0.00007	0.05668	-2.06880	0.00732	0.05424
N	0.00000	2.04945	-0.00006	0.00007	-2.04989	0.00001	-0.00007	2.03438	-0.00014
C	2.86827	1.10264	0.00608	-2.87197	-1.10768	-0.00163	2.89505	1.10000	-0.00139
C	4.24304	0.68181	0.10261	-4.26596	-0.67489	0.09861	4.26984	0.67253	0.09005
C	4.24304	-0.68181	0.10258	-4.26601	0.67455	0.09877	4.26437	-0.69356	0.09165
C	2.86827	-1.10265	0.00603	-2.87206	1.10746	-0.00140	2.89171	-1.11143	0.00020
C	2.44974	-2.45005	0.01470	-2.47094	2.44295	0.01265	2.46718	-2.45867	0.00440
C	1.10281	-2.86993	0.00896	-1.10194	2.87211	0.00828	1.11717	-2.85508	0.00347
C	0.68176	-4.24791	-0.00474	-0.68570	4.24638	-0.00376	0.68399	-4.22598	-0.00641
C	-0.68175	-4.24791	0.00483	0.68541	4.24643	0.00384	-0.68366	-4.22603	0.00627
C	-1.10281	-2.86993	-0.00897	1.10174	2.87218	-0.00825	-1.11695	-2.85516	-0.00360
C	-2.44972	-2.45006	-0.01473	2.47077	2.44312	-0.01264	-2.46699	-2.45885	-0.00444
C	-2.86826	-1.10265	-0.00610	2.87198	1.10766	0.00138	-2.89162	-1.11164	-0.00019
C	-4.24303	-0.68182	-0.10264	4.26596	0.67484	-0.09883	-4.26432	-0.69389	-0.09151
C	-4.24304	0.68180	-0.10268	4.26600	-0.67460	-0.09867	-4.26989	0.67220	-0.08992
C	-2.86827	1.10264	-0.00616	2.87205	-1.10748	0.00161	-2.89513	1.09978	0.00139
C	-2.44973	2.45005	-0.01483	2.47094	-2.44297	-0.01223	-2.48464	2.46228	-0.00974
C	-1.10281	2.86992	-0.00903	1.10194	-2.87213	-0.00803	-1.13722	2.87952	-0.00723
C	-0.68176	4.24790	0.00478	0.68570	-4.24641	0.00399	-0.70861	4.21904	0.00738
C	0.68176	4.24791	-0.00471	-0.68541	-4.24645	-0.00390	0.70829	4.21910	-0.00757
C	1.10281	2.86993	0.00900	-1.10174	-2.87221	0.00807	1.13701	2.87960	0.00708
C	2.44973	2.45006	0.01478	-2.47077	-2.44314	0.01224	2.48446	2.46246	0.00970
H	5.09168	1.34253	0.18896	-5.11033	-1.34074	0.19062	5.11816	1.33455	0.16950
H	5.09169	-1.34254	0.18889	-5.11043	1.34033	0.19094	5.10823	-1.36151	0.16974
H	1.34187	-5.10113	-0.02168	-1.34745	5.09810	-0.02164	1.34416	-5.07944	-0.02398
H	-1.34186	-5.10113	0.02185	1.34710	5.09819	0.02176	-1.34377	-5.07954	0.02388
H	-5.09168	-1.34255	-0.18892	5.11033	1.34068	-0.19102	-5.10813	-1.36190	-0.16954
H	-5.09169	1.34252	-0.18900	5.11042	-1.34040	-0.19070	-5.11827	1.33417	-0.16930
H	-1.34187	5.10112	0.02177	1.34744	-5.09813	0.02205	-1.35657	5.08172	0.03624
H	1.34186	5.10113	-0.02162	-1.34709	-5.09822	-0.02193	1.35620	5.08182	-0.03638
C	-3.50508	-3.49986	-0.03715	3.52097	3.49774	-0.03619	-3.51378	-3.51891	-0.02394
C	-4.39060	-3.63796	1.04589	4.39598	3.65282	1.05263	-4.35869	-3.70076	1.08378
C	-3.63096	-4.36065	-1.14143	3.65240	4.34934	-1.14707	-3.67449	-4.34373	-1.14992
C	-5.37535	-4.62687	1.02831	5.38159	4.64207	1.03129	-5.33984	-4.69459	1.06792
H	-4.29267	-2.98013	1.90434	4.29072	3.00624	1.91907	-4.23621	-3.06889	1.95880
C	-4.62987	-5.33512	-1.16386	4.64731	5.32795	-1.17131	-4.66310	-5.33009	-1.16754
H	-2.95677	-4.25056	-1.98557	2.98427	4.23029	-1.99506	-3.03242	-4.19999	-2.01435
C	-5.50028	-5.47394	-0.07773	5.51155	5.47890	-0.08131	-5.49552	-5.50952	-0.05798
H	-6.04388	-4.73523	1.87690	6.04463	4.75954	1.88305	-5.98007	-4.83273	1.93397
H	-4.72841	-5.98426	-2.02854	4.74899	5.97026	-2.04080	-4.78479	-5.95455	-2.04748
H	-6.27187	-6.23756	-0.09342	6.28095	6.24467	-0.09933	-6.26131	-6.27904	-0.07111
C	3.50509	-3.49985	0.03720	-3.52121	3.49750	0.03619	3.51405	-3.51865	0.02398
C	3.63095	-4.36057	1.14153	-3.65275	4.34905	1.14709	3.67472	-4.34346	1.14997
C	4.39061	-3.63803	-1.04584	-4.39619	3.65255	-1.05266	4.35906	-3.70044	-1.08367
C	4.62986	-5.33505	1.16402	-4.64773	5.32759	1.17133	4.66340	-5.32974	1.16767
H	2.95676	-4.25043	1.98566	-2.98464	4.23001	1.99510	3.03258	-4.19977	2.01435
C	5.37535	-4.62695	-1.02819	-5.38187	4.64174	-1.03133	5.34027	-4.69420	-1.06774
H	4.29268	-2.98026	-1.90433	-4.29085	3.00601	-1.91912	4.23659	-3.06858	-1.95871
C	5.50028	-5.47395	0.07790	-5.51193	5.47852	0.08130	5.49593	-5.50912	0.05818
H	4.72839	-5.98413	2.02875	-4.74948	5.96986	2.04083	4.78507	-5.95419	2.04761
H	6.04389	-4.73536	-1.87677	-6.04488	4.75920	-1.88311	5.98058	-4.83230	-1.93374
H	6.27185	-6.23757	0.09366	-6.28139	6.24423	0.09931	6.26177	-6.27858	0.07136
C	3.50508	3.49986	0.03736	-3.52099	-3.49775	0.03543	3.53717	3.51314	0.04183
C	3.63089	4.36054	1.14173	-3.65270	-4.34947	1.14618	3.67979	4.34766	1.16431
C	4.39065	3.63808	-1.04562	-4.39577	-3.65265	-1.05359	4.40695	3.68240	-1.04926
C	4.62979	5.33502	1.16431	-4.64766	-5.32806	1.17008	4.67347	5.32844	1.19520

H	2.95665	4.25036	1.98583	-2.98476	-4.23055	1.99434	3.02128	4.21271	2.01784
C	5.37538	4.62700	-1.02790	-5.38143	-4.64188	-1.03260	5.39287	4.67083	-1.02056
H	4.29276	2.98034	-1.90415	-4.29031	-3.00596	-1.91993	4.30069	3.04379	-1.92154
C	5.50025	5.47396	0.07824	-5.51166	-5.47884	0.07987	5.52980	5.49427	0.10195
H	4.72828	5.98407	2.02907	-4.74955	-5.97047	2.03947	4.78133	5.95827	2.07312
H	6.04395	4.73545	-1.87644	-6.04428	-4.75921	-1.88451	6.05192	4.79849	-1.87402
H	6.27183	6.23759	0.09405	-6.28109	-6.24458	0.09763	6.30013	6.25898	0.12513
C	-3.50508	3.49985	-0.03733	3.52124	-3.49751	-0.03544	-3.53744	3.51287	-0.04178
C	-4.39064	3.63800	1.04568	4.39606	-3.65232	1.05356	-4.40712	3.68208	1.04938
C	-3.63090	4.36061	-1.14163	3.65297	-4.34925	-1.14617	-3.68022	4.34736	-1.16426
C	-5.37538	4.62692	1.02803	5.38178	-4.64148	1.03256	-5.39312	4.67044	1.02077
H	-4.29274	2.98020	1.90416	4.29058	-3.00562	1.91989	-4.30073	3.04349	1.92167
C	-4.62981	5.33509	-1.16413	4.64799	-5.32776	-1.17008	-4.67399	5.32807	-1.19507
H	-2.95668	4.25049	-1.98575	2.98499	-4.23039	-1.99430	-3.02179	4.21245	-2.01786
C	-5.50026	5.47395	-0.07804	5.51204	-5.47846	-0.07989	-5.53022	5.49384	-0.10175
H	-6.04394	4.73531	1.87659	6.04467	-4.75875	1.88446	-6.05210	4.79806	1.87428
H	-4.72831	5.98420	-2.02885	4.74990	-5.97019	-2.03945	-4.78198	5.95787	-2.07299
H	-6.27183	6.23758	-0.09379	6.28152	-6.24415	-0.09766	-6.30062	6.25849	-0.12487
Pd	0.00000	0.00000	-0.00015	0.00000	-0.00001	0.00000	0.00000	0.01815	-0.00013

