Supporting Information

Interpretation of the UV-vis spectra of the *meso*(ferrocenyl)-containing porphyrins using TDDFT approach: is classic Gouterman's four-orbital model still in play?

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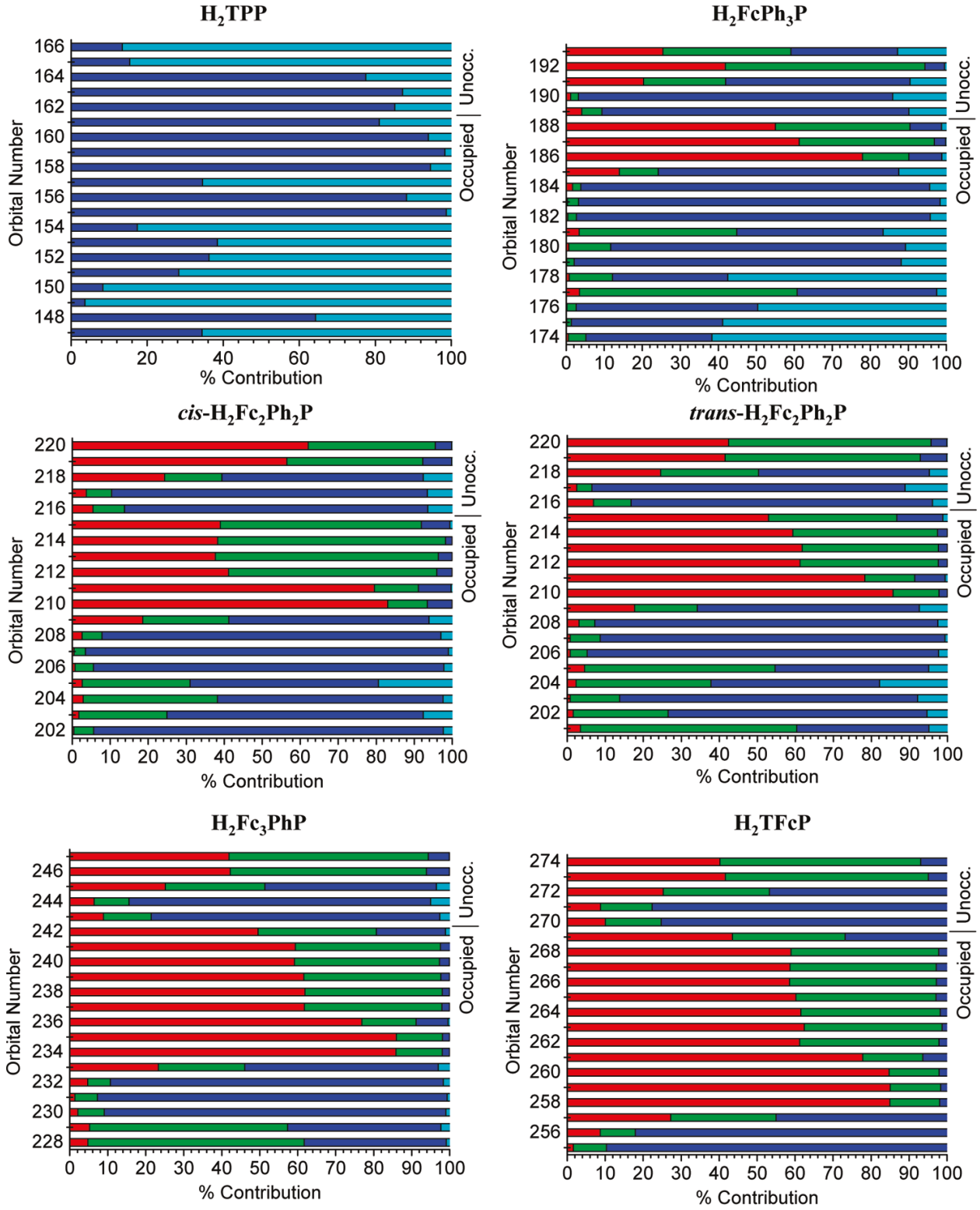
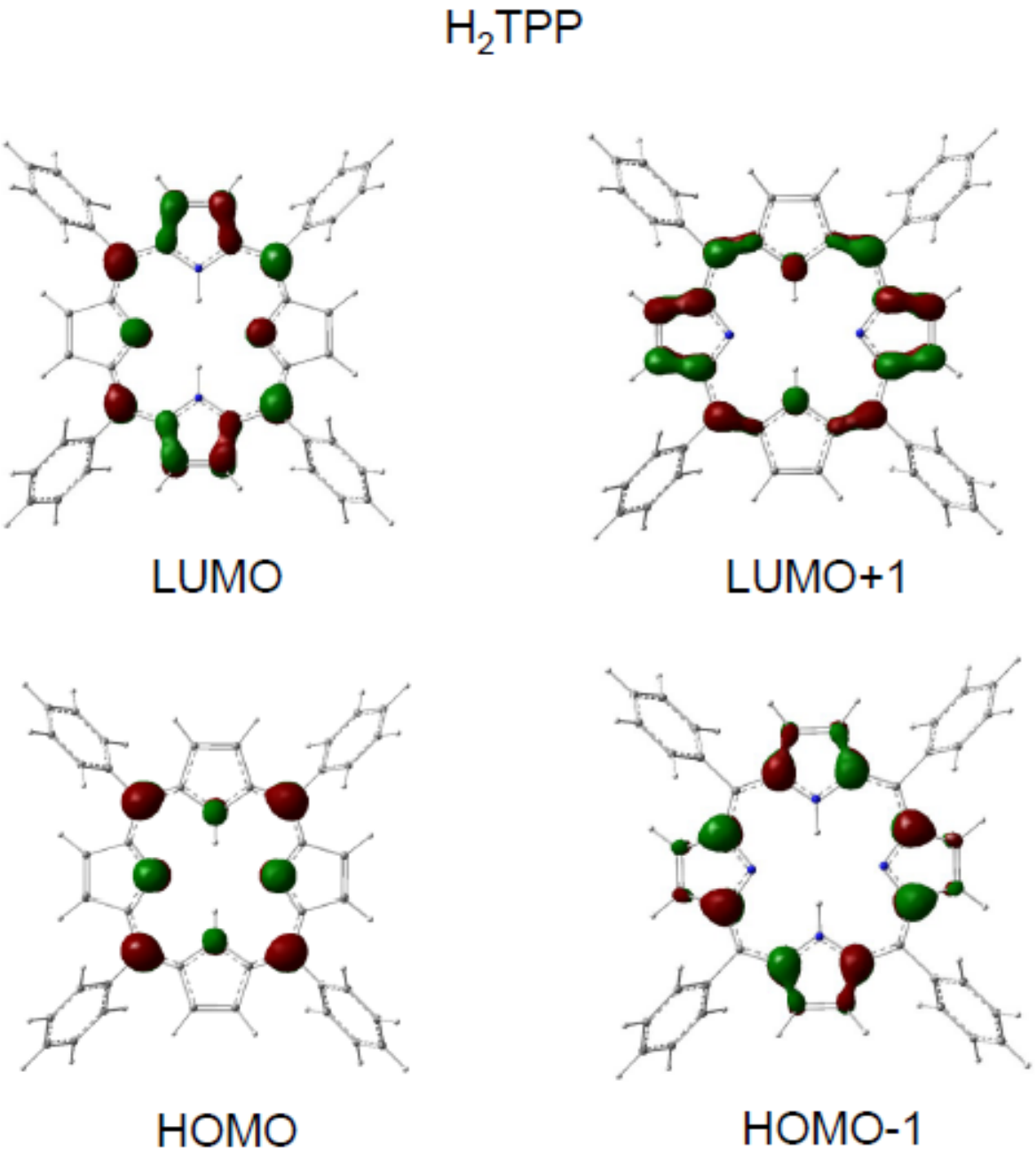
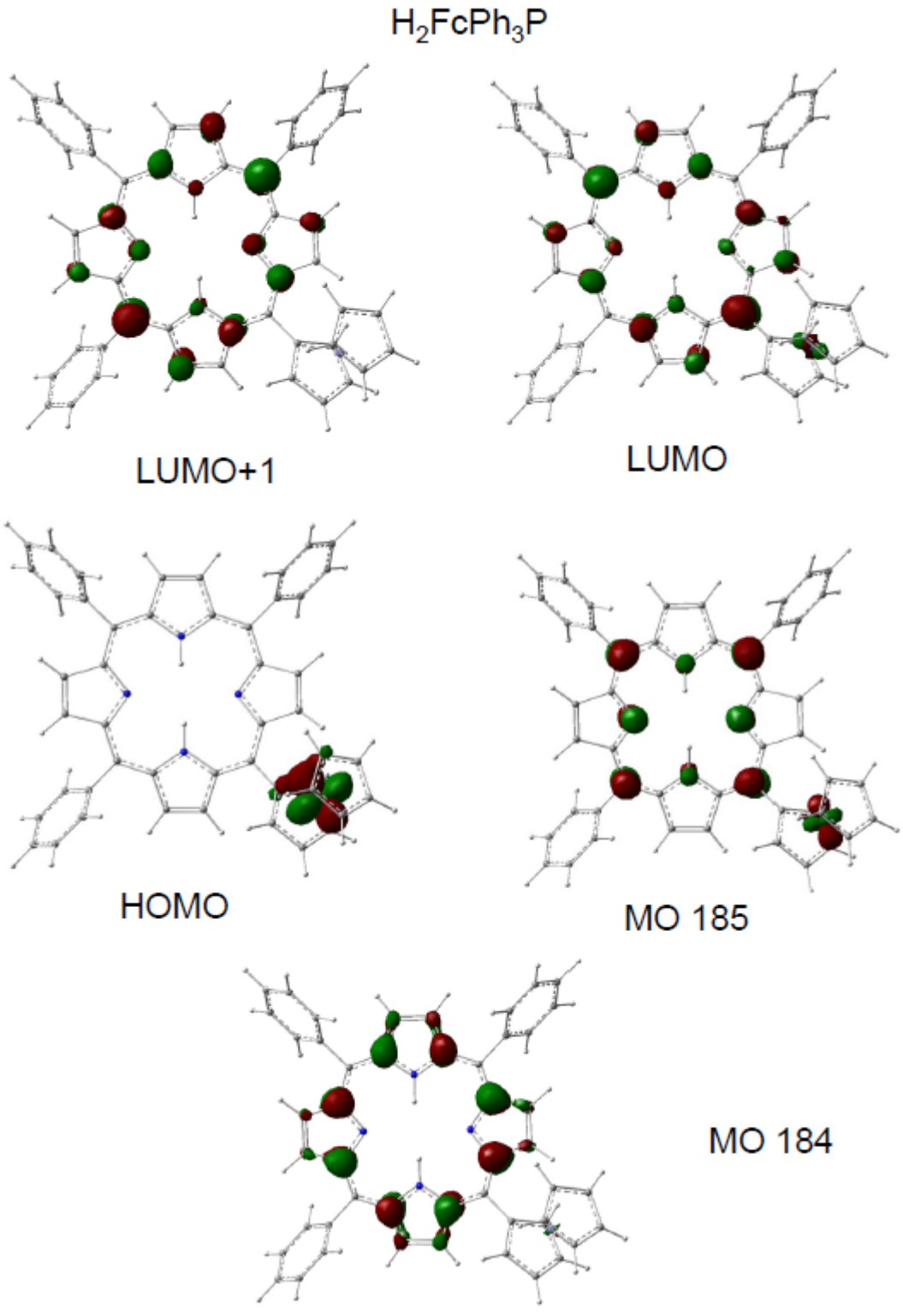