H-PdTPP, total charge 0

		Doublet			Quartet			Sextet	
N	0.16608	-2.04304	-0.04047	-1.37561	-1.40517	0.01257	2.06990	0.00005	-0.09395
N	-2.04185	-0.16791	-0.03779	-1.51735	1.46588	-0.26569	0.00142	-2.06819	-0.03671
N	-0.16748	2.04231	-0.02686	1.37290	1.59852	-0.25988	-2.06506	-0.00005	0.02082
N	2.04000	0.16747	-0.02212	1.49092	-1.26362	0.03499	0.00132	2.06819	-0.03671
C	1.33703	-2.76340	-0.00169	-1.13960	-2.68080	0.45024	2.88671	1.10877	-0.03435
C	1.02363	-4.17238	0.07766	-2.39368	-3.38684	0.51720	4.26148	0.68450	0.05483
C	-0.33377	-4.28335	0.08088	-3.36449	-2.53172	0.06263	4.26151	-0.68430	0.05480
C	-0.87208	-2.94405	0.00398	-2.72323	-1.28340	-0.24666	2.88676	-1.10864	-0.03439
C	-2.24002	-2.63824	-0.00872	-3.37807	-0.11048	-0.68558	2.46410	-2.46217	-0.01778
C	-2.76346	-1.33846	-0.04348	-2.79758	1.16807	-0.72768	1.11102	-2.88562	-0.02800
C	-4.17417	-1.02448	-0.08855	-3.43146	2.39349	-1.10457	0.68748	-4.26318	-0.04568
C	-4.28476	0.33293	-0.08752	-2.54880	3.41467	-0.81193	-0.68134	-4.26437	-0.04017
C	-2.94331	0.87043	-0.05526	-1.37453	2.80767	-0.26873	-1.10688	-2.88684	-0.04162
C	-2.63761	2.23733	-0.02599	-0.16130	3.47215	0.21698	-2.46004	-2.46329	-0.03268
C	-1.33890	2.76223	-0.00677	1.11433	2.92291	-0.24589	-2.88124	-1.10883	-0.03573
C	-1.02784	4.17362	0.01507	2.24012	3.63769	-0.76179	-4.25454	-0.68468	-0.14248
C	0.32944	4.28614	0.01944	3.20872	2.70098	-1.06211	-4.25457	0.68447	-0.14250
C	0.86955	2.94523	-0.01379	2.67735	1.41917	-0.71448	-2.88129	1.10869	-0.03577
C	2.23718	2.63912	-0.03446	3.36085	0.19209	-0.70888	-2.46016	2.46317	-0.03275
C	2.75993	1.33857	-0.05978	2.81285	-1.04013	-0.28948	-1.10702	2.88678	-0.04166
C	4.16843	1.02528	-0.14794	3.54751	-2.25627	-0.07659	-0.68154	4.26433	-0.04020
C	4.27980	-0.33206	-0.14736	2.65714	-3.19549	0.37837	0.68728	4.26321	-0.04565
C	2.94120	-0.87070	-0.05779	1.36317	-2.56546	0.42734	1.11089	2.88567	-0.02796
C	2.63687	-2.23882	-0.02466	0.14027	-3.22852	0.71608	2.46398	2.46229	-0.01771
H	1.75472	-4.96494	0.13535	-2.51985	-4.40269	0.85976	5.11017	1.34672	0.13208
H	-0.92649	-5.18393	0.14169	-4.42326	-2.72502	-0.02764	5.11024	-1.34649	0.13204
H	-4.96811	-1.75579	-0.11840	-4.41987	2.48097	-1.53089	1.35025	-5.11468	-0.06744
H	-5.18636	0.92704	-0.10858	-2.68410	4.47415	-0.97576	-1.34237	-5.11732	-0.03069
H	-1.76135	4.96621	0.02508	2.28523	4.70741	-0.90780	-5.10151	-1.34755	-0.23294
H	0.92105	5.18920	0.04152	4.19011	2.87959	-1.47606	-5.10158	1.34729	-0.23298
H	4.95971	1.75690	-0.21666	4.60802	-2.37808	-0.24043	-1.34261	5.11725	-0.03074
H	5.17983	-0.92478	-0.21569	2.85422	-4.22696	0.63030	1.35001	5.11474	-0.06740
C	-3.77966	3.20658	-0.01470	-0.22059	4.58294	1.12859	-3.51838	-3.51186	-0.04039
C	-4.14612	3.85879	1.17200	0.96184	5.18838	1.65522	-3.69069	-4.35393	-1.15199
C	-4.49883	3.47662	-1.18844	-1.46290	5.09289	1.61674	-4.36950	-3.67272	1.06615
C	-5.21130	4.76347	1.18525	0.89967	6.25300	2.54431	-4.68854	-5.33146	-1.15746
H	-3.59305	3.65003	2.08335	1.93185	4.79587	1.37857	-3.04144	-4.23147	-2.01411
C	-5.56387	4.38158	-1.17667	-1.51262	6.15783	2.50634	-5.36403	-4.65351	1.06333
H	-4.21664	2.97531	-2.10997	-2.38997	4.62706	1.30859	-4.24058	-3.02707	1.92999
C	-5.92290	5.02731	0.01065	-0.33547	6.76181	2.97014	-5.52751	-5.48547	-0.04905
H	-5.48548	5.25932	2.11219	1.82310	6.68452	2.92086	-4.81247	-5.96935	-2.02813
H	-6.11033	4.58273	-2.09386	-2.47856	6.51527	2.85262	-6.00844	-4.76916	1.93030
H	-6.75074	5.73058	0.02047	-0.37932	7.59616	3.66371	-6.30216	-6.24693	-0.05230
C	-3.20920	-3.77875	0.02013	-4.81021	-0.24099	-1.08003	3.51835	-3.51429	0.02374
C	-3.96188	-4.04417	1.17445	-5.81693	0.43727	-0.37310	3.66700	-4.33479	1.15475
C	-3.37988	-4.60058	-1.10442	-5.17384	-1.05921	-2.16255	4.38526	-3.70345	-1.06576
C	-4.86583	-5.10935	1.20424	-7.15724	0.29876	-0.74002	4.65831	-5.31802	1.19594
H	-3.83023	-3.41279	2.04845	-5.54181	1.05965	0.47276	3.00446	-4.19032	2.00318

C	-4.28529	-5.66469	-1.07671	-6.51319	-1.18742	-2.53653	5.37343	-4.69004	-1.02719
H	-2.80111	-4.39779	-2.00103	-4.39902	-1.58553	-2.71186	4.27449	-3.07521	-1.94492
C	-5.03048	-5.92226	0.07827	-7.50891	-0.51058	-1.82501	5.51388	-5.49981	0.10449
H	-5.43835	-5.30480	2.10661	-7.92584	0.82024	-0.17670	4.76417	-5.93875	2.08123
H	-4.40933	-6.28971	-1.95663	-6.77813	-1.81545	-3.38233	6.03072	-4.82752	-1.88124
H	-5.73371	-6.74988	0.10075	-8.55121	-0.61471	-2.11257	6.28359	-6.26564	0.13572
C	3.77959	-3.20521	-0.01430	0.23083	-4.62453	1.22966	3.51818	3.51446	0.02386
C	4.59602	-3.33035	1.12041	0.79159	-4.86984	2.49464	3.66675	4.33494	1.15490
C	4.05388	-4.00073	-1.13748	-0.21163	-5.71678	0.46449	4.38511	3.70369	-1.06561
C	5.66293	-4.23260	1.13271	0.89594	-6.17266	2.98696	4.65801	5.31822	1.19613
H	4.38551	-2.71914	1.99329	1.13819	-4.03015	3.08995	3.00420	4.19041	2.00330
C	5.12226	-4.90134	-1.12749	-0.10268	-7.02027	0.95455	5.37322	4.69033	-1.02699
H	3.42687	-3.90533	-2.01935	-0.62934	-5.53813	-0.52191	4.27439	3.07546	-1.94479
C	5.92946	-5.02023	0.00829	0.44903	-7.25233	2.21851	5.51359	5.50008	0.10471
H	6.28302	-4.32140	2.02031	1.32483	-6.34345	3.97036	4.76380	5.93894	2.08144
H	5.32462	-5.50704	-2.00639	-0.44331	-7.85393	0.34680	6.03052	4.82787	-1.88101
H	6.75941	-5.72101	0.01706	0.53219	-8.26591	2.60020	6.28326	6.26595	0.13598
C	3.20845	3.77814	-0.03520	4.79148	0.19048	-1.13245	-3.51854	3.51169	-0.04051
C	3.36652	4.58358	-1.17344	5.75687	0.90606	-0.40570	-4.36970	3.67255	1.06600
C	3.97865	4.05634	1.10444	5.19382	-0.53864	-2.26337	-3.69087	4.35372	-1.15214
C	4.27580	5.64470	-1.17301	7.09643	0.89066	-0.80064	-5.36427	4.65329	1.06313
H	2.77511	4.37013	-2.05924	5.45151	1.46168	0.47563	-4.24077	3.02692	1.92987
C	4.88654	5.11860	1.10697	6.53161	-0.54407	-2.66431	-4.68876	5.33121	-1.15766
H	3.85773	3.43700	1.98856	4.45036	-1.09313	-2.82811	-3.04158	4.23128	-2.01424
C	5.03798	5.91549	-0.03219	7.48700	0.16869	-1.93288	-5.52776	5.48521	-0.04927
H	4.38987	6.25684	-2.06326	7.83402	1.44024	-0.22275	-6.00871	4.76893	1.93008
H	5.47269	5.32410	1.99830	6.82664	-1.10470	-3.54670	-4.81269	5.96907	-2.02835
H	5.74428	6.74080	-0.03101	8.52830	0.16015	-2.24194	-6.30244	6.24664	-0.05257
Pd	-0.00105	-0.00051	0.05218	-0.00869	0.10871	0.00725	0.00333	0.00000	0.04750
H	-0.01194	-0.01157	1.91494	-0.02817	0.25761	1.83780	0.06790	0.00000	1.88574

O=Ti(IV)TPP, total charge 0

		Singlet			Triplet			Quintet	
N	-2.04631	-0.05671	-0.03992	-1.21638	-1.52428	0.02781	-1.59819	1.37246	-0.22424
N	-0.05611	2.04160	-0.02594	-1.64940	1.31115	-0.20912	1.27699	1.66888	-0.23808
N	2.04343	0.05537	-0.01582	1.19992	1.71558	-0.25183	1.56251	-1.16138	0.06877
N	0.05331	-2.04303	-0.04891	1.60552	-1.11821	0.05446	-1.27567	-1.46203	0.03050
C	-2.83890	-1.18574	-0.08437	-0.87217	-2.79238	0.45356	-2.82177	1.00517	-0.75455
C	-4.22616	-0.79739	-0.18222	-2.05936	-3.60070	0.55205	-3.47771	2.17651	-1.26979
C	-4.26316	0.56610	-0.17895	-3.10616	-2.83157	0.11259	-2.65540	3.25382	-0.99577
C	-2.89825	1.02798	-0.09306	-2.57731	-1.53663	-0.21231	-1.51058	2.73840	-0.32379
C	-2.51461	2.37862	-0.06856	-3.33161	-0.43939	-0.69268	-0.36146	3.47921	0.20603
C	-1.18680	2.83439	-0.04104	-2.85974	0.88254	-0.76300	0.94768	3.00208	-0.24395
C	-0.80136	4.22500	-0.06812	-3.54440	2.01657	-1.29599	2.02748	3.77009	-0.76735
C	0.56196	4.26438	-0.06351	-2.76446	3.12685	-1.02576	3.05265	2.88475	-1.04235
C	1.02751	2.89768	-0.04792	-1.61351	2.65883	-0.32809	2.57855	1.57197	-0.69731
C	2.37865	2.51449	-0.07660	-0.49155	3.45603	0.19504	3.34373	0.37464	-0.72820
C	2.83287	1.18465	-0.09515	0.84251	3.02586	-0.21131	2.85427	-0.88708	-0.31224
C	4.21549	0.79677	-0.24259	1.92067	3.84569	-0.66186	3.64311	-2.10671	-0.24620
C	4.25271	-0.56672	-0.24195	2.97016	2.99811	-0.95681	2.81918	-3.09655	0.20446
C	2.89336	-1.02938	-0.09333	2.52621	1.66755	-0.68598	1.50793	-2.51545	0.37681
C	2.51184	-2.38186	-0.06701	3.31486	0.50470	-0.72881	0.33364	-3.24604	0.66053
C	1.18309	-2.83789	-0.03787	2.88927	-0.78727	-0.35278	-0.97207	-2.75318	0.45895
C	0.79438	-4.22751	0.00021	3.70582	-1.96570	-0.33871	-2.18898	-3.52519	0.53662
C	-0.56907	-4.26422	0.00139	2.91933	-3.00022	0.10600	-3.20293	-2.72608	0.09166
C	-1.03196	-2.89764	-0.03544	1.60631	-2.46193	0.32637	-2.62482	-1.43172	-0.22476
C	-2.38381	-2.51479	-0.05699	0.45400	-3.23993	0.64392	-3.35454	-0.31376	-0.70806
H	-5.05810	-1.48252	-0.25192	-2.09396	-4.62356	0.89560	-4.43085	2.18563	-1.77713
H	-5.13119	1.20604	-0.23760	-4.14537	-3.11660	0.03788	-2.81517	4.29298	-1.24676
H	-1.48904	5.05749	-0.09446	-4.49178	1.98980	-1.81427	2.01541	4.84006	-0.91856
H	1.19882	5.13635	-0.07713	-2.95699	4.15470	-1.29875	4.03625	3.11010	-1.42709
H	5.04260	1.48218	-0.35433	1.88574	4.92012	-0.77122	4.68329	-2.18644	-0.52401
H	5.11609	-1.20582	-0.35347	3.95383	3.26887	-1.31182	3.05783	-4.13879	0.35821
H	1.47832	-5.06268	0.02949	4.74182	-2.01132	-0.64014	-2.25612	-4.54845	0.87479
H	-1.20738	-5.13477	0.03143	3.19570	-4.03726	0.22663	-4.25112	-2.97147	0.00773
C	3.41228	3.59659	-0.11049	-0.70392	4.58329	1.06175	4.75648	0.46811	-1.19788
C	4.21888	3.84042	1.01183	0.38648	5.26406	1.68420	5.82534	0.29812	-0.30236
C	3.59653	4.37884	-1.26100	-2.01440	5.03398	1.40530	5.04346	0.74056	-2.54566

C	5.18728	4.84743	0.98557	0.17881	6.34509	2.53018	7.14754	0.39261	-0.74395
H	4.07816	3.23878	1.90520	1.39753	4.91179	1.52321	5.61217	0.09861	0.74404
C	4.56652	5.38429	-1.28927	-2.20997	6.11617	2.25328	6.36530	0.83615	-2.98826
H	2.97808	4.19071	-2.13402	-2.87881	4.51408	1.01242	4.22253	0.87231	-3.24487
C	5.36409	5.62184	-0.16536	-1.11875	6.79417	2.81432	7.42172	0.66163	-2.08867
H	5.80082	5.02747	1.86383	1.03459	6.83394	2.98755	7.96199	0.26203	-0.03685
H	4.70028	5.97876	-2.18871	-3.22311	6.43052	2.48848	6.56907	1.04295	-4.03520
H	6.11752	6.40406	-0.18644	-1.27661	7.64070	3.47582	8.44952	0.73568	-2.43227
C	-3.59980	3.41111	-0.08665	-4.73140	-0.70551	-1.12662	-0.51405	4.60309	1.08355
C	-3.94341	4.09698	1.08792	-5.81040	-0.04679	-0.51228	0.61437	5.27513	1.64488
C	-4.28562	3.70921	-1.27351	-4.99625	-1.62641	-2.15490	-1.80177	5.06434	1.49454
C	-4.95448	5.06175	1.07629	-7.12216	-0.30635	-0.91408	0.46020	6.35427	2.50441
H	-3.41588	3.86685	2.00923	-5.61248	0.65551	0.29148	1.61275	4.92083	1.41946
C	-5.29633	4.67445	-1.28641	-6.30738	-1.87546	-2.56507	-1.94302	6.14573	2.35347
H	-4.02014	3.18264	-2.18591	-4.16650	-2.13545	-2.63594	-2.68887	4.54945	1.14644
C	-5.63346	5.35303	-0.11105	-7.37441	-1.21824	-1.94404	-0.81718	6.81201	2.85884
H	-5.21199	5.58302	1.99399	-7.94623	0.20104	-0.42072	1.34267	6.83791	2.91412
H	-5.81736	4.89686	-2.21343	-6.49503	-2.58145	-3.36901	-2.93935	6.46811	2.64326
H	-6.41918	6.10306	-0.12040	-8.39481	-1.41647	-2.25930	-0.93273	7.65764	3.53011
C	-3.41529	-3.59944	-0.05825	0.69009	-4.64079	1.09145	-4.75712	-0.52977	-1.14921
C	-3.61122	-4.40209	-1.19260	1.36483	-4.88043	2.30099	-5.05311	-1.44896	-2.17270
C	-4.20453	-3.82854	1.07946	0.27890	-5.73960	0.31821	-5.82154	0.17017	-0.55153
C	-4.57661	-5.41239	-1.19056	1.60771	-6.18565	2.73362	-6.36961	-1.66053	-2.58701
H	-3.00518	-4.22634	-2.07686	1.68833	-4.03513	2.90131	-4.23951	-1.99007	-2.64728
C	-5.16827	-4.84031	1.08348	0.52849	-7.04514	0.74754	-7.13839	-0.04270	-0.96354
H	-4.05358	-3.21202	1.96092	-0.22327	-5.56357	-0.62842	-5.60825	0.87188	0.24931
C	-5.35740	-5.63464	-0.05185	1.19045	-7.27241	1.95825	-7.41793	-0.95800	-1.98387
H	-4.71965	-6.02284	-2.07780	2.12155	-6.35318	3.67596	-6.57579	-2.36953	-3.38402
H	-5.76826	-5.00879	1.97331	0.21104	-7.88348	0.13375	-7.94682	0.50102	-0.48272
H	-6.10719	-6.42063	-0.04928	1.38234	-8.28776	2.29316	-8.44243	-1.12266	-2.30498
C	3.60190	-3.40684	-0.08554	4.72885	0.65840	-1.18631	0.50564	-4.66002	1.10481
C	4.43430	-3.57674	1.03182	5.01021	0.97470	-2.52441	1.09879	-4.93097	2.34875
C	3.81329	-4.21039	-1.21671	5.79270	0.49791	-0.28490	0.10905	-5.73510	0.29310
C	5.45440	-4.53148	1.01948	6.33138	1.12026	-2.95462	1.28105	-6.24846	2.77605
H	4.27234	-2.95938	1.91071	4.18899	1.09893	-3.22410	1.40674	-4.10204	2.97941
C	4.83531	-5.16313	-1.23133	7.11299	0.65224	-0.71407	0.29665	-7.05255	0.71819
H	3.17490	-4.07967	-2.08582	5.57778	0.26072	0.75280	-0.33423	-5.53220	-0.67744
C	5.65823	-5.32690	-0.11253	7.38606	0.96116	-2.05040	0.88090	-7.31277	1.96199
H	6.08702	-4.65480	1.89399	6.53539	1.35760	-3.99484	1.73376	-6.44226	3.74427
H	4.98966	-5.77420	-2.11624	7.92664	0.53287	-0.00435	-0.00843	-7.87411	0.07623
H	6.45205	-6.06832	-0.12289	8.41305	1.07785	-2.38431	1.02499	-8.33719	2.29315
O	-0.01726	-0.01615	2.15168	-0.02941	0.28212	2.11615	-0.03844	0.29875	2.11927
Ti	-0.00413	-0.00330	0.53533	-0.02083	0.15162	0.50753	-0.01707	0.16684	0.50972

O=Ti(IV)TPP, total charge 1

		Doublet			Quartet			Sextet	
N	0.33574	2.02596	-0.08428	-0.00001	2.05234	-0.03776	-1.29950	1.42827	0.00146
N	2.02614	-0.33746	-0.00553	2.05218	0.00001	-0.02234	1.54212	1.14128	0.02808
N	-0.33849	-2.02392	-0.01282	0.00001	-2.05234	-0.03777	1.27546	-1.68705	-0.29807
N	-2.02714	0.33678	-0.07567	-2.05218	-0.00001	-0.02234	-1.63287	-1.40391	-0.24014
C	-0.61852	3.01874	-0.01136	-1.10271	2.87550	0.06111	-2.65816	1.38080	-0.17922
C	0.01853	4.29772	0.15169	-0.68742	4.23160	0.26697	-3.25133	2.61235	0.27159
C	1.36732	4.07408	0.15840	0.68737	4.23161	0.26697	-2.23111	3.41306	0.72290
C	1.55920	2.65783	-0.00204	1.10268	2.87551	0.06111	-1.00803	2.69674	0.51342
C	2.82079	2.01849	-0.06611	2.47083	2.44609	-0.05987	0.30437	3.20397	0.67928
C	3.01109	0.61627	-0.13765	2.86643	1.10868	-0.16306	1.48073	2.48442	0.31820
C	4.27508	-0.02024	-0.39581	4.23106	0.67574	-0.45838	2.77033	3.10154	0.05095
C	4.04984	-1.36851	-0.39641	4.23106	-0.67569	-0.45838	3.58748	2.13113	-0.43153
C	2.64731	-1.56007	-0.13930	2.86644	-1.10865	-0.16306	2.83005	0.88336	-0.42449
C	2.01246	-2.82413	-0.08138	2.47085	-2.44606	-0.05988	3.33860	-0.36367	-0.81145
C	0.61244	-3.02200	-0.00935	1.10271	-2.87550	0.06110	2.59703	-1.57923	-0.73005
C	-0.03069	-4.30810	0.04364	0.68742	-4.23161	0.26696	3.11562	-2.89596	-0.99016
C	-1.37840	-4.08140	0.03389	-0.68737	-4.23161	0.26696	2.11347	-3.79020	-0.69473
C	-1.56446	-2.65523	0.00685	-1.10267	-2.87551	0.06110	0.98689	-3.01735	-0.25206
C	-2.82375	-2.01563	-0.06901	-2.47082	-2.44609	-0.05988	-0.33299	-3.50285	0.16608
C	-3.01906	-0.61689	-0.15298	-2.86642	-1.10868	-0.16306	-1.48248	-2.79830	-0.41491
C	-4.30076	0.02262	-0.29089	-4.23106	-0.67574	-0.45838	-2.57219	-3.31041	-1.15324
C	-4.07443	1.37002	-0.30689	-4.23107	0.67569	-0.45838	-3.42598	-2.25398	-1.39275
C	-2.65676	1.56021	-0.14639	-2.86644	1.10865	-0.16305	-2.82062	-1.06489	-0.77621
C	-2.01998	2.82233	-0.07267	-2.47085	2.44606	-0.05987	-3.38786	0.26801	-0.71557