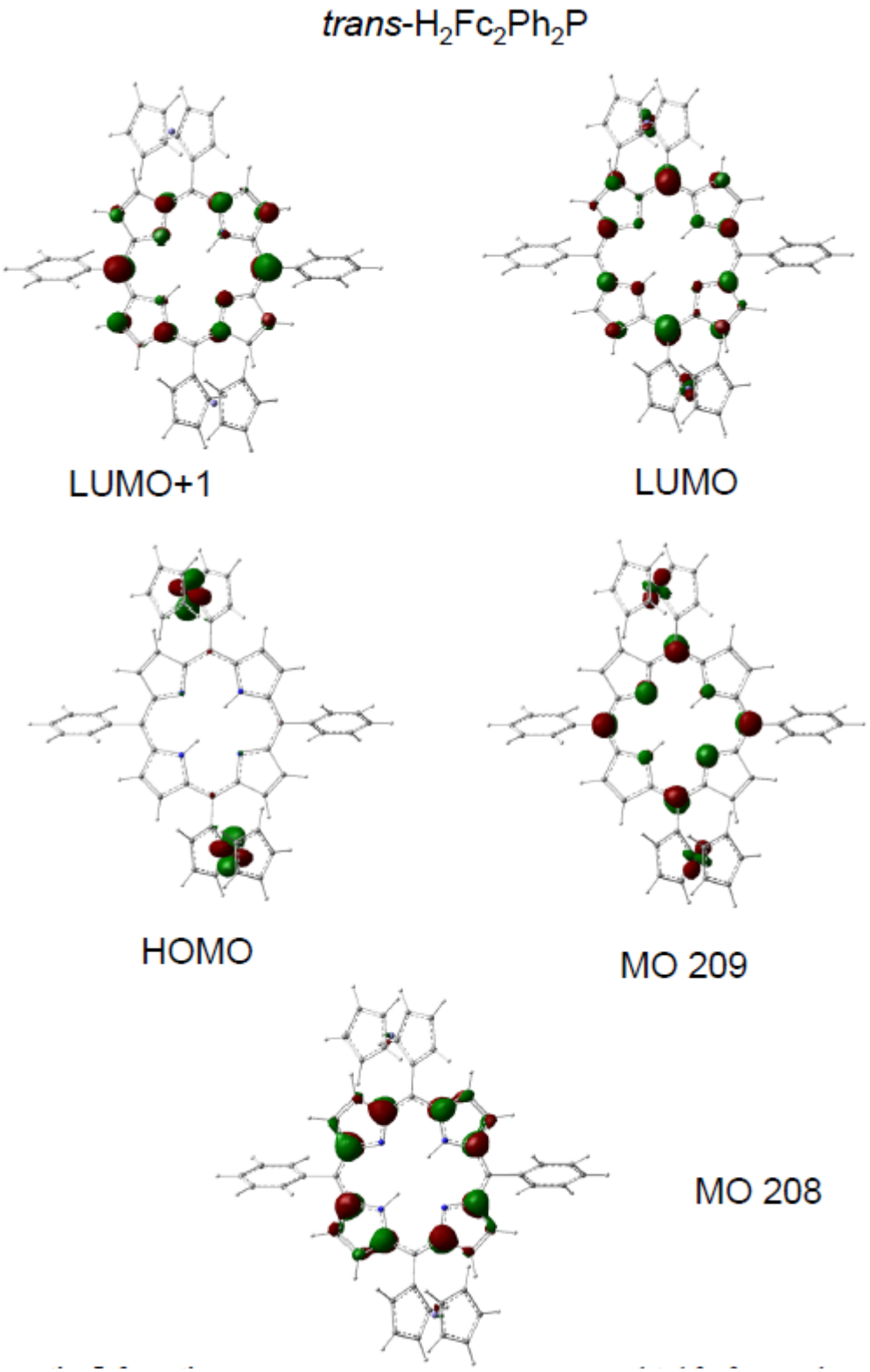
Supporting Information Figure 1. Molecular orbital compositions for frontier orbitals in ferrocenyl-containing porphyrins and H_2TPP predicted at the DFT level. Contributions from iron AOs are in red, cyclopentadienyl ligands are in green, porphyrin core is in blue, and phenyl substituents are in cyan.



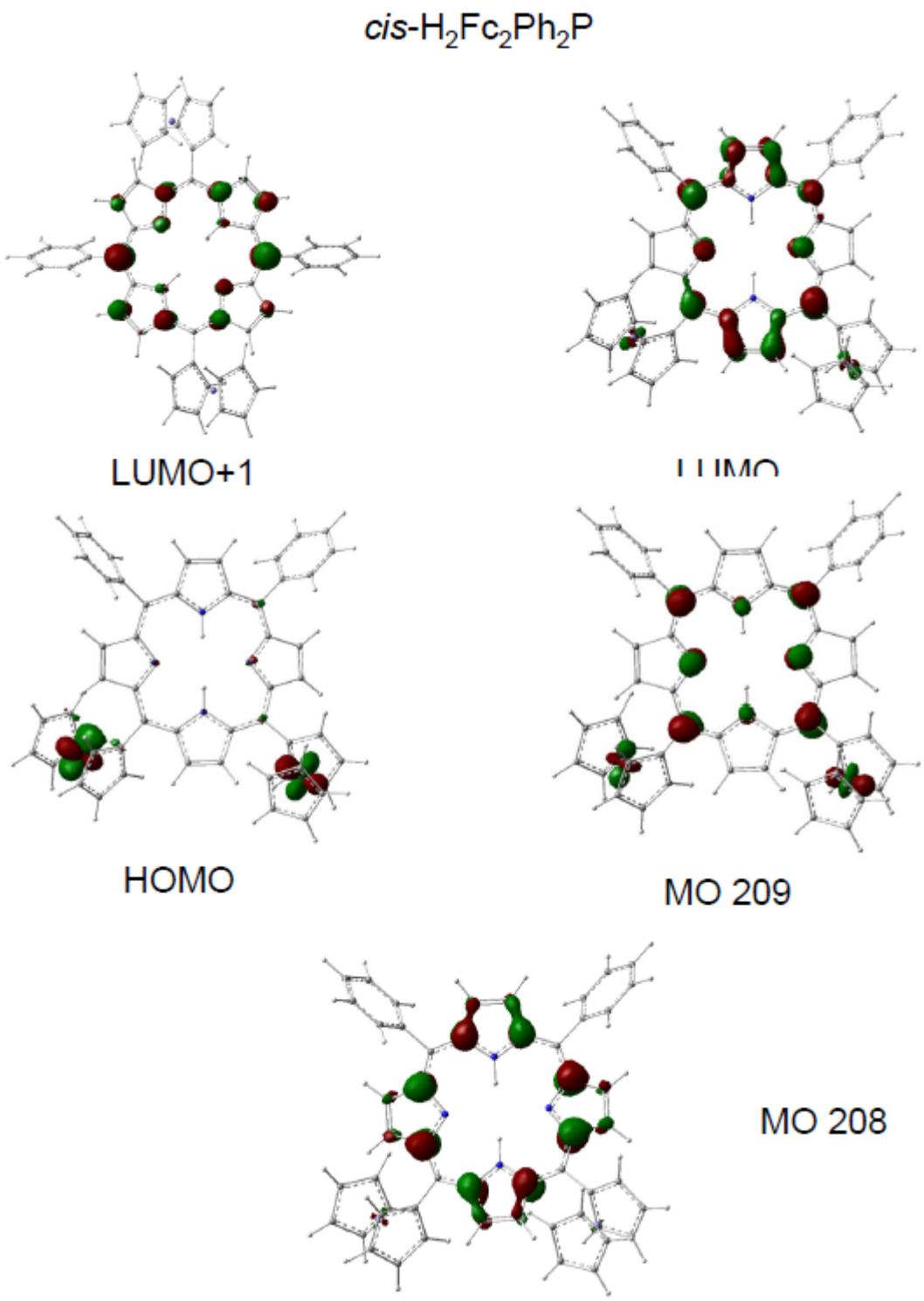
Supporting Information Figure 2. Important frontier orbitals calculated for ferrocenyl-containing porphyrins and H_2TPP.