H	-0.49179	5.24121	0.26956	-1.34687	5.07377	0.40926	-4.30941	2.82733	0.28279
H	2.15332	4.80277	0.28374	1.34682	5.07379	0.40925	-2.31689	4.39683	1.15820
H	5.20538	0.49228	-0.58706	5.05476	1.33970	-0.67262	2.98840	4.15242	0.16963
H	4.76304	-2.15573	-0.58723	5.05478	-1.33965	-0.67262	4.60506	2.23085	-0.77788
H	0.47496	-5.26065	0.07750	1.34687	-5.07378	0.40924	4.11601	-3.11069	-1.33473
H	-2.16986	-4.81513	0.03278	-1.34682	-5.07379	0.40925	2.13440	-4.86764	-0.77822
H	-5.24924	-0.48628	-0.36712	-5.05476	-1.33970	-0.67261	-2.69237	-4.34091	-1.45604
H	-4.80227	2.15821	-0.42330	-5.05478	1.33965	-0.67261	-4.35688	-2.26915	-1.93904
C	2.88618	-4.02656	-0.12250	3.52092	-3.49620	-0.08676	4.75262	-0.45198	-1.27833
C	2.79048	-4.95099	-1.17827	3.52146	-4.48712	-1.08587	5.04076	-0.78403	-2.61202
C	3.82901	-4.24574	0.89828	4.53223	-3.51184	0.89111	5.81354	-0.21914	-0.38767
C	3.62601	-6.06787	-1.21392	4.51893	-5.46217	-1.11225	6.36492	-0.87245	-3.04830
H	2.07703	-4.77811	-1.97840	2.75072	-4.47619	-1.85089	4.22504	-0.96111	-3.30751
C	4.64710	-5.37573	0.87025	5.51950	-4.49859	0.87122	7.13762	-0.31116	-0.82478
H	3.90130	-3.53926	1.71970	4.52665	-2.76164	1.67642	5.59694	0.02262	0.64912
C	4.55105	-6.28615	-0.18736	5.51761	-5.47285	-0.13193	7.41587	-0.63669	-2.15558
H	3.55595	-6.76573	-2.04267	4.51853	-6.21143	-1.89804	6.57511	-1.12100	-4.08427
H	5.35839	-5.54465	1.67287	6.28607	-4.50826	1.64002	7.94904	-0.13356	-0.12534
H	5.19434	-7.16038	-0.21231	6.28866	-6.23697	-0.14969	8.44465	-0.70751	-2.49529
C	4.03450	2.87422	-0.07282	3.52088	3.49624	-0.08676	0.48932	4.59285	1.15931
C	5.00673	2.72940	0.93449	4.53219	3.51189	0.89110	1.29756	4.83540	2.28763
C	4.23131	3.83491	-1.08212	3.52140	4.48717	-1.08586	-0.10397	5.68615	0.49785
C	6.14273	3.53900	0.93854	5.51945	4.49865	0.87121	1.48553	6.13501	2.75574
H	4.85440	1.99834	1.72265	4.52664	2.76168	1.67640	1.75352	3.99726	2.80623
C	5.38023	4.62608	-1.08731	4.51885	5.46223	-1.11225	0.10397	6.98667	0.95675
H	3.49340	3.94010	-1.87165	2.75065	4.47623	-1.85087	-0.69777	5.51273	-0.39406
C	6.33486	4.48464	-0.07436	5.51754	5.47292	-0.13194	0.89188	7.21437	2.09028
H	6.87640	3.43221	1.73161	6.28603	4.50833	1.64000	2.09306	6.30660	3.63900
H	5.53087	5.35088	-1.88147	4.51844	6.21149	-1.89804	-0.34325	7.82228	0.42708
H	7.22405	5.10760	-0.07483	6.28858	6.23705	-0.14971	1.04695	8.22681	2.45039
C	-2.88684	4.03000	-0.06011	-3.52092	3.49620	-0.08675	-4.75130	0.48876	-1.20609
C	-3.81083	4.22780	0.98215	-4.53223	3.51184	0.89111	-5.81877	-0.36960	-0.84657
C	-2.79282	4.98879	-1.08507	-3.52145	4.48713	-1.08586	-5.03873	1.59309	-2.04753
C	-4.61506	5.36777	1.00268	-5.51950	4.49859	0.87121	-7.11162	-0.12645	-1.29696
H	-3.87785	3.49763	1.78300	-4.52666	2.76163	1.67641	-5.63419	-1.20007	-0.17212
C	-3.61492	6.11607	-1.07234	-4.51892	5.46217	-1.11225	-6.32991	1.82012	-2.51391
H	-2.09008	4.83525	-1.89854	-2.75070	4.47620	-1.85087	-4.23005	2.25043	-2.35041
C	-4.52323	6.31092	-0.02636	-5.51761	5.47285	-0.13194	-7.37357	0.96481	-2.13932
H	-5.31154	5.51959	1.82154	-6.28608	4.50826	1.64000	-7.92151	-0.78024	-0.98804
H	-3.54681	6.84076	-1.87790	-4.51851	6.21144	-1.89804	-6.52437	2.65945	-3.17445
H	-5.15594	7.19310	-0.01325	-6.28865	6.23697	-0.14971	-8.38171	1.14351	-2.50017
C	-4.03366	-2.88564	-0.07374	-3.52088	-3.49624	-0.08676	-0.49960	-4.50165	1.16730
C	-4.37809	-3.61657	1.07599	-3.52141	-4.48716	-1.08587	0.62481	-5.06607	1.85801
C	-4.83769	-2.98732	-1.22146	-4.53219	-3.51189	0.89111	-1.80274	-4.94641	1.57361
C	-5.51511	-4.42656	1.07891	-4.51886	-5.46222	-1.11226	0.45279	-6.01843	2.84574
H	-3.76287	-3.53474	1.96724	-2.75066	-4.47622	-1.85089	1.62547	-4.72779	1.61784
C	-5.96400	-3.81212	-1.21959	-5.51945	-4.49865	0.87122	-1.95781	-5.90103	2.56295
H	-4.56852	-2.43314	-2.11590	-4.52662	-2.76169	1.67641	-2.68231	-4.52655	1.10083
C	-6.30760	-4.52920	-0.06890	-5.51755	-5.47291	-0.13194	-0.83620	-6.45389	3.20555
H	-5.78089	-4.97612	1.97674	-4.51845	-6.21148	-1.89805	1.32186	-6.42835	3.35107
H	-6.57118	-3.89494	-2.11588	-6.28602	-4.50833	1.64001	-2.95552	-6.22279	2.84529
H	-7.18770	-5.16489	-0.06703	-6.28859	-6.23704	-0.14970	-0.96328	-7.20692	3.97664
O	-0.03944	0.05431	2.11058	0.00000	-0.00001	2.12586	-0.04553	-0.34271	2.06793
Ti	-0.00727	0.01019	0.50506	0.00000	-0.00001	0.51829	-0.02286	-0.18610	0.46647

O=V(IV)TPP, total charge 0

		Doublet			Quartet			Sextet	
N	-0.00014	2.02287	-0.04487	-1.24607	-1.46802	0.01905	1.29755	1.40868	0.02848
N	2.02314	0.00014	-0.04142	-1.58264	1.34426	-0.24291	1.53656	-1.39716	-0.25052
N	0.00013	-2.02287	-0.04487	1.22989	1.66287	-0.27078	-1.29533	-1.61993	-0.26043
N	-2.02315	-0.00013	-0.04142	1.55078	-1.14773	0.03793	-1.51193	1.18226	0.05366
C	-1.10443	2.85432	-0.02120	-0.94785	-2.74453	0.45551	1.03585	2.70427	0.47160
C	-0.68170	4.23155	0.04520	-2.15621	-3.51903	0.54613	2.27129	3.44457	0.54907
C	0.68113	4.23164	0.04523	-3.17498	-2.72458	0.08696	3.25949	2.62600	0.08376
C	1.10404	2.85447	-0.02120	-2.60458	-1.44895	-0.23694	2.64390	1.35222	-0.23999
C	2.44270	2.44409	-0.06940	-3.32674	-0.33841	-0.72837	3.34330	0.22696	-0.74218
C	2.84984	1.10390	-0.11920	-2.81379	0.96469	-0.78806	2.77503	-1.07312	-0.77654
C	4.21984	0.68174	-0.27774	-3.48188	2.12783	-1.27642	3.41163	-2.26834	-1.25930

C	4.21993	-0.68118	-0.27780	-2.67918	3.21206	-0.97414	2.56964	-3.32196	-0.95752
C	2.84999	-1.10352	-0.11919	-1.52866	2.69556	-0.31181	1.43217	-2.76509	-0.30883
C	2.44303	-2.44376	-0.06939	-0.39154	3.45213	0.22334	0.27461	-3.47012	0.23879
C	1.10442	-2.85432	-0.02120	0.91881	2.98434	-0.20703	-1.01202	-2.96397	-0.22945
C	0.68169	-4.23154	0.04524	2.01372	3.77861	-0.65855	-2.11137	-3.71432	-0.73502
C	-0.68114	-4.23163	0.04518	3.03256	2.90401	-0.98000	-3.10749	-2.80652	-1.03838
C	-1.10405	-2.85446	-0.02119	2.55082	1.58613	-0.71775	-2.59489	-1.50175	-0.72077
C	-2.44271	-2.44408	-0.06938	3.31147	0.40846	-0.76066	-3.33312	-0.29203	-0.76350
C	-2.84985	-1.10389	-0.11918	2.84764	-0.86082	-0.36343	-2.81210	0.94783	-0.33006
C	-4.21985	-0.68174	-0.27776	3.63684	-2.05575	-0.31895	-3.57427	2.18179	-0.24576
C	-4.21994	0.68118	-0.27776	2.82412	-3.06028	0.14466	-2.72997	3.14397	0.22473
C	-2.85000	1.10352	-0.11918	1.52346	-2.48603	0.33995	-1.43360	2.52984	0.38595
C	-2.44303	2.44377	-0.06939	0.35801	-3.23139	0.66699	-0.25026	3.23149	0.68837
H	-1.34509	5.08229	0.09244	-2.22216	-4.53762	0.89749	2.36618	4.46114	0.90041
H	1.34441	5.08246	0.09249	-4.22092	-2.97951	-0.00124	4.31297	2.84387	-0.00955
H	5.06340	1.34619	-0.39238	-4.43647	2.13625	-1.78176	4.36741	-2.30773	-1.76001
H	5.06357	-1.34551	-0.39249	-2.85446	4.25328	-1.20455	2.71166	-4.37133	-1.17418
H	1.34508	-5.08228	0.09251	2.00930	4.85532	-0.74907	-2.13020	-4.78814	-0.85476
H	-1.34442	-5.08246	0.09241	4.02102	3.14764	-1.34139	-4.09733	-3.01022	-1.41920
H	-5.06340	-1.34619	-0.39243	4.67322	-2.13099	-0.61290	-4.61156	2.28866	-0.52495
H	-5.06358	1.34552	-0.39242	3.07401	-4.10042	0.29304	-2.94442	4.18816	0.39948
C	3.50495	-3.49762	-0.08065	-0.56327	4.56288	1.11768	0.39696	-4.57395	1.14423
C	3.68843	-4.31999	-1.20308	0.55295	5.20680	1.73417	-0.74955	-5.20405	1.71796
C	4.33824	-3.67716	1.03447	-1.85753	5.03358	1.49557	1.67187	-5.05613	1.57145
C	4.68395	-5.30051	-1.21137	0.38393	6.27315	2.60691	-0.62449	-6.26499	2.60441
H	3.04889	-4.18240	-2.07029	1.55317	4.83806	1.54484	-1.73816	-4.83133	1.47940
C	5.33177	-4.65964	1.02870	-2.01408	6.10068	2.37021	1.78374	-6.11883	2.45756
H	4.19818	-3.04483	1.90646	-2.73984	4.54004	1.10845	2.57227	-4.57195	1.21351
C	5.50789	-5.47363	-0.09473	-0.89834	6.74320	2.92519	0.64026	-6.74478	2.97511
H	4.81682	-5.92610	-2.08960	1.25831	6.73448	3.05773	-1.51984	-6.71703	3.02225
H	5.96545	-4.78989	1.90145	-3.01575	6.43099	2.63138	2.77095	-6.45834	2.75887
H	6.28103	-6.23665	-0.10011	-1.02580	7.57848	3.60723	0.73295	-7.57631	3.66721
C	3.50450	3.49808	-0.08065	-4.73060	-0.56772	-1.17104	4.74498	0.41427	-1.19934
C	4.33779	3.67769	1.03445	-5.79912	0.10044	-0.54928	5.80462	-0.29788	-0.60806
C	3.68784	4.32050	-1.20307	-5.00846	-1.46644	-2.21510	5.04411	1.32238	-2.23160
C	5.33119	4.66029	1.02869	-7.11404	-0.12707	-0.96056	7.12017	-0.10862	-1.03590
H	4.19783	3.04532	1.90643	-5.59125	0.78496	0.26725	5.58930	-0.99030	0.20029
C	4.68325	5.30114	-1.21135	-6.32246	-1.68366	-2.63439	6.35917	1.51052	-2.66166
H	3.04831	4.18285	-2.07027	-4.18651	-1.98429	-2.70018	4.23389	1.87408	-2.69977
C	5.50718	5.47434	-0.09473	-7.37935	-1.01643	-2.00675	7.40281	0.79525	-2.06546
H	5.96488	4.79060	1.90142	-7.93035	0.38764	-0.46188	7.92523	-0.66176	-0.56015
H	4.81602	5.92676	-2.08957	-6.52021	-2.37303	-3.45026	6.56779	2.21142	-3.46517
H	6.28024	6.23745	-0.10010	-8.40202	-1.18985	-2.32918	8.42620	0.94153	-2.39883
C	-3.50496	3.49763	-0.08065	0.55271	-4.62941	1.14164	-0.38831	4.63973	1.16038
C	-4.33827	3.67714	1.03445	1.20622	-4.86480	2.36354	-0.97374	4.90012	2.41025
C	-3.68840	4.32002	-1.20307	0.12349	-5.73118	0.38257	0.03195	5.72148	0.36965
C	-5.33179	4.65962	1.02868	1.41093	-6.16787	2.82186	-1.12499	6.21270	2.86398
H	-4.19823	3.04479	1.90644	1.54442	-4.01749	2.95285	-1.30109	4.06636	3.02457
C	-4.68392	5.30054	-1.21136	0.33421	-7.03481	0.83785	-0.12406	7.03425	0.82124
H	-3.04884	4.18244	-2.07026	-0.36223	-5.55942	-0.57338	0.46877	5.52779	-0.60568
C	-5.50788	5.47364	-0.09474	0.97543	-7.25735	2.06054	-0.70069	7.28341	2.07082
H	-5.96550	4.78986	1.90142	1.90934	-6.33157	3.77315	-1.57249	6.39772	3.83637
H	-4.81677	5.92614	-2.08958	0.00291	-7.87560	0.23480	0.19943	7.86105	0.19518
H	-6.28103	6.23666	-0.10012	1.13732	-8.27114	2.41546	-0.82042	8.30413	2.42248
C	-3.50449	-3.49808	-0.08065	4.72527	0.52133	-1.22911	-4.74191	-0.35129	-1.24836
C	-3.68782	-4.32051	-1.20307	5.00326	0.81442	-2.57319	-5.01866	-0.62535	-2.59808
C	-4.33779	-3.67771	1.03445	5.79239	0.34826	-0.33396	-5.81788	-0.15136	-0.36750
C	-4.68321	-5.30116	-1.21137	6.32397	0.92406	-3.01541	-6.33669	-0.69227	-3.05689
H	-3.04827	-4.18285	-2.07026	4.17951	0.94934	-3.26792	-4.19237	-0.78128	-3.28591
C	-5.33118	-4.66032	1.02867	7.11247	0.46618	-0.77525	-7.13627	-0.21732	-0.82525
H	-4.19784	-3.04534	1.90643	5.58035	0.13014	0.70852	-5.61341	0.04809	0.68064
C	-5.50715	-5.47437	-0.09475	7.38194	0.75170	-2.11751	-7.39995	-0.48748	-2.17186
H	-4.81597	-5.92678	-2.08958	6.52507	1.14394	-4.06003	-6.53211	-0.90061	-4.10513
H	-5.96487	-4.79064	1.90140	7.92884	0.33711	-0.07034	-7.95624	-0.06394	-0.12916
H	-6.28020	-6.23749	-0.10013	8.40866	0.84032	-2.46080	-8.42482	-0.53931	-2.52802
O	-0.00001	0.00000	2.05315	-0.02685	0.30084	2.00731	0.02755	-0.32303	2.01135
V	-0.00001	0.00000	0.48032	-0.01610	0.15012	0.44372	0.01189	-0.16464	0.44688

O=V(IV)TPP, total charge 1

	Singlet			Triplet			Quintet		
N	-1.81510	-0.73281	-0.04149	-0.32786	-2.00852	-0.07237	1.24364	-1.45749	0.02527
N	-0.72479	1.80043	-0.00298	-2.00178	0.32838	-0.03039	-1.54208	-1.14012	0.05125
N	1.79584	0.70855	-0.01943	0.33102	2.00572	-0.01912	-1.22661	1.65332	-0.25946
N	0.72300	-1.83106	-0.02407	2.00461	-0.32898	-0.08373	1.57532	1.33927	-0.24225
C	-2.18864	-2.01779	-0.40448	0.62374	-3.00459	-0.00185	2.60556	-1.43880	-0.24106
C	-3.60459	-2.17263	-0.21833	-0.00749	-4.28513	0.16115	3.17809	-2.73299	0.06999
C	-4.07788	-1.00486	0.31168	-1.35593	-4.06453	0.16627	2.16687	-3.52290	0.51847
C	-2.97503	-0.08706	0.36749	-1.54746	-2.64959	0.00461	0.94596	-2.73313	0.44073
C	-3.07174	1.29648	0.60012	-2.80940	-2.02167	-0.06814	-0.35457	-3.23003	0.66703
C	-2.02052	2.18238	0.29793	-2.99195	-0.62301	-0.15144	-1.50966	-2.47662	0.34154
C	-2.19266	3.57581	-0.00217	-4.25925	0.00752	-0.39971	-2.82769	-3.06024	0.14328
C	-1.01827	4.01864	-0.54539	-4.03749	1.35555	-0.40080	-3.63583	-2.06469	-0.30995
C	-0.08566	2.92778	-0.50107	-2.63462	1.54744	-0.15421	-2.84174	-0.85464	-0.34891
C	1.29091	3.01868	-0.75484	-2.01394	2.81358	-0.08664	-3.31598	0.40761	-0.75786
C	2.17385	1.97343	-0.44741	-0.61753	3.00669	-0.00989	-2.54345	1.57787	-0.71976
C	3.59996	2.10522	-0.33563	0.01906	4.29395	0.05579	-3.01370	2.90732	-1.02167
C	4.07895	0.94264	0.20117	1.36655	4.07062	0.04707	-1.99485	3.77059	-0.72292
C	2.95971	0.05684	0.35855	1.55287	2.64607	0.00749	-0.90672	2.96774	-0.21890
C	3.05962	-1.32442	0.60143	2.81298	2.01779	-0.07064	0.39099	3.44299	0.24525
C	2.01285	-2.21580	0.30827	3.00073	0.62212	-0.15941	1.51927	2.68885	-0.30137
C	2.15847	-3.62974	0.10355	4.28390	-0.01163	-0.29391	2.67713	3.21543	-0.97671
C	0.98656	-4.08128	-0.43628	4.06063	-1.35873	-0.30818	3.47720	2.14310	-1.27735
C	0.07085	-2.97433	-0.46193	2.64422	-1.54886	-0.14988	2.80666	0.96748	-0.78496
C	-1.30832	-3.07065	-0.69551	2.02132	-2.81302	-0.06795	3.33291	-0.33593	-0.73110
H	-4.15476	-3.07906	-0.42266	0.50688	-5.22626	0.27981	4.22471	-2.98309	-0.02006
H	-5.08861	-0.78071	0.61710	-2.14218	-4.79303	0.29052	2.22408	-4.54294	0.86662
H	-3.11384	4.12446	0.12649	-5.18918	-0.50889	-0.58174	-3.06661	-4.10358	0.28592
H	-0.79959	5.00139	-0.93515	-4.75290	2.14264	-0.58332	-4.67050	-2.13595	-0.60971
H	4.15767	2.98848	-0.60911	-0.49108	5.24375	0.09766	-3.99831	3.14653	-1.39548
H	5.10335	0.68744	0.42852	2.15786	4.80438	0.05506	-1.97321	4.84482	-0.83535
H	3.05441	-4.19678	0.30591	5.23043	0.50115	-0.36763	2.84314	4.25867	-1.20403
H	0.75262	-5.08356	-0.76194	4.78891	-2.14704	-0.42037	4.42915	2.14935	-1.78697
C	1.86834	4.30248	-1.24481	-2.89102	4.01384	-0.11825	-4.72722	0.51745	-1.23002
C	2.49982	4.34400	-2.49889	-2.80089	4.94341	-1.16983	-4.99785	0.81867	-2.57439
C	1.81603	5.46842	-0.46337	-3.83023	4.22653	0.90704	-5.79456	0.33246	-0.33674
C	3.05466	5.53605	-2.96936	-3.63872	6.05890	-1.19716	-6.31777	0.92455	-3.01942
H	2.54374	3.44457	-3.10639	-2.08939	4.77606	-1.97288	-4.17451	0.95623	-3.26951
C	2.38158	6.65596	-0.93180	-4.65084	5.35494	0.88731	-7.11279	0.44884	-0.78314
H	1.34984	5.43646	0.51700	-3.89842	3.51577	1.72514	-5.58899	0.11290	0.70704
C	2.99786	6.69334	-2.18668	-4.56051	6.27051	-0.16633	-7.37676	0.74188	-2.12497
H	3.53026	5.55987	-3.94513	-3.57277	6.76096	-2.02270	-6.51720	1.14795	-4.06307
H	2.34490	7.54904	-0.31537	-5.35969	5.51858	1.69319	-7.93150	0.31373	-0.08292
H	3.43402	7.61841	-2.55104	-5.20560	7.14357	-0.18484	-8.40213	0.82807	-2.47118
C	-4.36772	1.89342	1.02478	-4.02215	-2.87938	-0.06996	-0.54825	-4.62715	1.14244
C	-4.43168	2.58467	2.24664	-4.98920	-2.73864	0.94254	-1.18854	-4.85408	2.37299
C	-5.51578	1.81575	0.21860	-4.22221	-3.83806	-1.08019	-0.13360	-5.72897	0.37514
C	-5.62999	3.16647	2.66488	-6.12391	-3.55021	0.95059	-1.39578	-6.15654	2.83280
H	-3.54514	2.65062	2.87068	-4.83465	-2.00826	1.73094	-1.50870	-4.00635	2.97223
C	-6.70836	2.41115	0.63343	-5.36968	-4.63157	-1.08119	-0.34751	-7.03046	0.83397
H	-5.46473	1.31243	-0.74229	-3.48760	-3.94070	-1.87316	0.33696	-5.56360	-0.58994
C	-6.76975	3.08178	1.85935	-6.31949	-4.49408	-0.06325	-0.97581	-7.24693	2.06486
H	-5.67204	3.68583	3.61740	-6.85398	-3.44612	1.74736	-1.88186	-6.31829	3.79015
H	-7.58660	2.35614	-0.00263	-5.52274	-5.35522	-1.87594	-0.03035	-7.87389	0.22803
H	-7.69952	3.53990	2.18241	-7.20754	-5.11865	-0.06058	-1.13926	-8.25927	2.42153
C	-1.89724	-4.37053	-1.12890	2.89188	-4.01819	-0.05255	4.73477	-0.55944	-1.17447
C	-1.86252	-5.50011	-0.29506	3.81242	-4.21415	0.99289	5.79921	0.12345	-0.55987
C	-2.52753	-4.45989	-2.38075	2.80455	-4.97632	-1.07848	5.01152	-1.46708	-2.21220
C	-2.44258	-6.70025	-0.71094	4.62005	-5.35177	1.01565	7.11328	-0.10127	-0.97328
H	-1.39895	-5.42964	0.68459	3.87513	-3.48378	1.79394	5.59433	0.80932	0.25670
C	-3.09742	-5.66469	-2.79838	3.62973	-6.10144	-1.06342	6.32548	-1.67828	-2.63317
H	-2.55966	-3.58779	-3.02760	2.10404	-4.82439	-1.89419	4.19277	-1.99019	-2.69762
C	-3.05696	-6.78620	-1.96441	4.53471	-6.29452	-0.01427	7.37873	-0.99842	-2.01303
H	-2.41910	-7.56485	-0.05455	5.31428	-5.50191	1.83673	7.92875	0.42001	-0.48128
H	-3.57231	-5.72603	-3.77287	3.56646	-6.82585	-1.86963	6.52608	-2.37106	-3.44470
H	-3.50465	-7.72097	-2.28768	5.16989	-7.17489	0.00055	8.40097	-1.16815	-2.33696
C	4.38697	-1.85324	1.02829	4.02219	2.88870	-0.07090	0.55178	4.55268	1.13308
C	4.85143	-1.56730	2.32222	4.37134	3.60791	1.08460	-0.57483	5.21106	1.71615
C	5.19544	-2.59794	0.15474	4.82078	3.00299	-1.22112	1.84550	5.00448	1.53836