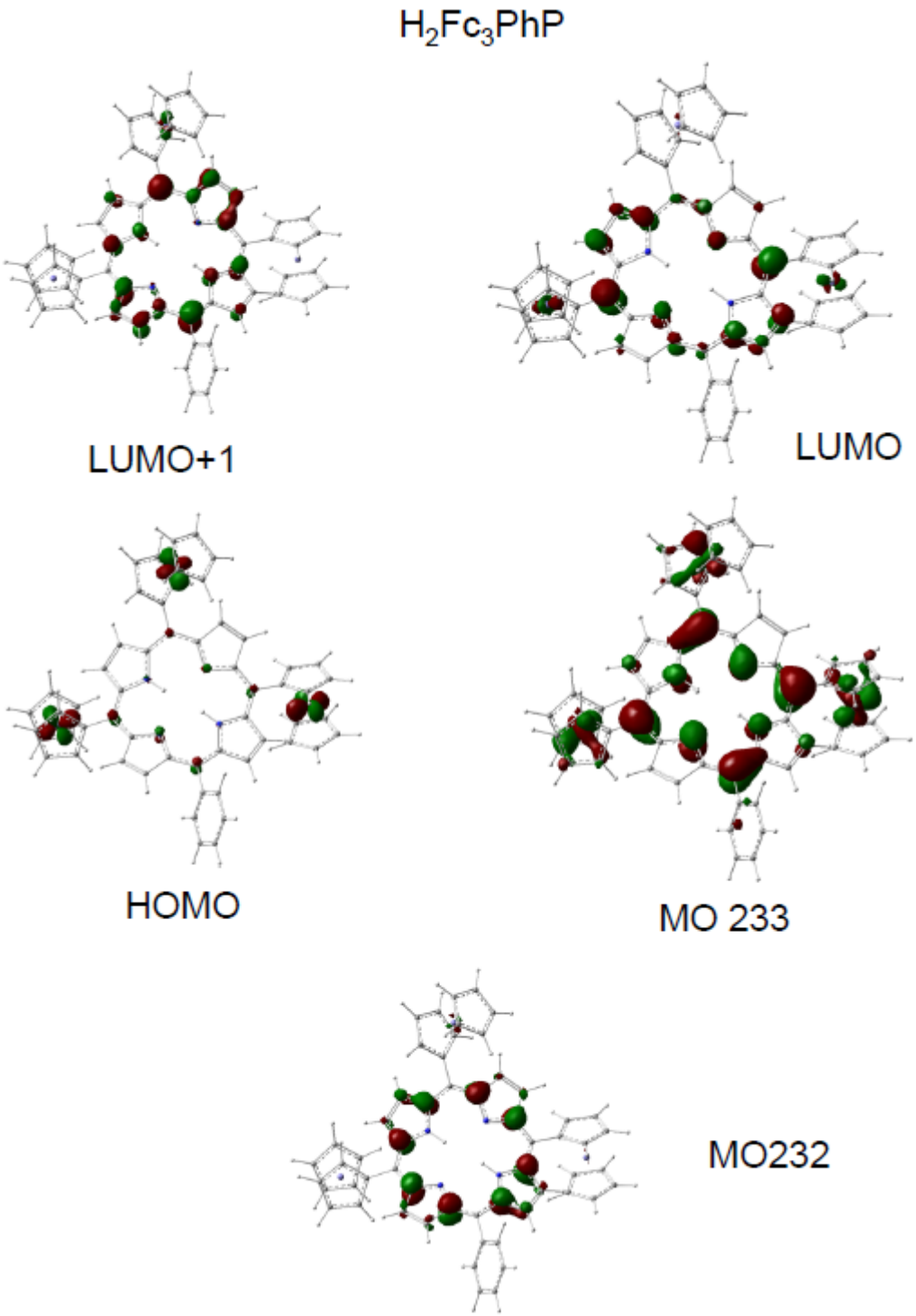
Supporting Information Figure 2. Important frontier orbitals calculated for ferrocenyl-containing porphyrins and H_2TPP.



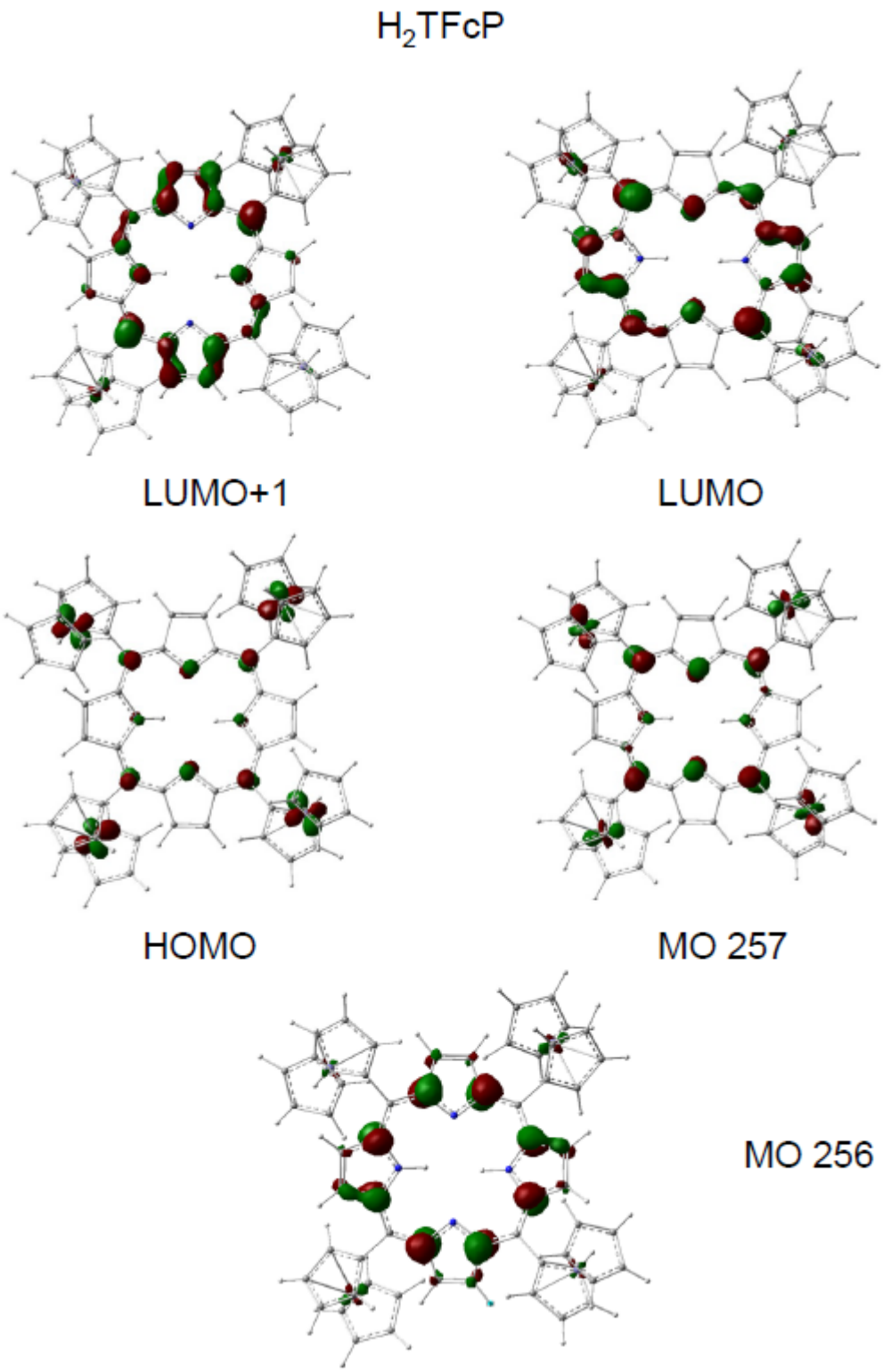
Supporting Information Figure 2. Important frontier orbitals calculated for ferrocenyl-containing porphyrins and H_2TPP.



Supporting Information Figure 2. Important frontier orbitals calculated for ferrocenyl-containing porphyrins and H_2TPP.



Supporting Information Figure 2. Important frontier orbitals calculated for ferrocenyl-containing porphyrins and H_2TPP.



Supporting Information Figure 2. Importantfrontier orbitals calculated for ferrocenyl-containing porphyrins and H_2TPP.

Supporting Information Table 1. Selected energies, oscillator strengths, and expansion coefficients for vertical transitions in **H_2TPP** calculated using a TDDFT approach. [a]

Transition	Symmetry	E, eV	E, nm	*f*	Predominant character	Major expansion coefficients for single-electron transitions
1	^{1}B	2.0165	615	0.0303	$\pi \rightarrow \pi^*$	**160** → **162**, -0.39790; **161** → **163**, 0.55138
2	^{1}B	2.1338	581	0.0457	$\pi \rightarrow \pi^*$	**160** → **163**, 0.40203; **161** → **162**, 0.52474
4	^{1}B	2.8495	435	0.2398	$\pi \rightarrow \pi^*$	158 → **163**, 0.53841; **160** → **162**, 0.32933; **161** → **163**, 0.16544
6	^{1}B	2.9025	427	0.0838	$\pi \rightarrow \pi^*$	158 → **162**, 0.63080; **160** → **163**, -0.18218; **161** → **162**, 0.13232
7	^{1}B	3.0789	403	0.9825	$\pi \rightarrow \pi^*$	146 → **162**, 0.16064; 148 → **162**, -0.17478; 149 → **163**, 0.13823; 158 → **162**, 0.27031; **160** → **163**, 0.39842; **161** → **162**, -0.23093; **161** → 172, 0.11122
8	^{1}B	3.1189	398	0.8390	$\pi \rightarrow \pi^*$	146 → **163**, -0.13842; 148 → **163**, 0.19171; 149 → **162**, 0.11183; 155 → **163**, 0.10506; 158 → **163**, -0.39913; 159 → 164, 0.12241; **160** → **162**, 0.31290; **161** → **163**, 0.20578; **161** → 170, 0.10295
12	^{1}B	3.2849	377	0.0191	$\pi \rightarrow \pi^*$	154 → **162**, 0.16926; 155 → **163**, 0.67322
15	^{1}B	3.2981	376	0.0537	$\pi \rightarrow \pi^*$	154 → **162**, -0.21832; 154 → **163**, 0.64136; 155 → **162**, 0.15482
16	^{1}B	3.2984	376	0.0358	$\pi \rightarrow \pi^*$	154 → **162**, 0.63779; 154 → **163**, 0.21944; 155 → **163**, -0.16112
17	^{1}B	3.3140	374	0.0114	$\pi \rightarrow \pi^*$	154 → **163**, -0.15825; 155 → **162**, 0.67844
18	^{1}A	3.3451	371	0.0010	$\pi \rightarrow \pi^*$	153 → **162**, 0.67284
23	^{1}B	3.4201	363	0.0217	$\pi \rightarrow \pi^*$	146 → **162**, -0.17958; 149 → **163**, -0.10296; 151 → **162**, 0.65620; **161** → 167, -0.10196
26	^{1}B	3.4569	359	0.0074	$\pi \rightarrow \pi^*$	146 → **163**, 0.10145; 148 → **163**, -0.12344; 149 → **162**, 0.67604
27	^{1}B	3.4620	358	0.0190	$\pi \rightarrow \pi^*$	146 → **162**,-0.10520; 148 → **162**, 0.18283; 149 → **163**, 0.65954
28	^{1}B	3.5142	353	0.0616	$\pi \rightarrow \pi^*$	148 → **163**, -0.26036; **161** → 166, 0.64551
29	^{1}B	3.5242	352	0.0710	$\pi \rightarrow \pi^*$	148 → **162**, -0.29662; **161** → 167, 0.62006
31	^{1}B	3.5602	348	0.0028	$\pi \rightarrow \pi^*$	148 → **162**, 0.48115; **161** → 167, 0.26779; **161** → 172, 0.40972
34	^{1}A	3.5701	347	0.0012	$\pi \rightarrow \pi^*$	**160** → 164, 0.23556; **161** → 169, 0.64501
40	^{1}B	3.6680	338	0.0599	$\pi \rightarrow \pi^*$	148 → **163**, 0.40367; 149 → **162**, 0.10417; **160** → 172, 0.12879; **161** → 166, 0.14084; **161** → 170, 0.46050

[a] Only transitions with oscillator strengths greater than 0.001 are shown. Gouterman's four-orbital model MOs are shown in bold.