C	6.09789	-2.03780	2.74157	5.50755	4.41915	1.09068	-0.41327	6.27566	2.58963
H	4.23030	-0.98700	2.99852	3.75993	3.51685	1.97759	-1.57656	4.86014	1.49908
C	6.44578	-3.05731	0.57399	5.94648	3.82870	-1.21592	1.99386	6.07083	2.41224
H	4.85283	-2.79730	-0.85649	4.54821	2.45735	-2.11979	2.73187	4.49937	1.17400
C	6.89701	-2.78253	1.86890	6.29471	4.53432	-0.05958	0.86954	6.72617	2.93693
H	6.44344	-1.82116	3.74780	5.77676	4.96002	1.99277	-1.28957	6.75418	3.01624
H	7.06808	-3.62430	-0.11175	6.54962	3.92104	-2.11401	2.99074	6.39265	2.69788
H	7.86789	-3.14338	2.19431	7.17422	5.17081	-0.05522	0.99091	7.56160	3.61906
O	-0.01103	-0.03407	2.02960	0.02752	-0.03529	2.01836	0.03641	0.30293	2.01994
V	-0.00524	-0.01417	0.47495	0.00574	-0.00629	0.45458	0.01905	0.14961	0.46110

ZnTPP, total charge 0

	Singlet			Triplet			Quintet		
N	-2.01605	0.39031	0.00141	-2.06035	-0.00013	-0.04239	2.06797	0.00000	-0.04620
N	0.39049	2.01615	0.00090	-0.00013	2.07772	0.00003	0.00000	-2.06913	0.00002
N	2.01609	-0.39033	0.00116	2.06035	0.00013	0.04239	-2.06797	0.00000	0.04617
N	-0.39042	-2.01616	0.00128	0.00013	-2.07772	0.00003	0.00000	2.06913	0.00002
C	-3.03139	-0.54039	0.00421	-2.88525	-1.10439	0.02015	2.89242	1.10768	0.00887
C	-4.30881	0.13972	-0.00229	-4.24028	-0.69432	0.13307	4.26834	0.68511	0.10947
C	-4.04950	1.47885	0.00353	-4.24037	0.69377	0.13307	4.26834	-0.68511	0.10948
C	-2.61045	1.63289	-0.00205	-2.88539	1.10402	0.02015	2.89242	-1.10767	0.00888
C	-1.93765	2.86842	0.00063	-2.44196	2.47187	0.01478	2.46312	-2.46372	0.00981
C	-0.54028	3.03142	0.00365	-1.10829	2.90033	0.00848	1.10789	-2.89516	0.00490
C	0.13972	4.30888	-0.00215	-0.68077	4.28634	-0.00267	0.68510	-4.27463	-0.00479
C	1.47888	4.04965	0.00357	0.68024	4.28642	0.00243	-0.68510	-4.27463	0.00448
C	1.63302	2.61060	-0.00212	1.10792	2.90047	-0.00852	-1.10789	-2.89516	-0.00500
C	2.86860	1.93779	0.00061	2.44164	2.47217	-0.01475	-2.46311	-2.46372	-0.00981
C	3.03145	0.54036	0.00365	2.88525	1.10439	-0.02002	-2.89242	-1.10767	-0.00878
C	4.30885	-0.13978	-0.00308	4.24031	0.69432	-0.13271	-4.26836	-0.68511	-0.10916
C	4.04952	-1.47892	0.00281	4.24040	-0.69377	-0.13271	-4.26836	0.68511	-0.10916
C	2.61047	-1.63293	-0.00236	2.88539	-1.10402	-0.02002	-2.89242	1.10767	-0.00877
C	1.93768	-2.86847	0.00047	2.44196	-2.47186	-0.01476	-2.46312	2.46372	-0.00979
C	0.54031	-3.03146	0.00374	1.10829	-2.90033	-0.00853	-1.10789	2.89516	-0.00499
C	-0.13973	-4.30891	-0.00202	0.68078	-4.28633	0.00242	-0.68511	4.27463	0.00449
C	-1.47889	-4.04963	0.00386	-0.68023	-4.28642	-0.00267	0.68510	4.27463	-0.00480
C	-1.63297	-2.61059	-0.00157	-1.10792	-2.90047	0.00847	1.10789	2.89517	0.00490
C	-2.86852	-1.93780	0.00126	-2.44164	-2.47218	0.01478	2.46312	2.46373	0.00979
H	-5.27331	-0.34658	-0.00997	-5.09411	-1.34890	0.22300	5.11905	1.34439	0.19427
H	-4.76280	2.29003	0.01032	-5.09428	1.34825	0.22300	5.11905	-1.34439	0.19428
H	-0.34652	5.27343	-0.00983	-1.33878	5.14239	-0.01488	1.34357	-5.12993	-0.01847
H	2.28994	4.76307	0.01099	1.33814	5.14256	0.01451	-1.34357	-5.12993	0.01802
H	5.27337	0.34647	-0.01119	5.09415	1.34890	-0.22251	-5.11908	-1.34439	-0.19383
H	4.76282	-2.29011	0.00927	5.09432	-1.34825	-0.22251	-5.11908	1.34439	-0.19382
H	0.34649	-5.27347	-0.00980	1.33880	-5.14238	0.01451	-1.34358	5.12993	0.01803
H	-2.28997	-4.76303	0.01126	-1.33813	-5.14256	-0.01488	1.34356	5.12994	-0.01848
C	4.11013	2.77661	-0.00057	3.50579	3.51763	-0.03348	-3.52054	-3.51443	-0.03219
C	4.89686	2.88957	1.15593	4.37062	3.67279	1.06292	-4.38556	-3.68238	1.06250
C	4.50704	3.46362	-1.15813	3.66708	4.35929	-1.14616	-3.67753	-4.35376	-1.14829
C	6.05461	3.67239	1.15623	5.36250	4.65545	1.05239	-5.37787	-4.66539	1.04400
H	4.59309	2.36227	2.05580	4.25499	3.02126	1.92392	-4.27026	-3.03927	1.93022
C	5.66531	4.24566	-1.16015	4.66631	5.33575	-1.16121	-4.67287	-5.33365	-1.17007
H	3.90385	3.37763	-2.05748	3.00876	4.23776	-2.00133	-3.01714	-4.22762	-2.00136
C	6.44236	4.35257	-0.00242	5.51497	5.48902	-0.06080	-5.52564	-5.49382	-0.07313
H	6.65088	3.75215	2.06093	6.01606	4.76963	1.91265	-6.03304	-4.78534	1.90235
H	5.96081	4.76854	-2.06551	4.78193	5.97398	-2.03272	-4.78392	-5.96886	-2.04447
H	7.34235	4.96087	-0.00309	6.28982	6.25024	-0.07067	-6.29850	-6.25698	-0.08891
C	-2.77654	4.10996	0.00007	-3.50624	3.51718	0.03347	3.52054	-3.51443	0.03219
C	-2.89287	4.89366	1.15830	-3.66749	4.35902	1.14603	3.67736	-4.35395	1.14817
C	-3.46020	4.50971	-1.15843	-4.37124	3.67203	-1.06284	4.38574	-3.68220	-1.06239
C	-3.67575	6.05136	1.15932	-4.66685	5.33535	1.16104	4.67269	-5.33384	1.16995
H	-2.36818	4.58749	2.05891	-3.00905	4.23772	2.00113	3.01683	-4.22795	2.00116
C	-4.24240	5.66790	-1.15968	-5.36325	4.65457	-1.05234	5.37806	-4.66520	-1.04389
H	-3.37161	3.90886	-2.05910	-4.25565	3.02037	-1.92374	4.27058	-3.03894	-1.93002
C	-4.35266	6.44199	-0.00029	-5.51568	5.48831	0.06072	5.52565	-5.49382	0.07313
H	-3.75816	6.64533	2.06530	-4.78244	5.97371	2.03246	4.78361	-5.96919	2.04426
H	-4.76277	5.96566	-2.06573	-6.01695	4.76851	-1.91253	6.03337	-4.78501	-1.90216
H	-4.96106	7.34191	-0.00039	-6.29063	6.24943	0.07056	6.29850	-6.25698	0.08890
C	-4.11005	-2.77669	-0.00026	-3.50579	-3.51763	0.03347	3.52054	3.51443	0.03216