Supporting Information Table 2. Selected energies, oscillator strengths, and expansion coefficients for vertical transitions in **H_2FcPh_3P** calculated using a TDDFT approach. [a]

Transition	Symmetry	E, eV	E, nm	*f*	Predominant character	Major expansion coefficients for single-electron transitions
1	^{1}A	1.3351	929	0.0046	Fc → π*	**187** → **189**, -0.30138; **7** → **190**,-0.11808; **188** → **189**, 0.46008; **188** → **190**; 0.40698
3	^{1}A	1.3910	891	0.0023	Fc → π*	**187** → **190**; 0.68734; **188** → **189**, 0.13185
4	^{1}A	1.4007	885	0.0393	Fc → π*	185 → **189**, 0.11304; 186 → **189,** 0.10017; **187** → **189**, 0.25297; **188** → **189**, 0.46234; **188** → **190**, -0.38741
5	^{1}A	1.6206	765	0.0048	Fc → π*	185 → **189**, -0.14865; 186 → **189,** 0.65188; 186 → **190**, 0.19447
6	^{1}A	1.6648	745	0.0122	Fc → π*	185 → **189**, 0.11687; 185 → **190**, -0.13998; 186 → **189**. -0.17020; 186 → **190,** 0.65054
7	^{1}A	1.9972	621	0.0451	π → π*	184 → **189,** -0.20520; 184 → **190**, 0.32081; 185 → **189**, 0.45162; 185 → **190**, 0.31736
8	^{1}A	2.1089	588	0.0492	π → π*	184 → **189**, -0.34707; 184 → **190**, -0.18964; 185 → **189**, -0.29592; 185 → **190**, 0.42413
9	^{1}A	2.4686	502	0.0126	Fc → π*	**187** → 192, -0.19971; **188** → 191, 0.64746
10	^{1}A	2.5050	495	0.0014	Fc → π*	**187** → 191, 0.64055; **188** → 192, 0.26636
11	^{1}A	2.7078	458	0.0178	Fc → π*	186 → 191, 0.42789; **187** → 192, -0.26163; **187** → 193, -0.25715; **188** → 192, -0.37050
12	^{1}A	2.7348	453	0.0104	Fc → π*	186 → 191, 0.11596; 186 → 192, 0.11488; **187** → 192, -0.37325; **187** → 193, 0.23117; **188** → 192, 0.29748; **188** → 193, 0.39874
13	^{1}A	2.7566	450	0.0264	Fc → π*	186 → 191, 0.44375; **187** → 192, 0.14528; **187** → 193, 0.28888; **188** → 192, 0.17089; **188** → 193, -0.35702
14	^{1}A	2.7919	444	0.0335	π → π*	183 → **189**, 0.61956; 183 → **190**, 0.20477
15	^{1}A	2.8078	442	0.2073	π → π*	182 → **189**, 0.39710; 182 → **190**, 0.20762; 183 → **189**, -0.15796; 183 → **190**, -0.12077; 184 → **189**, 0.18825; 184 → **190**, -0.24398; 185 → **190**, 0.11069; 185 → 191, -0.11488; 186 → 191, 0.19948
16	^{1}A	2.8685	432	0.2583	π → π*	182 → **189**, -0.30528; 182 → **190**, 0.38525; 184 → **189**, 0.25611; 184 → **190**, 0.11871; 185 → **190**, 0.15304; 185 → 191, 0.14506
18	^{1}A	2.8993	428	0.0045	Fc → π*	182 → **189**, 0.12552; 185 → 191, 0.10757; 186 → 192, 0.55573;

						187 → 192, -0.14994; **187** → 193, -0.21330; **188** → 193, -0.23947
19	^{1}A	2.9662	418	0.1399	π → π*	181 → **189**, -0.14939; 182 → **189**, 0.23926; 182 → **190**, -0.11763; 184 → **190**, 0.12190; 185 → 191, 0.53220; 186 → 192, -0.16420; 186 → 193, 0.10030
20	^{1}A	3.0053	413	0.3264	π → π*	181 → **190**, 0.15028; 182 → **190**, 0.34690; 184 → **189**, -0.19730; 184 → **190**, -0.13133; 185 → **190**, -0.10642; 185 → 191, 0.14230; 185 → 192, 0.19392; 186 → 193, 0.20632; **187** → 193, 0.18330; **188** → 195, -0.14404
21	^{1}A	3.0097	412	0.0126	Fc → π*	185 → 192, -0.14151; 186 → 193, -0.19663; **187** → 193, -0.15827; **188** → 194, -0.60778
22	^{1}A	3.0162	411	0.1301	Fc → π*	181 → **190**, -0.13126; 182 → **190**, -0.16014; 184 → **189**, 0.11665; 185 → 191, -0.13779; 185 → 192, 0.21496; 186 → 193, 0.29284; **187** → 193, 0.21912; **188** → 192, -0.11630; **188** → 194, -0.34725; **188** → 195, 0.11748
23	^{1}A	3.0324	409	0.0290	Fc → π*	182 → **190**, 0.10249; **188** → 195, 0.67289
24	^{1}A	3.0440	407	0.4706	π → π*	172 → **189**, 0.13254; 181 → **189**, -0.31121; 182 → **189**, -0.29491; 182 → **190**, -0.25753; 184 → **190**, -0.22047; 185 → **189**, 0.11804; 185 → 191, 0.10526; **188** → 199, -0.17426
25	^{1}A	3.0676	404	0.0019	Fc → π*	**187** → 194, 0.70417
27	^{1}A	3.0787	403	0.0055	Fc → π*	185 → 192, 0.45237; 186 → 192, 0.14678; 186 → 193, -0.31339; **188** → 196, 0.19059; **188** → 197, 0.30152; **188** → 198, 0.10951
29	^{1}A	3.0959	400	0.0060	Fc → π*	**187** → 195, 0.70375
30	^{1}A	3.1061	399	0.0022	Fc → π*	186 → 193, 0.10569; **188** → 198, 0.68232
31	^{1}A	3.1206	397	0.0306	Fc → π*	181 → **189**, -0.16345; **188** → 199, 0.66991
33	^{1}A	3.1484	394	0.0053	Fc → π*	181 → **190**, 0.15454; 185 → 192, -0.10447; **187** → 197, 0.65603
34	^{1}A	3.1513	393	0.0526	π → π*	181 → **189**, 0.29723; 181 → **190**, 0.48280; 184 → 191, -0.27964; **187** → 197, -0.21300
35	^{1}A	3.1617	392	0.0018	Fc → π*	**187** → 198, 0.69805
36	^{1}A	3.1734	391	0.0018	Fc → π*	**187** → 199, 0.69890
37	^{1}A	3.2110	386	0.1106	π → π*	176 → **189**, 0.20670; 177 → **189**, -0.16234; 180 → **189**, 0.35252; 181 → **189**, -0.29686, 181 → **190**, 0.25840; 184 → **190**, 0.12255; 185 → 191, -0.14076

38	^{1}A	3.2129	386	0.0186	$\pi \rightarrow \pi^*$	176 → **189**, -0.16957; 179 → **189**, 0.10653; 180 → **189**, 0.56142; 180 → **190**, 0.17676; 181 → **189**, 0.16985; 181 → **190**, -0.13684; 184 → 191, -0.12232
39	^{1}A	3.2425	382	0.0050	$\pi \rightarrow \pi^*$	179 → **189**, 0.64757; 179 → **190**, 0.16236; 185 → 193, -0.11999
40	^{1}A	3.2559	381	0.0316	$\pi \rightarrow \pi^*$	178 → **189**, 0.50717; 179 → **189**, 0.10237; 180 → **190**, -0.36706; 185 → 193, 0.21882

[a] Only transitions with oscillator strengths greater than 0.001 are shown. Gouterman's four-orbital model MOs are shown in bold.

Supporting Information Table 3. Selected energies, oscillator strengths, and expansion coefficients for vertical transitions in ***cis*-$H_2PFc_2Ph_2$** calculated using a TDDFT approach.[a]

Transition	Symmetry	E, eV	E, nm	*f*	Predominant character	Major expansion coefficients for single-electron transitions
1	^{1}A	1.3202	939	0.0028	Fc → π*	213 → **216**, -0.11103; **214** → **216**, 0.48313; **215** → **216**, -0.15779; **215** → **217**, -0.45682
2	^{1}A	1.3301	932	0.0098	Fc → π*	209 → **216**, 0.10595; 213 → **216**, 0.15304; 213 → **217**; -0.12761; **214** → **217**, -0.36773; **215** → **216**, 0.50391; **215** → **217**; -0.16653
3	^{1}A	1.3547	915	0.0018	Fc → π*	212 → **216**, 0.46806; 213 → **216**, 0.36638; 213 → **217**, -0.14222; **214** → **216**, 0.24522; **214** → **217**, 0.16878; **215** → **217**, 0.17367
4	^{1}A	1.3584	913	0.0025	Fc → π*	212 → **216**, -0.41486; 212 → **217**, -0.13611; 213 → **216**, 0.52123; **215** → **216**, -0.15290
6	^{1}A	1.3839	896	0.0030	Fc → π*	212 → **216**, -0.11593; 212 → **217**, 0.48919; 213 → **217**, -0.15913; **214** → **216**, -0.13954; **214** → **217**, 0.39709; **215** → **216**, 0.10177; **215** → **217**, -0.12746
7	^{1}A	1.4050	882	0.0440	Fc → π*	212 → **216,** -0.28207; 213 → **216**, -0.13434; 213 → **217**, 0.10825; **214** → **216**, 0.38059; **214** → **217**, 0.18675; **215** → **216**, 0.23613; **215** → **217**, 0.31916
8	^{1}A	1.4282	868	0.0331	Fc → π*	212 → **217**, 0.43710; **214** → **216**, 0.13792; **214** → **217**, -0.35479; **215** → **216**, -0.23608; **215** → **217**, 0.22188
9	^{1}A	1.6228	764	0.0059	Fc → π*	209 → **216**, 0.16088; 210 → **216**, 0.13636; 210 → **217**, -0.18752; 211 → **216**, 0.63533
10	^{1}A	1.6317	760	0.0032	Fc → π*	210 → **216**, 0.56372; 211 → **216**, -0.10067; 211 → **217**, -0.39470
11	^{1}A	1.6583	748	0.0170	Fc → π*	209 → **217**, 0.15115; 210 → **216**, 0.38694; 210 → **217**, 0.10104; 211 → **217**, 0.54381
12	^{1}A	1.6684	743	0.0064	Fc → π*	210 → **217**, 0.66617; 211 → **216**, 0.17706
13	^{1}A	1.9911	623	0.0320	π → π*	208 → **216**, 0.37623; 209 → **216**, 0.18667; 209 → **217**, 0.51808
14	^{1}A	2.0881	594	0.0638	π → π*	208 → **217**, -0.36624; 209 → **216**, 0.49542; 209 → **217**, -0.17197; 211 → **216**, -0.10312
15	^{1}A	2.3444	529	0.0209	Fc → π*	**215** → 218, 0.66960
16	^{1}A	2.3909	519	0.0034	Fc → π*	**214** → 218, 0.67143; **215** → 219, 0.12823

18	^{1}A	2.4201	512	0.0015	Fc → π*	212 → 218, 0.67426
19	^{1}A	2.5746	482	0.0028	Fc → π*	212 → 220, -0.10415; **214** → 219, 0.25914; **214** → 220, 0.13691; **215** → 219, 0.57816; **215** → 220, 0.17920
20	^{1}A	2.5871	479	0.0021	Fc → π*	213 → 221, -0.10240; **214** → 219, 0.24493; **214** → 220, -0.25283; **215** → 219, -0.18451; **215** → 220, 0.55221
21	^{1}A	2.6329	471	0.0133	Fc → π*	212 → 219, 0.10098; 213 → 219, -0.34890; **215** → 221, 0.56741
22	^{1}A	2.6386	470	0.0038	Fc → π*	211 → 218, 0.12730; 212 → 219, 0.11620; 212 → 220, 0.14211; 213 → 219, 0.49453; 213 → 220, 0.16873; **214** → 220, 0.37371; **215** → 221, 0.15231
23	^{1}A	2.6428	469	0.0165	Fc → π*	211 → 218, 0.61586; 213 → 220, -0.13926; **214** → 219, -0.22187;
24	^{1}A	2.6536	467	0.0013	Fc → π*	210 → 218, -0.12326; 212 → 219, 0.39768; 212 → 220, -0.35396; 213 → 219, 0.10097; 213 → 220, 0.31440; 213 → 221, 0.10684; **214** → 220, -0.25884
25	^{1}A	2.6684	465	0.0061	Fc → π*	210 → 218, 0.61394; 212 → 220, -0.29636; **214** → 219, 0.10320
26	^{1}A	2.6798	463	0.0020	Fc → π*	211 → 218, 0.17773; 212 → 219, -0.25575; 212 → 221, 0.30584; 213 → 220, 0.10829; 213 → 221, 0.15832; **214** → 219, 0.26464; **214** → 221, 0.39311; **215** → 220, -0.14217
29	^{1}A	2.7663	448	0.3195	π → π*	206 → **216**, -0.14808; 206 → **217**, -0.35729; 208 → **216**, 0.34288; 209 → **217**, -0.15862; 209 → 218, 0.18170
30	^{1}A	2.7841	445	0.0138	π → π*	207 → **216**, 0.38265; 207 → **217**, 0.50241; **215** → 222, -0.19565
31	^{1}A	2.7878	445	0.0400	Fc → π*	206 → **216**, -0.10766; 207 → **216**, 0.13713; 208 → **217**, -0.11072; 213 → 219, -0.10023; 213 → 220, 0.22963; **214** → 221, -0.15682; **214** → 222, 0.11422; **215** → 222, 0.52282
32	^{1}A	2.7993	443	0.0862	Fc → π*	206 → **216**, -0.22516; 207 → **217**, -0.26388; 208 → **217**, -0.16539; 209 → 218, 0.10348; 211 → 219, 0.16917; 212 → 219, 0.17630; 212 → 220, 0.11494; 212 → 222, -0.15642; 213 → 219, -0.13416; **214** → 220, 0.11993; **214** → 222, 0.23290; **215** → 221, -0.10334; **215** → 222, -0.23411
33	^{1}A	2.8247	439	0.0032	π → π*	206 → **216**, -0.15223; 207 → **216**, 0.48661; 207 → **217**, -0.34376; **214** → 222, -0.17233
34	^{1}A	2.8314	438	0.0035	Fc → π*	210 → 220, 0.12927; 211 → 221, -0.13065; 212 → 220, 0.11864; 212 → 222, 0.22941; 213 → 221, -0.32927; 213 → 222, 0.37525; **214** → 220, -0.17630; **214** → 222, 0.20416; **215** → 220, -0.11155

35	^{1}A	2.8342	437	0.0016	Fc → π*	210 → 221, 0.14546; 212 → 221, 0.36636; 212 → 222, 0.29709; 213 → 222, -0.30534; **214** → 219, -0.18544; **214** → 222, 0.24541; **215** → 220, 0.10462
36	^{1}A	2.8570	434	0.0453	π → π*	206 → **216**, 0.46278; 206 → **217**, -0.18229; 207 → **216**, 0.23057; 207 → **217**, -0.10942; 208 → **217**, 0.11540; **214** → 222, 0.18681; **215** → 221, -0.10103
37	^{1}A	2.8833	430	0.0066	π → π*	205 → **216**, 0.16104; 206 → **217**, 0.25065; 209 → 218, 0.43744; 210 → 219, 0.18732; 211 → 22, -0.25281; 212 → 219, -0.10243; 213 → 220, 0.11419; 213 → 222, 0.11281; **214** → 221, -0.12280; **215** → 222, -0.12420
38	^{1}A	2.8916	429	0.0040	Fc → π*	210 → 219, 0.12503; 211 → 219, 0.58837; **214** → 222, -0.32034
39	^{1}A	2.9065	427	0.0964	π → π*	205 → **216**, 0.16942; 206 → **216**, -0.16120; 206 → **217**, 0.14239; 208 → **217**, 0.13826; 209 → 218, 0.24016; 211 → 220, 0.46755; **214** → 222, 0.10592; **215** → 222, 0.16568
40	^{1}A	2.9106	426	0.1210	Fc → π*	206 → **216**, 0.17562; 208 → **217**, -0.15364; 210 → 219, 0.48499; 211 → 220, 0.36348
41	^{1}A	2.9203	425	0.2376	π → π*	206 → **216**, -0.24687; 208 → **217**, 0.22368; 208 → 218, -0.11154; 209 → **216**, 0.10054; 209 → 218, -0.24746; 210 → 219, 0.30762; 210 → 220, -0.19537; 211 → 221, 0.14412; 213 → 222, 0.11667; **215** → 222, -0.11299
42	^{1}A	2.9301	423	0.0127	Fc → π*	210 → 219, 0.10266; 210 → 220, 0.55863; 211 → 221, 0.15464; 212 → 222, -0.28142; 213 → 222, -0.10930; **214** → 222; 0.18315
43	^{1}A	2.9572	419	0.0588	Fc → π*	206 → **217**, 0.12620; 209 → 221, 0.10109; 211 → 221, 0.53592; 212 → 222, 0.28514; 213 → 222, 0.10073; **214** → 222, 0.10507
44	^{1}A	2.9666	418	0.0117	Fc → π*	210 → 221, 0.53775; 212 → 221, 0.11597; 212 → 222, -0.14354; 213 → 222, 0.33369
45	^{1}A	2.9889	415	0.3656	π → π*	196 → **217**, -0.10782; 204 → **217**, 0.15280; 205 → **216**, -0.11783; 206 → **217**, 0.38602; 208 → **216**, 0.20162; 209 → **217**, -0.11928; 209 → 218, -0.11671; 211 → 221, -0.10682; **215** → 223, -0.26611; **215** → 226, -0.14498
46	^{1}A	3.0004	413	0.0633	Fc → π*	206 → **217**, 0.13949; **215** → 223, 0.64175
47	^{1}A	3.0458	407	0.0026	Fc → π*	205 → **216**, 0.11016; **215** → 224, 0.68714
50	^{1}A	3.0701	404	0.0139	π → π*	205 → **216**, -0.29428; 209 → 220, 0.38596; 210 → 221

						0.19230, 211 → 222, -0.16418; **215** → 225, 0.26482; **215** → 226, 0.23002
51	^{1}A	3.0724	404	0.0145	Fc → π*	205 → **216**, 0.14608; 209 → 220, -0.10371; **215** → 225, 0.63889; **215** → 226, -0.14894
52	^{1}A	3.0742	403	0.0107	π → π*	205 → **216**, -0.29390; 205 → **217**, 0.11492; 209 → 220, -0.37033; 210 → 221, -0.18242; **215** → 226, 0.36694
54	^{1}A	3.0875	402	0.0058	π → π*	204 → **216**, 0.13391; 205 → **216**, 0.17374; 205 → **217**, 0.56267; 208 → 218, -0.30425
55	^{1}A	3.0924	401	0.0105	Fc → π*	204 → **217**, 0.19775; 205 → **216**, 0.26524; 209 → 220, 0.10386; 211 → 222, 0.13919; 212 → 223, -0.31905; **215** → 226, 0.42565
56	^{1}A	3.0936	401	0.0022	Fc → π*	204 → **217**, 0.10374; 205 → **216**, 0.14075; 212 → 223, 0.62819; **215** → 226, 0.20321
58	^{1}A	3.1252	397	0.0012	Fc → π*	209 → 220, 0.22391; 211 → 222, 0.45980; 213 → 224, -0.27660; **214** → 225, -0.21178; **214** → 226, -0.13744; **215** → 226, -0.11165
59	^{1}A	3.1340	396	0.0016	Fc → π*	210 → 222, -0.10669; 213 → 224, 0.49072; **214** → 225, -0.40368; **214** → 226, -0.23058

[a] Only transitions with oscillator strengths greater than 0.001 are shown. Gouterman's four-orbital model MOs are shown in bold.

Supporting Information Table 4. Selected energies, oscillator strengths, and expansion coefficients for vertical transitions in ***trans*-$H_2Fc_2Ph_2P$** calculated using a TDDFT approach.[a]