C	-4.50848	-3.46064	-1.15910	-3.66693	-4.35949	1.14603	3.67737	4.35396	1.14813
C	-4.89531	-2.89250	1.15695	-4.37077	-3.67259	-1.06284	4.38574	3.68219	-1.06242
C	-5.66688	-4.24247	-1.16174	-4.66617	-5.33594	1.16104	4.67270	5.33385	1.16990
H	-3.90628	-3.37250	-2.05891	-3.00851	-4.23811	2.00113	3.01684	4.22797	2.00113
C	-6.05323	-3.67510	1.15660	-5.36266	-4.65525	-1.05234	5.37805	4.66520	-1.04394
H	-4.59030	-2.36774	2.05790	-4.25526	-3.02092	-1.92374	4.27057	3.03893	-1.93005
C	-6.44257	-4.35215	-0.00335	-5.51498	-5.48902	0.06072	5.52565	5.49383	0.07307
H	-5.96358	-4.76299	-2.06806	-4.78168	-5.97432	2.03246	4.78363	5.96921	2.04420
H	-6.64845	-3.75705	2.06180	-6.01634	-4.76928	-1.91253	6.03335	4.78500	-1.90221
H	-7.34274	-4.96018	-0.00450	-6.28984	-6.25023	0.07057	6.29851	6.25698	0.08883
C	2.77653	-4.11001	-0.00019	3.50624	-3.51718	-0.03348	-3.52055	3.51443	-0.03216
C	3.46015	-4.50972	-1.15874	4.37109	-3.67223	1.06293	-4.38555	3.68237	1.06254
C	2.89286	-4.89377	1.15800	3.66763	-4.35883	-1.14616	-3.67755	4.35376	-1.14825
C	4.24230	-5.66794	-1.16007	5.36309	-4.65476	1.05239	-5.37787	4.66538	1.04405
H	3.37156	-3.90880	-2.05937	4.25537	-3.02072	1.92392	-4.27024	3.03925	1.93026
C	3.67571	-6.05151	1.15893	4.66699	-5.33516	-1.16121	-4.67288	5.33365	-1.17002
H	2.36820	-4.58765	2.05864	3.00931	-4.23738	-2.00134	-3.01716	4.22763	-2.00133
C	4.35256	-6.44210	-0.00072	5.51567	-5.48832	-0.06080	-5.52565	5.49382	-0.07307
H	4.76263	-5.96566	-2.06616	6.01667	-4.76886	1.91265	-6.03303	4.78533	1.90241
H	3.75812	-6.64552	2.06488	4.78269	-5.97337	-2.03272	-4.78395	5.96886	-2.04441
H	4.96094	-7.34204	-0.00089	6.29062	-6.24944	-0.07067	-6.29851	6.25697	-0.08884
Zn	0.00003	-0.00002	0.00152	0.00000	0.00000	0.00002	0.00000	0.00000	0.00000

ZnTPP, total charge 1

		Doublet			Quartet			Sextet	
N	2.06062	-0.00001	-0.06796	2.06069	0.00018	-0.05835	-2.08335	0.00000	-0.07665
N	-0.00001	-2.06073	0.00000	0.00017	-2.05913	-0.00001	0.01688	2.03651	-0.00600
N	-2.06062	0.00001	0.06796	-2.06068	-0.00018	0.05831	2.14026	0.00000	0.02165
N	0.00001	2.06074	0.00000	-0.00016	2.05914	-0.00001	0.01688	-2.03651	-0.00600
C	2.88062	1.10209	-0.00068	2.88257	1.10748	0.00045	-2.90371	-1.10674	-0.02216
C	4.25463	0.68311	0.12432	4.27807	0.67585	0.11013	-4.29362	-0.67874	0.07146
C	4.25463	-0.68315	0.12433	4.27819	-0.67514	0.11015	-4.29362	0.67874	0.07147
C	2.88061	-1.10212	-0.00067	2.88277	-1.10701	0.00048	-2.90371	1.10674	-0.02216
C	2.45233	-2.45278	0.00715	2.47375	-2.44454	0.01091	-2.46999	2.44950	-0.00443
C	1.10247	-2.88315	0.00387	1.10167	-2.88385	0.00463	-1.11148	2.86703	-0.00318
C	0.68306	-4.26252	-0.00753	0.68723	-4.25916	-0.00657	-0.69290	4.23924	-0.00812
C	-0.68310	-4.26252	0.00741	-0.68649	-4.25928	0.00610	0.67820	4.24549	0.00718
C	-1.10250	-2.88314	-0.00391	-1.10116	-2.88402	-0.00481	1.10465	2.87207	-0.00558
C	-2.45235	-2.45275	-0.00715	-2.47333	-2.44495	-0.01095	2.48924	2.47442	-0.01244
C	-2.88062	-1.10209	0.00072	-2.88257	-1.10748	-0.00041	2.95841	1.14185	-0.02447
C	-4.25464	-0.68311	-0.12420	-4.27809	-0.67584	-0.10988	4.30212	0.73535	-0.13398
C	-4.25464	0.68315	-0.12419	-4.27820	0.67515	-0.10986	4.30212	-0.73535	-0.13398
C	-2.88061	1.10212	0.00073	-2.88277	1.10702	-0.00039	2.95841	-1.14185	-0.02447
C	-2.45232	2.45277	-0.00713	-2.47374	2.44453	-0.01089	2.48924	-2.47442	-0.01243
C	-1.10247	2.88315	-0.00391	-1.10166	2.88385	-0.00476	1.10466	-2.87207	-0.00558
C	-0.68306	4.26252	0.00741	-0.68722	4.25917	0.00618	0.67820	-4.24549	0.00718
C	0.68310	4.26252	-0.00755	0.68649	4.25928	-0.00653	-0.69289	-4.23925	-0.00813
C	1.10250	2.88314	0.00386	1.10116	2.88403	0.00462	-1.11148	-2.86703	-0.00319
C	2.45235	2.45276	0.00713	2.47334	2.44495	0.01087	-2.46999	-2.44951	-0.00444
H	5.10408	1.34031	0.23090	5.12453	1.33854	0.20831	-5.14180	-1.34143	0.15362
H	5.10407	-1.34035	0.23092	5.12476	-1.33768	0.20835	-5.14180	1.34142	0.15362
H	1.33917	-5.11903	-0.02904	1.34538	-5.11398	-0.02490	-1.35380	5.09208	-0.02608
H	-1.33922	-5.11901	0.02887	-1.34450	-5.11421	0.02426	1.33240	5.10336	0.02403
H	-5.10410	-1.34030	-0.23073	-5.12456	-1.33853	-0.20795	5.16251	1.37873	-0.24379
H	-5.10409	1.34036	-0.23071	-5.12479	1.33769	-0.20790	5.16251	-1.37873	-0.24378
H	-1.33917	5.11903	0.02887	-1.34538	5.11399	0.02437	1.33241	-5.10336	0.02402
H	1.33921	5.11901	-0.02908	1.34450	5.11421	-0.02487	-1.35379	-5.09208	-0.02609
C	-3.50920	-3.50130	-0.03382	-3.52445	-3.49950	-0.03467	3.52536	3.54381	-0.02460
C	-4.41060	-3.62671	1.03803	-4.40799	-3.64669	1.04852	4.38416	3.71108	1.07599
C	-3.62377	-4.37359	-1.13068	-3.64990	-4.35916	-1.14022	3.67431	4.38737	-1.13880
C	-5.39754	-4.61331	1.01766	-5.39463	-4.63492	1.02730	5.36698	4.70395	1.06430
H	-4.32293	-2.96036	1.89100	-4.30861	-2.99418	1.91122	4.26617	3.07294	1.94758
C	-4.62495	-5.34556	-1.15685	-4.64576	-5.33680	-1.16495	4.66377	5.37305	-1.15275
H	-2.93888	-4.27375	-1.96742	-2.97598	-4.24707	-1.98458	3.01795	4.26270	-1.99529
C	-5.51015	-5.47141	-0.08115	-5.51793	-5.47941	-0.08022	5.51062	5.53498	-0.05108
H	-6.07768	-4.71113	1.85830	-6.06385	-4.74551	1.87516	6.01501	4.83079	1.92633
H	-4.71391	-6.00288	-2.01641	-4.74198	-5.98494	-2.03076	4.77376	6.01260	-2.02335
H	-6.28353	-6.23316	-0.09942	-6.28812	-6.24440	-0.09836	6.27580	6.30511	-0.06136
C	3.50917	-3.50133	0.03382	3.52504	-3.49891	0.03469	-3.51911	3.50832	0.03348
C	3.62367	-4.37369	1.13063	3.65043	-4.35870	1.14014	-3.66606	4.32797	1.16544

C	4.41063	-3.62669	-1.03799	4.40879	-3.64582	-1.04837	-4.38273	3.69231	-1.05923
C	4.62484	-5.34566	1.15681	4.64646	-5.33618	1.16493	-4.66010	5.30816	1.20449
H	2.93873	-4.27389	1.96735	2.97634	-4.24683	1.98440	-3.00757	4.18505	2.01734
C	5.39756	-4.61330	-1.01762	5.39559	-4.63389	-1.02711	-5.36929	4.68033	-1.02258
H	4.32300	-2.96030	-1.89092	4.30945	-2.99322	-1.91101	-4.27002	3.06736	-1.94061
C	5.51009	-5.47146	0.08114	5.51884	-5.47851	0.08033	-5.51185	5.48843	0.10999
H	4.71375	-6.00304	2.01634	4.74263	-5.98441	2.03067	-4.77025	5.92796	2.08926
H	6.07774	-4.71108	-1.85823	6.06498	-4.74427	-1.87486	-6.02364	4.81959	-1.87788
H	6.28347	-6.23323	0.09942	6.28915	-6.24337	0.09851	-6.28192	6.25323	0.13956
C	3.50921	3.50130	0.03379	3.52445	3.49950	0.03458	-3.51911	-3.50833	0.03347
C	3.62372	4.37367	1.13059	3.64974	4.35935	1.14001	-3.66605	-4.32798	1.16542
C	4.41066	3.62663	-1.03803	4.40816	3.64652	-1.04850	-4.38272	-3.69231	-1.05924
C	4.62490	5.34563	1.15675	4.64560	5.33699	1.16473	-4.66009	-5.30817	1.20447
H	2.93879	4.27389	1.96731	2.97569	4.24740	1.98429	-3.00756	-4.18507	2.01732
C	5.39760	4.61323	-1.01768	5.39480	4.63474	-1.02729	-5.36929	-4.68033	-1.02260
H	4.32303	2.96023	-1.89096	4.30891	2.99387	-1.91111	-4.27001	-3.06735	-1.94062
C	5.51015	5.47140	0.08107	5.51794	5.47942	0.08011	-5.51185	-5.48844	0.10996
H	4.71382	6.00301	2.01627	4.74169	5.98526	2.03045	-4.77024	-5.92798	2.08923
H	6.07778	4.71100	-1.85829	6.06415	4.74520	-1.87506	-6.02364	-4.81959	-1.87790
H	6.28354	6.23316	0.09934	6.28813	6.24440	0.09825	-6.28191	-6.25324	0.13952
C	-3.50917	3.50133	-0.03379	-3.52504	3.49891	-0.03458	3.52537	-3.54380	-0.02458
C	-4.41055	3.62674	1.03808	-4.40857	3.64594	1.04865	4.38416	-3.71107	1.07601
C	-3.62375	4.37363	-1.13064	-3.65067	4.35856	-1.14011	3.67433	-4.38736	-1.13878
C	-5.39748	4.61336	1.01773	-5.39538	4.63400	1.02747	5.36698	-4.70393	1.06433
H	-4.32287	2.96040	1.89104	-4.30905	2.99343	1.91134	4.26616	-3.07293	1.94760
C	-4.62492	5.34560	-1.15679	-4.64671	5.33603	-1.16481	4.66378	-5.37304	-1.15272
H	-2.93887	4.27379	-1.96739	-2.97675	4.24659	-1.98449	3.01797	-4.26269	-1.99528
C	-5.51010	5.47146	-0.08107	-5.51887	5.47848	-0.08004	5.51063	-5.53497	-0.05105
H	-6.07761	4.71118	1.85838	-6.06460	4.74447	1.87535	6.01501	-4.83077	1.92636
H	-4.71389	6.00293	-2.01635	-4.74306	5.98415	-2.03060	4.77378	-6.01259	-2.02332
H	-6.28347	6.23322	-0.09933	-6.28919	6.24333	-0.09816	6.27581	-6.30510	-0.06132
Zn	0.00000	0.00000	0.00000	0.00000	0.00000	-0.00001	-0.05162	0.00000	-0.02057