Transition	Symmetry	E, eV	E, nm	*f*	Predominant character	Major expansion coefficients for single-electron transitions
1	^{1}B	1.2959	957	0.0196	Fc → π*	213 → **216**, 0.37417; **215** → **216**, 0.51858; **215** → **217**, -0.23004
3	^{1}B	1.3131	944	0.0101	Fc → π*	213 → **216**, 0.58501; **215** → **216**, -0.26662; **215** → **217**, 0.25311
4	^{1}A	1.3435	923	0.0017	Fc → π*	212 → **216**, 0.54430; **214** → **216**, -0.33504; **214** → **217**, 0.27295
5	^{1}B	1.3807	898	0.0582	Fc → π*	209 → **216**, -0.11128; 209 → **217**, -0.10350; 211 → **217**, 0.10995; **215** → **216**, 0.29146; **215** → **217**, 0.57980
6	^{1}A	1.3995	886	0.0018	Fc → π*	212 → **216**, -0.13109; 212 → **217**, 0.37730; **214** → **216**, 0.15180; **214** → **217**, 0.55518
7	^{1}B	1.4010	885	0.0016	Fc → π*	213 → **217**, 0.70022
8	^{1}A	1.4180	874	0.0015	Fc → π*	212 → **216**, 0.12867; 212 → **217**, 0.59374; **214** → **216**, -0.11727; **214** → **217**, -0.32445
9	^{1}B	1.5789	785	0.0076	Fc → π*	209 → **216**, 0.14977; 211 → **216**, 0.67399
11	^{1}B	1.6721	742	0.0160	Fc → π*	209 → **216**, 0.11096; 209 → **217**, 0.13409; 211 → **217**, 0.67328
12	^{1}A	1.6894	734	0.0017	Fc → π*	210 → **217**, 0.69788
13	^{1}B	1.9873	629	0.0564	π → π*	208 → **216**, -0.14131; 208 → **217**, -0.33835; 209 → **216**, 0.49825; 209 → **217**, -0.25430
14	^{1}B	2.1017	590	0.0350	π → π*	208 → **216**, 0.39210; 208 → **217**, -0.11435; 209 → **216**, 0.23177; 209 → **217**, 0.45976
15	^{1}A	2.3535	527	0.0046	Fc → π*	**215** → 218, 0.67450
16	^{1}B	2.3970	517	0.0039	Fc → π*	**214** → 218, 0.67287; **215** → 219, -0.13437
18	^{1}B	2.4200	512	0.0026	Fc → π*	212 → 218, 0.67672
19	^{1}B	2.5857	480	0.0075	Fc → π*	212 → 220, 0.19850; 213 → 221, -0.13148; **214** → 220, -0.23485; **215** → 219, 0.60331
21	^{1}B	2.6403	470	0.0218	Fc → π*	213 → 219, 0.32867; **214** → 220, 0.13901; **215** → 221, 0.58570
22	^{1}B	2.6429	469	0.0034	Fc → π*	212 → 220, 0.24518; 213 → 219, -0.45423; **214** → 220, 0.45557
25	^{1}B	2.6673	465	0.0127	Fc → π*	210 → 218, 0.62370; 212 → 220, 0.29470
30	^{1}B	2.7633	449	0.2217	π → π*	204 → **216**, -0.10810; 206 → **216**, 0.31825; 206 → **217**, -0.14043; 208 → **216**, 0.19624; 208 → **217**, 0.26827; 209 → **217**, -0.14294;

						210 → 218, -0.15892; 211 → 219, 0.12197; 212 → 220, 0.12664; 212 → 222, -0.12292; 213 → 219, 0.15511; **214** → 220, 0.11539; **214** → 222, 0.17639
32	^{1}B	2.8191	440	0.1415	Fc → π*	206 → **217**, -0.15201; 208 → **216**, 0.20063; 209 → **217**, -0.12451; 210 → 220, -0.18948; 211 → 219, -0.12091; 212 → 222, 0.37256; 213 → 219, -0.20300; 213 → 221, -0.17796; **214** → 220, -0.22328; **215** → 221, 0.16551
33	^{1}B	2.8308	438	0.0213	Fc → π*	206 → **216**, 0.19298; 211 → 219, -0.14310; 212 → 220, -0.20098; 212 → 222, -0.13765; 213 → 221, 0.25431; **214** → 222, -0.49140; **215** → 219, 0.10644
35	^{1}B	2.8536	434	0.2244	π → π*	204 → **217**, -0.10104; 206 → **216**, 0.40676; 206 → **217**, 0.22455; 208 → **216**, -0.23823; 208 → **217**, 0.12411; 209 → **217**, 0.15771; 212 → 222, 0.17422
36	^{1}A	2.8877	429	0.0031	Fc → π*	207 → **217**, -0.22406; 209 → 218, -0.33798; 210 → 219, 0.23086; 211 → 220, 0.37903; 212 → 219, 0.11318; 213 → 220, 0.12145; 213 → 222, 0.15426; **214** → 221, -0.13729; **215** → 222, -0.16632
40	^{1}A	2.9237	424	0.0011	π → π*	205 → **216**, 0.20731; 205 → **217**, 0.13138; 209 → 218, 0.45083; 210 → 219, 0.40855; **215** → 222, -0.13855
41	^{1}B	2.9275	424	0.0021	Fc → π*	210 → 220, 0.58551; 212 → 222, 0.35590
42	^{1}B	2.9574	419	0.0319	Fc → π*	206 → **216**, -0.12362; 211 → 219, -0.12411; 211 → 221, 0.58938; 212 → 222, -0.18544; 213 → 221, -0.11745; **214** → 222, -0.18805
44	^{1}B	2.9826	416	0.0514	Fc → π*	206 → **216**, -0.10987; 206 → **217**, -0.18144; **215** → 223, 0.65126
45	^{1}B	2.9986	413	0.4533	π → π*	204 → **217**, 0.10973; 206 → **216**, 0.24996; 206 → **217,** 0.29848; 208 → **216**, 0.14550; 208 → **217**, -0.22268; 209 → **216**, -0.10328; 209 → 221, 0.18202; 212 → 222, -0.12005; **215** → 223, 0.25250; **215** → 226, 0.17145
48	^{1}B	3.0323	409	0.1248	π → π*	204 → **216**, -0.20601, 206 → **216**, -0.16615; 206 → **217**, 0.43784; **215** → 226, -0.35925
50	^{1}B	3.0600	405	0.1249	Fc → π*	204 → **216**, -0.14613; 206 → **216**, -0.13246; 206 → **217**, 0.16013; 209 → 221, -0.13182; 212 → 224, 0.11684; **214** → 224, -0.11205; **215** → 226, 0.56738
51	^{1}A	3.0673	404	0.0092	π → π*	205 → **216,** 0.51653; 205 → **217**, -0.31920; 208 → 218, 0.22382; 209 → 218, -0.11606; 211 → 222, 0.10877

52	^{1}B	3.0680	404	0.0022	Fc → π*	209 → 219, 0.10270; 213 → 223, 0.66742; **214** → 224, 0.16147;
53	^{1}B	3.0721	404	0.0013	Fc → π*	209 → 219, 0.26808; 209 → 221, -0.10935; 210 → 222, -0.18289; 211 → 221, 0.18663; 212 → 224, 0.12908; 213 → 223, -0.22420; **214** → 224, 0.47280
56	^{1}B	3.0873	402	0.0182	Fc → π*	209 → 219, 0.42903; 210 → 222, -0.11579; 211 → 221, 0.10308; 212 → 224, 0.15143; **214** → 224, -0.45958
57	^{1}B	3.0983	400	0.0031	Fc → π*	**214** → 225, 0.69410
59	^{1}B	3.1118	398	0.0197	Fc → π*	209 → 219, -0.16450; 210 → 222, 0.10010; 212 → 224, 0.64336; 212 → 225, 0.12501

[a] Only transitions with oscillator strengths greater than 0.001 are shown. Gouterman's four-orbital model MOs are shown in bold.

Supporting Information Table 5. Selected energies, oscillator strengths, and expansion coefficients for vertical transitions in **H_2Fc_3PhP** calculated using a TDDFT approach.[a]

Transition	Symmetry	E, eV	E, nm	*f*	Predominant character	Expansion coefficients for single-electron transitions
1	^{1}A	1.3038	951	0.0183	Fc → π*	233 → **243**, -0.11109; 240 → **243**, -0.21684; **241** → **243**, 0.40994; **241** → **244**, 0.10755; **242** → **243**, 0.40828; **242** → **244**, 0.20998
2	^{1}A	1.3159	942	0.0195	Fc → π*	238 → **243**, -0.15257; 239 → **244**, -0.10869; **241** → **243**, -0.31337; **241** → **244**, 0.13861; **242** → **243**, 0.39337; **242** → **244**, -0.36181
3	^{1}A	1.3330	930	0.0022	Fc → π*	238 → **243**, -0.38102; 239 → **243**, 0.43209; 240 → **243**, -0.25197; **241** → **243**, -0.21187; **242** → **244**, 0.18173
4	^{1}A	1.3348	929	0.0011	Fc → π*	37 → **243**, 0.31611; 238 → **243**, 0.42240; 239 → **243**, 0.37750; 240 → **243**, -0.15939; **241** → **244**, 0.10463; **242** → **244**, -0.18059
6	^{1}A	1.3634	909	0.0079	Fc → π*	237 → **243**, -0.23021; 238 → **243**, 0.26656; 239 → **243**, -0.18119; 240 → **243**, -0.24020; 240 → **244**, 0.35302; **241** → **243**, -0.26618; **241** → **244**, 0.18055; **242** → **244**, 0.19145
7	^{1}A	1.3849	895	0.0427	Fc → π*	237 → **243**, -0.28448; 237 → **244**, -0.14724; 239 → **244**, 0.28051; 240 → **243**, -0.18436; **241** → **243**, 0.21221; **241** → **244**, 0.22203; **242** → **243**, -0.19142; **242** → **244**, -0.30862
8	^{1}A	1.4019	884	0.0109	Fc → π*	237 → **244**, 0.22265; 238 → **244**, -0.26271; 239 → **244**, 0.51893; 240 → **244**, -0.23907; **241** → **243**, -0.14028
9	^{1}A	1.4051	882	0.0055	Fc → π*	237 → **244**, 0.43177; 238 → **244**, 0.17250; 239 → **244**, -0.12781; 240 → **244**, -0.21171; **241** → **244**, 0.43959; **242** → **243**, -0.10053
10	^{1}A	1.4109	879	0.0100	Fc → π*	237 → **244**, -0.23387; 238 → **244**, 0.53854; 239 → **244**, 0.30201; 240 → **243**, 0.12026; **241** → **244**, 0.10606
11	^{1}A	1.4208	873	0.0095	Fc → π*	237 → **243**, 0.19025; 237 → **244**, 0.13011; 238 → **243**, -0.12680; 238 → **244**, -0.13002; 239 → **244**, 0.14216; 240 → **243**, 0.28501; 240 → **244**, 0.47153; **241** → **243**, 0.13633; **241** → **244**, 0.16810
12	^{1}A	1.4494	855	0.0276	Fc → π*	237 → **244**, 0.39735; 238 → **244**, 0.27632; 240 → **243**, -0.11230; 240 → **244**, 0.15408; **241** → **244**, -0.34671; **242** → **244**, -0.19207
13	^{1}A	1.5993	775	0.0112	Fc → π*	233 → **243**, 0.16221; 236 → **243**, 0.65973
14	^{1}A	1.6146	768	0.0044	Fc → π*	234 → **243**, 0.13465; 235 → **243**, 0.67075; 236 → **244**, -0.13843
15	^{1}A	1.6236	763	0.0012	Fc → π*	234 → **243**, 0.66453; 235 → **243**, -0.14563; 236 → **244**, -0.11389

16	^{1}A	1.6689	743	0.0185	Fc → π*	233 → **244**, 0.14965; 234 → **243**, 0.11863; 235 → **243**, 0.10242; 235 → **244**, 0.11369; 236 → **244**, 0.64065
17	^{1}A	1.6870	735	0.0020	Fc → π*	234 → **244**, -0.29657; 235 → **244**, 0.61962
18	^{1}A	1.6912	733	0.0055	Fc → π*	234 → **244**, 0.62547; 235 → **244**, 0.28775
19	^{1}A	1.9799	626	0.0285	π → π*	232 → **243**, 0.35785; 232 → **244**, -0.14097; 233 → **243**, 0.30621; 233 → **244**, 0.45950
20	^{1}A	2.0585	602	0.0753	π → π*	232 → **243**, -0.16786; 232 → **244**, -0.32216; 233 → **243**, 0.44957; 233 → **244**, -0.29306
21	^{1}A	2.2454	552	0.0237	Fc → π*	**242** → 245, 0.67525
22	^{1}A	2.3173	535	0.0028	Fc → π*	**241** → 245, 0.68251
23	^{1}A	2.3295	532	0.0035	Fc → π*	239 → 245, -0.11667; 240 → 245, 0.67094
25	^{1}A	2.3408	530	0.0014	Fc → π*	238 → 245, 0.68401
26	^{1}A	2.3475	528	0.0020	Fc → π*	237 → 245, 0.68344
27	^{1}A	2.5253	491	0.0054	Fc → π*	**241** → 246, -0.13361; **242** → 246, 0.62267; **242** → 247, -0.19479
28	^{1}A	2.5374	489	0.0043	Fc → π*	240 → 246, -0.15151; **242** → 246, 0.19248; **242** → 247, 0.61969
29	^{1}A	2.5428	488	0.0019	Fc → π*	236 → 245, -0.11211; **241** → 247, -0.11229; **241** → 248, 0.12052; **242** → 248, 0.64203
30	^{1}A	2.5733	482	0.0176	Fc → π*	236 → 245, 0.64540; **242** → 249, 0.15470
31	^{1}A	2.5837	480	0.0218	Fc → π*	236 → 245, -0.16679; 238 → 246, 0.13389; **242** → 249, 0.61842
32	^{1}A	2.5987	477	0.0078	Fc → π*	235 → 245, 0.67205
33	^{1}A	2.6035	476	0.0210	Fc → π*	234 → 245, 0.61103; **242** → 250, -0.26146
34	^{1}A	2.6094	475	0.0234	Fc → π*	234 → 245, 0.28565; 239 → 247, 0.11453; **241** → 246, -0.10962; **242** → 250, 0.57676
38	^{1}A	2.6408	470	0.0013	Fc → π*	238 → 246, 0.14258; 238 → 248, -0.10568; 239 → 248, 0.10283; 240 → 247, -0.22014; 240 → 248, 0.42190; **241** → 246, -0.15035; **241** → 247, 0.26776; **241** → 248, -0.31759
45	^{1}A	2.6804	463	0.0027	Fc → π*	237 → 246, 0.10425; 237 → 249, 0.31168; 238 → 246, -0.13470; 238 → 249, 0.28115; 240 → 246, 0.23575; 240 → 249, -0.11604; **241** → 246, -0.22348; **241** → 247, 0.17533; **241** → 248, 0.14899; **241** → 249, -0.26065
50	^{1}A	2.7049	458	0.0070	Fc → π*	238 → 249, -0.18713; 238 → 250, -0.12502; 239 → 248, 0.15130; 239 → 249, 0.33978; 239 → 250, 0.23626; 240 → 247, 0.11429;

						240 → 248, -0.11141; 240 → 249, -0.10855; **241** → 248, -0.13807; **241** → 250, 0.40063
51	^{1}A	2.7172	456	0.0080	Fc → π*	237 → 247, -0.14103; 237 → 249, 0.12590; 238 → 250, -0.11795; 239 → 248, 0.12458; 239 → 250, 0.15712; 240 → 250, 0.55236; **241** → 250, -0.17098
52	^{1}A	2.7241	455	0.2342	π → π*	230 → **243**, -0.21211; 230 → **244**, -0.22616; 231 → **243**, 0.22309; 232 → **243**, 0.27711; 232 → **244**, -0.10280; 233 → **244**, -0.13357; 233 → 245, 0.10170; 237 → 249, 0.13287; 237 → 250, -0.12176; 238 → 250, 0.16769; 239 → 250, 0.13848
53	^{1}A	2.7291	454	0.0500	Fc → π*	230 → **244**, 0.10510; 231 → **243**, -0.10521; 232 → **243**, -0.12343; 237 → 249, 0.30032; 237 → 250, -0.34217; 238 → 250, 0.31687; 239 → 250, 0.22385; 240 → 247, -0.12672
54	^{1}A	2.7370	453	0.0021	Fc → π*	237 → 250, 0.46670; 238 → 249, 0.16557; 238 → 250, 0.45060; 239 → 250, 0.12486
55	^{1}A	2.7522	451	0.0564	π → π*	230 → **243**, 0.11803; 230 → **244**, 0.11030; 231 → **243**, 0.57422; 231 → **244**, 0.24138; 232 → **243**, -0.12330
56	^{1}A	2.7721	447	0.1525	π → π*	230 → **243**, 0.36694; 231 → **244**, 0.10011; 232 → **243**, 0.12549; 232 → **244**, 0.21054; 233 → 245, 0.30894; **242** → 251, -0.18665
57	^{1}A	2.8050	442	0.0169	π → π*	230 → **243**, -0.27623; 231 → **243**, -0.18468; 231 → **244**, 0.48847; 233 → 245, 0.25336; **242** → 251, -0.11037
58	^{1}A	2.8131	441	0.0048	Fc → π*	231 → **243**, -0.12007; 231 → **244**, 0.23959; 233 → 245, -0.10756; 237 → 246, 0.10007; 240 → 249, 0.11079; **242** → 251, 0.54332
59	^{1}A	2.8281	438	0.1721	π → π*	230 → **243**, 0.38105; 230 → **244**, -0.14990; 231 → **244**, 0.22522; 232 → **244**, -0.19028; 233 → 245, -0.14846; 236 → 246, 0.11144; 236 → 247, 0.12726; 240 → 251, -0.12956
60	^{1}A	2.8382	437	0.0601	π → π*	229 → **243**, 0.21917; 230 → **243**, -0.11148; 231 → **244**, 0.19396; 232 → **244**, 0.10965; 233 → 245, -0.41412; 236 → 248, 0.12435; 239 → 248, 0.11606; **241** → 250, -0.11693; **242** → 251, -0.16935
61	^{1}A	2.8530	435	0.0065	Fc → π*	230 → **244**, 0.19768; 234 → 247, 0.11669; 235 → 246, -0.11078; 236 → 246, 0.43092; 237 → 247, -0.12268; 238 → 246, 0.15129; 240 → 250, -0.1425; **241** → 249, -0.13185; **241** → 251, 0.17359; **242** → 249, -0.10142
63	^{1}A	2.8747	431	0.0133	Fc → π*	230 → **244**, -0.14015; 234 → 246, -0.14779; 234 → 247, -0.13802;

						234 → 248, -0.10745; 234 → 249, 0.21042; 235 → 248, 0.14854; 237 → 249, 0.24656; 237 → 250, 0.17201; 237 → 251, 0.18901; 238 → 251, -0.23167; 239 → 250, -0.14474; 239 → 251, -0.11489; 240 → 246, -0.14598; 240 → 247, -0.10462
64	^{1}A	2.8862	430	0.0140	Fc → π*	235 → 247, -0.10533; 235 → 248, 0.26053; 235 → 250, 0.16502; 236 → 246, -0.13093; 236 → 250, 0.11292; 238 → 250, 0.19020; 239 → 250, -0.22041; 239 → 251, 0.31845; 240 → 251, -0.11252; **241** → 248, -0.13028
65	^{1}A	2.8937	428	0.1073	Fc → π*	232 → **244**, 0.15204; 236 → 247, 0.60119
66	^{1}A	2.8981	428	0.0112	Fc → π*	235 → 246, 0.24486; 236 → 246, 0.29547; 236 → 248, 0.42676; 240 → 251, 0.14843, **241** → 251, -0.17902; **242** → 251, 0.13571
67	^{1}A	2.9027	427	0.0069	Fc → π*	235 → 246, -0.25755; 236 → 246, -0.26885; 236 → 248, 0.46750; 236 → 249, 0.12128; 239 → 251, -0.14908; **241** → 251, 0.16059
68	^{1}A	2.9122	426	0.0669	Fc → π*	232 → **244**, 0.11515; 234 → 246, 0.49722; 235 → 246, -0.15669; 236 → 247, -0.16136; 240 → 251, -0.18812; **241** → 251, -0.13315
69	^{1}A	2.9169	425	0.0017	Fc → π*	234 → 246, 0.17169; 234 → 247, 0.27406; 235 → 246, 0.40116; 235 → 247, -0.15360; 235 → 248, 0.18030; 236 → 246, -0.15039; 236 → 248, -0.10768; 236 → 249, 0.11822; 239 → 251, -0.16008; **241** → 251, 0.16614; **242** → 251, 0.11798
70	^{1}A	2.9199	425	0.0235	Fc → π*	230 → **244**, -0.16341; 234 → 246, 0.15374; 234 → 247, -0.14855; 235 → 246, -0.32002; 235 → 247, -0.36115; 235 → 248, 0.15250; 236 → 248, -0.13289; 239 → 251, -0.13759; 240 → 251, 0.21736
71	^{1}A	2.9267	424	0.0125	Fc → π*	234 → 246, 0.25631; 234 → 247, -0.12114; 235 → 247, 0.50207; 235 → 248, 0.26450; 240 → 251, 0.14000; **241** → 251, 0.19884
72	^{1}A	2.9357	422	0.1624	π → π*	230 → **244**, -0.38333; 232 → **243**, -0.11836; 234 → 247, 0.27217; 235 → 248, -0.21975; 236 → 249, -0.18393; **241** → 251, 0.17650; **242** → 252, 0.13319; **242** → 253, 0.11301
73	^{1}A	2.9375	422	0.0120	Fc → π*	230 → **244**, -0.10029; 234 → 247, -0.26816; 234 → 248, 0.58797; 240 → 251, -0.16824
74	^{1}A	2.9453	421	0.0353	Fc → π*	230 → **244**, -0.11919; 234 → 247, 0.19710; 234 → 248, 0.22134; 235 → 248, 0.10278; 236 → 249, 0.43067; 237 → 251, 0.16466; 240 → 251, 0.15124; **241** → 251, -0.30204
75	^{1}A	2.9525	420	0.0132	Fc → π*	234 → 246, 0.10542; 235 → 248, -0.30625; 236 → 249, 0.26003;

						236 → 250, 0.20195; 238 → 251, -0.25918; 239 → 251, 0.18435; 240 → 251, 0.29237; **241** → 251, 0.24048
76	^{1}A	2.9643	418	0.0340	Fc → π*	230 → **244**, -0.11222; 234 → 247, -0.20371; 234 → 248, -0.18455; 235 → 249, 0.30243; 236 → 249, 0.27094; 236 → 250, -0.13586; 237 → 251, -0.27250; 239 → 251, 0.10722; 240 → 251, -0.26945; **242** → 252, 0.10561
77	^{1}A	2.9777	416	0.0183	Fc → π*	234 → 249, 0.26876; 235 → 249, 0.32113; 236 → 250, -0.23391; 237 → 251, 0.26152; 238 → 251, 0.18162; 239 → 251, 0.29620; **242** → 253, -0.10844
78	^{1}A	2.9783	416	0.0133	Fc → π*	234 → 249, 0.15565; 235 → 249, -0.41994; 236 → 250, -0.39024; 237 → 251, -0.13630; 238 → 251, -0.22141; 239 → 251, 0.17835
79	^{1}A	2.9799	416	0.0113	Fc → π*	234 → 249, 0.41590; 235 → 249, -0.13193; 236 → 250, 0.16738; 237 → 251, -0.30079; 238 → 251, 0.36605
80	^{1}A	2.9942	414	0.0048	Fc → π*	234 → 249, 0.15194; 234 → 250, -0.17447; 235 → 250, 0.50439; 236 → 250, -0.24784; 239 → 251, -0.27773

[a] Only transitions with oscillator strengths greater than 0.001 are shown. Gouterman's four-orbital model MOs are shown in bold.