H-ZnTPP, total charge 0

		Doublet			Quartet			Sextet	
N	2.05878	-0.00003	-0.06880	2.05955	0.00135	-0.07336	-1.42003	-1.37348	-0.00834
N	0.00135	-2.05783	-0.02748	-0.00159	-2.07834	-0.02207	-1.49745	1.51199	-0.23330
N	-2.05689	0.00003	0.01365	-2.06361	-0.00135	0.03495	1.44293	1.56742	-0.23015
N	0.00140	2.05785	-0.02752	-0.00430	2.07834	-0.02206	1.47073	-1.30559	0.05045
C	2.87839	1.10027	-0.03799	2.88373	1.10695	-0.00997	-1.20834	-2.67843	0.41477
C	4.26579	0.68149	0.01771	4.23788	0.69787	0.09629	-2.48486	-3.34441	0.55492
C	4.26577	-0.68159	0.01773	4.23879	-0.69232	0.09629	-3.44777	-2.45193	0.17757
C	2.87836	-1.10035	-0.03799	2.88518	-1.10317	-0.00994	-2.76964	-1.21312	-0.17189
C	2.44516	-2.44278	-0.03561	2.44066	-2.47125	-0.00388	-3.42035	-0.02068	-0.59667
C	1.10220	-2.87646	-0.03673	1.10712	-2.89966	-0.00713	-2.78092	1.25358	-0.66622
C	0.68409	-4.26448	-0.07133	0.68068	-4.28623	-0.00746	-3.36742	2.48022	-1.14246
C	-0.67915	-4.26557	-0.06594	-0.68033	-4.28716	-0.00143	-2.43193	3.48063	-0.94056
C	-1.09900	-2.87787	-0.04562	-1.10881	-2.90143	-0.02167	-1.29364	2.86565	-0.34613
C	-2.44114	-2.44378	-0.05154	-2.44306	-2.47362	-0.02462	-0.06276	3.50896	0.12571
C	-2.87382	-1.10044	-0.04456	-2.88713	-1.10601	-0.03174	1.19830	2.91314	-0.33008
C	-4.25747	-0.68161	-0.15521	-4.24204	-0.69676	-0.15160	2.32671	3.57446	-0.89811
C	-4.25745	0.68171	-0.15521	-4.24295	0.69122	-0.15159	3.29533	2.60812	-1.10011
C	-2.87380	1.10051	-0.04456	-2.88857	1.10224	-0.03173	2.73896	1.35620	-0.65074
C	-2.44108	2.44384	-0.05155	-2.44629	2.47043	-0.02461	3.41461	0.10016	-0.60199
C	-1.09893	2.87791	-0.04563	-1.11260	2.89998	-0.02167	2.80696	-1.11652	-0.19024
C	-0.67904	4.26561	-0.06596	-0.68594	4.28627	-0.00143	3.51704	-2.36630	0.04103
C	0.68419	4.26448	-0.07128	0.67507	4.28713	-0.00749	2.58689	-3.29429	0.41215
C	1.10227	2.87645	-0.03675	1.10333	2.90112	-0.00716	1.29887	-2.63395	0.40406
C	2.44522	2.44272	-0.03562	2.43744	2.47444	-0.00393	0.05655	-3.26945	0.63023
H	5.11924	1.34167	0.06649	5.09244	1.35218	0.18112	-2.62609	-4.35832	0.89915
H	5.11921	-1.34179	0.06653	5.09421	-1.34549	0.18113	-4.51734	-2.60082	0.16208
H	1.34444	-5.11856	-0.10218	1.33935	-5.14186	-0.01375	-4.34682	2.57488	-1.58778
H	-1.33825	-5.12105	-0.07733	-1.33754	-5.14368	0.01790	-2.51855	4.52882	-1.19036
H	-5.10727	-1.34202	-0.24606	-5.09497	-1.35177	-0.24672	2.38342	4.62841	-1.13150
H	-5.10724	1.34214	-0.24606	-5.09674	1.34511	-0.24671	4.27941	2.74029	-1.52497
H	-1.33813	5.12110	-0.07735	-1.34428	5.14193	0.01790	4.58300	-2.50426	-0.06257
H	1.34458	5.11854	-0.10208	1.33261	5.14362	-0.01380	2.75123	-4.33543	0.64852
C	-3.50284	-3.49737	-0.08182	-3.50670	-3.51932	-0.03740	-0.09091	4.65462	0.99233
C	-4.32443	-3.70880	1.03644	-3.66489	-4.37067	-1.14329	1.10811	5.25485	1.48695
C	-3.69844	-4.28534	-1.22678	-4.37457	-3.66542	1.05798	-1.31936	5.21296	1.46321

C	-5.31723	-4.69149	1.01235	-4.66383	-5.34743	-1.15265	1.07438	6.35198	2.33744
H	-4.17638	-3.10179	1.92486	-3.00457	-4.25608	-1.99787	2.06758	4.83534	1.21079
C	-4.69599	-5.26312	-1.25381	-5.36599	-4.64849	1.05326	-1.34016	6.31053	2.31350
H	-3.06815	-4.12253	-2.09622	-4.26138	-3.00653	1.91366	-2.25811	4.76096	1.16772
C	-5.50694	-5.47035	-0.13348	-5.51530	-5.49162	-0.05317	-0.14692	6.90273	2.75172
H	-5.94093	-4.84800	1.88794	-4.77713	-5.99296	-2.01907	2.00927	6.77894	2.69039
H	-4.83981	-5.86075	-2.14955	-6.02172	-4.75559	1.91279	-2.29596	6.70518	2.64756
H	-6.28078	-6.23238	-0.15345	-6.28990	-6.25314	-0.05858	-0.16824	7.76278	3.41424
C	3.50317	-3.50046	-0.02274	3.50487	-3.51645	0.02458	-4.86243	-0.10459	-0.94643
C	3.70030	-4.29655	1.11641	3.66774	-4.34534	1.14658	-5.82014	0.68503	-0.28266
C	4.31563	-3.71160	-1.14758	4.36793	-3.68422	-1.07132	-5.30696	-0.98714	-1.94879
C	4.69139	-5.28109	1.13149	4.66694	-5.32159	1.17129	-7.17451	0.59491	-0.60922
H	3.07611	-4.13459	1.99037	3.01055	-4.21393	2.00116	-5.49386	1.36113	0.50203
C	5.30202	-4.70102	-1.13543	5.36002	-4.66655	-1.05092	-6.66100	-1.07667	-2.27763
H	4.16575	-3.09916	-2.03200	4.25073	-3.04291	-1.93978	-4.57806	-1.59712	-2.47465
C	5.49383	-5.48745	0.00490	5.51411	-5.48732	0.07150	-7.60109	-0.28570	-1.60908
H	4.83658	-5.88488	2.02284	4.78376	-5.94994	2.04978	-7.89774	1.20745	-0.07787
H	5.91885	-4.85713	-2.01596	6.01230	-4.79060	-1.91079	-6.98084	-1.75972	-3.05973
H	6.26258	-6.25481	0.01558	6.28901	-6.24835	0.08895	-8.65473	-0.35502	-1.86392
C	3.50327	3.50037	-0.02274	3.50030	3.52102	0.02451	0.09418	-4.69633	1.07137
C	3.70045	4.29641	1.11644	3.66214	4.35011	1.14650	0.59746	-5.03209	2.33872
C	4.31572	3.71151	-1.14759	4.36315	3.68984	-1.07139	-0.35620	-5.72559	0.22879
C	4.69157	5.28092	1.13153	4.66012	5.32760	1.17120	0.64324	-6.36444	2.75675
H	3.07626	4.13445	1.99040	3.00514	4.21787	2.00110	0.94758	-4.24083	2.99541
C	5.30214	4.70089	-1.13541	5.35401	4.67342	-1.05099	-0.30674	-7.05856	0.64422
H	4.16579	3.09910	-2.03201	4.24677	3.04837	-1.93983	-0.73685	-5.47420	-0.75689
C	5.49400	5.48728	0.00493	5.50707	5.49439	0.07141	0.19158	-7.38186	1.91034
H	4.83680	5.88467	2.02289	4.77616	5.95610	2.04970	1.02970	-6.60644	3.74278
H	5.91897	4.85701	-2.01596	6.00614	4.79827	-1.91087	-0.65331	-7.84344	-0.02219
H	6.26277	6.25461	0.01562	6.28103	6.25639	0.08885	0.22883	-8.41808	2.23402
C	-3.50276	3.49746	-0.08183	-3.51127	3.51476	-0.03736	4.85355	0.06709	-0.98100
C	-4.32437	3.70888	1.03641	-4.37928	3.65977	1.05806	5.80406	0.83372	-0.28258
C	-3.69830	4.28546	-1.22678	-3.67056	4.36594	-1.14322	5.29740	-0.73613	-2.04712
C	-5.31714	4.69160	1.01233	-5.37194	4.64160	1.05339	7.15426	0.79694	-0.63689
H	-4.17635	3.10185	1.92483	-4.26522	3.00103	1.91374	5.47575	1.45129	0.54832
C	-4.69584	5.26327	-1.25381	-4.67073	5.34143	-1.15255	6.64721	-0.77261	-2.40374
H	-3.06799	4.12266	-2.09620	-3.01012	4.25219	-1.99782	4.57228	-1.32694	-2.59952
C	-5.50681	5.47049	-0.13350	-5.52234	5.48455	-0.05303	7.58144	-0.00607	-1.69970
H	-5.94086	4.84810	1.88790	-6.02776	4.74788	1.91294	7.87329	1.39081	-0.07933
H	-4.83962	5.86091	-2.14954	-4.78486	5.98683	-2.01896	6.96783	-1.39518	-3.23447
H	-6.28063	6.23254	-0.15346	-6.29790	6.24509	-0.05841	8.63155	-0.03414	-1.97615
Zn	0.00372	0.00000	0.50945	-0.00338	0.00000	-0.00039	-0.00261	0.12125	0.05174
H	0.07274	0.00022	2.13897	1.08613	-0.00045	2.39274	-0.16744	0.54603	2.00144