Supporting Information Table 6. Selected energies, oscillator strengths, and expansion coefficients for vertical transitions in **H_2TFcP** calculated using a TDDFT approach.[a]

Transition	Symmetry	E, eV	E, nm	*f*	Predominant character	Expansion coefficients for single-electron transitions
1	^{1}B	1.3843	896	0.0249	Fc → π*	257 → **270**, -0.12196; 263 → **270**, -0.11033; **268** → **270**, 0.31364; **269** → **270**, 0.27646; **269** → **271**, 0.49630
2	^{1}B	1.4011	885	0.0489	Fc → π*	257 → **270**, -0.15391; 257 → **271**, 0.12240; 261 → **270**, -0.12805; 265 → **271**, -0.16206; **268** → **270**, -0.11866; **268** → **271**, 0.18240; **269** → **270**, 0.51032; **269** → **271**, -0.26907
3	^{1}A	1.4495	855	0.0022	Fc → π*	264 → **270**, -0.27589; 266 → **270**, -0.10454; 266 → **271**, -0.23894; 267 → **270**, 0.56945; 267 → **271**, 0.15501
4	^{1}B	1.4557	852	0.0021	Fc → π*	263 → **270**, 0.48995; 265 → **270**, 0.37565; **268** → **270**, 0.26234; **268** → **271**, 0.18285
9	^{1}B	1.4899	832	0.0067	Fc → π*	263 → **271**, 0.42882; 265 → **270**, -0.15041; 265 → **271**, 0.17464; **268** → **270**, -0.19560; **268** → **271**, 0.44819
10	^{1}B	1.4914	831	0.0109	Fc → π*	263 → **270**, -0.28378; 263 → **271**, -0.28766; 265 → **271**, 0.47120; **268** → **270**, 0.16698; **268** → **271**, 0.23909; **269** → **271**, -0.11039
13	^{1}B	1.5101	821	0.0555	Fc → π*	263 → **270**, -0.24399; 263 → **271**, 0.26698; 265 → **271**, -0.27330; **268** → **270**, 0.42033; **269** → **270**, -0.10942; **269** → **271**, -0.20508
14	^{1}B	1.5195	816	0.0457	Fc → π*	263 → **271**, -0.36845; 265 → **271**, -0.36016; **268** → **271**, 0.38584; **269** → **270**, -0.16848; **269** → **271**, 0.10024
15	^{1}A	1.5277	812	0.0166	Fc → π*	262 → **270**, 0.11281; 262 → **271**, 0.25891; 264 → **270**, 0.14394; 266 → **270**, 0.17428; 266 → **271**, 0.49171; 267 → **270**, 0.30704
17	^{1}B	1.6617	746	0.0155	Fc → π*	257 → **270**, -0.1**271**1; 259 → **271**, -0.10745; 261 → **270**, 0.65862
18	^{1}B	1.6801	738	0.0031	Fc → π*	259 → **270**, 0.52557; 261 → **271**, -0.46152
19	^{1}A	1.6839	736	0.0012	Fc → π*	258 → **270**, 0.47024; 258 → **271**, -0.20020; 260 → **270**, -0.48162
20	^{1}A	1.6886	734	0.0017	Fc → π*	258 → **270**, 0.46962; 260 → **270**, 0.44400; 260 → **271**, 0.26555
21	^{1}B	1.7033	728	0.0190	Fc → π*	257 → **271**, -0.10449; 259 → **270**, 0.45611; 261 → **271**, 0.49153
22	^{1}A	1.7206	721	0.0021	Fc → π*	258 → **271**, 0.27640; 260 → **270**, -0.23613; 260 → **271**, 0.59410
23	^{1}B	1.7225	720	0.0110	Fc → π*	259 → **271**, 0.68845

24	^{1}A	1.7277	718	0.0029	Fc → π*	258 → **270**, 0.20995; 258 → **271**, 0.60972; 260 → **271**, -0.26185
25	^{1}B	1.9996	620	0.0253	π → π*	256 → **270**, 0.38715; 257 → **270**, 0.13461; 257 → **271**, 0.54117
26	^{1}B	2.0671	600	0.0629	π → π*	256 → **271**, -0.36498; 257 → **270**, 0.52454; 257 → **271**, -0.12871; **269** → **270**, 0.11397
27	^{1}A	2.2808	544	0.0360	Fc → π*	**269** → 272, 0.67478
28	^{1}B	2.4076	515	0.0141	Fc → π*	267 → 272, 0.68876
30	^{1}B	2.4178	513	0.0125	Fc → π*	266 → 272, 0.68787
32	^{1}B	2.4264	511	0.0045	Fc → π*	264 → 272, 0.69174
34	^{1}B	2.4306	510	0.0075	Fc → π*	262 → 272, 0.69035
35	^{1}A	2.6043	476	0.0028	Fc → π*	261 → 272, 0.69028
36	^{1}B	2.6244	472	0.0761	Fc → π*	256 → **270**, -0.16228; 258 → 272, 0.10666; 260 → 272, 0.58473; **269** → 274, 0.25455; **269** → 275, 0.11772
37	^{1}B	2.6316	471	0.0286	Fc → π*	256 → **271**, 0.10868; 258 → 272, 0.63795; 260 → 272, -0.13867; **269** → 274, 0.12331; **269** → 275, -0.17869
40	^{1}B	2.6505	468	0.0324	Fc → π*	258 → 272, -0.13779; 260 → 272, -0.30768; **269** → 274, 0.56063; **269** → 275, 0.12709
41	^{1}B	2.6580	466	0.0116	Fc → π*	258 → 272, 0.19839; **269** → 274, -0.14322; **269** → 275, 0.61976
43	^{1}B	2.6892	461	0.2299	Fc → π*	254 → **271**, 0.17658; 256 → **270**, 0.25629; 257 → **271**, -0.10650; 260 → 272, 0.14265; **269** → 274, 0.19719; **269** → 278, 0.48048
45	^{1}B	2.7160	457	0.1929	Fc → π*	254 → **270**, -0.15153; 256 → **271**, 0.24605; **269** → 279, 0.54334
47	^{1}B	2.7744	447	0.0875	Fc → π*	254 → **270**, -0.22114; 254 → **271**, -0.29130; 256 → **270**, -0.19877; **269** → 278, 0.43618
49	^{1}B	2.8143	441	0.0205	π → π*	254 → **270**, 0.51732; 254 → **271**, -0.19553; 267 → 273, -0.15176; **269** → 279, 0.28229
52	^{1}B	2.8230	439	0.0022	Fc → π*	266 → 273, 0.45344; 267 → 273, 0.12371; **268** → 274, 0.41163; **268** → 275, -0.30841
55	^{1}B	2.8321	438	0.0100	Fc → π*	254 → **270**, 0.10646; 266 → 273, 0.33800; 267 → 276, 0.51178; **268** → 274, -0.25976
57	^{1}B	2.8369	437	0.0024	Fc → π*	263 → 274, 0.13051; 264 → 273, 0.33734; 265 → 274, 0.35167; 266 → 273, -0.10500; 266 → 276, -0.20866; 267 → 273, -0.14442; 267 → 276, 0.13535; **268** → 275, -0.35247
59	^{1}B	2.8382	437	0.0202	Fc → π*	254 → **270**, 0.10960; 262 → 273, 0.12858; 262 → 276, 0.11452;

						263 → 275, 0.17824; 264 → 273, 0.44531; 265 → 274, 0.19387; 266 → 276, 0.21416; 267 → 273, 0.16241; **268** → 275, 0.28926
61	^{1}A	2.8417	436	0.0091	π → π*	253 → **270**, -0.24761; 255 → **271**, 0.15644; 257 → 272, 0.59743; **269** → 280, 0.12971
62	^{1}B	2.8426	436	0.0113	Fc → π*	262 → 273, 0.55922; 263 → 274, -0.27239; 264 → 273, -0.13592; 265 → 275, -0.22818
63	^{1}B	2.8446	436	0.0032	Fc → π*	262 → 273, -0.12931; 263 → 274, -0.31629; 263 → 275, -0.23322; 264 → 273, -0.15257; 265 → 274, 0.41065; 265 → 275, 0.26134; 266 → 276, 0.13253; 267 → 276, -0.15146
64	^{1}B	2.8479	435	0.0026	Fc → π*	263 → 274, -0.22857; 263 → 275, 0.20092; 264 → 273, 0.11113; 265 → 274, -0.16182; 265 → 275, 0.45441; 266 → 276, -0.38143
67	^{1}B	0.13564	434	0.0696	Fc → π*	254 → **270**, 0.13564; 256 → **271**, 0.13373; 262 → 273, 0.11973; 263 → 274, 0.38112; 264 → 276, 0.41119; 265 → 275, 0.12274; 266 → 276, -0.14958; 267 → 276, -0.15096
69	^{1}B	2.8585	434	0.0272	Fc → π*	262 → 276, -0.38338; 263 → 275, 0.46980; 264 → 276, 0.18014; 266 → 276, 0.18115
71	^{1}B	2.8638	433	0.2320	Fc → π*	254 → **270**, 0.18921; 256 → **271**, 0.24630; 257 → **270**, 0.10293; 262 → 273, -0.11603; 262 → 276, -0.23044; 263 → 275, 0.10385; 264 → 276, -0.29154; 266 → 277, -0.19813; **269** → 279, -0.20267
75	^{1}B	2.8803	430	0.0095	Fc → π*	262 → 273, 0.15306; 262 → 276, 0.13694; 262 → 277, -0.18806; 263 → 278, -0.12572; 264 → 276, -0.22931; 264 → 277, 0.36245; 266 → 273, 0.15485; 266 → 276, 0.12941; 266 → 277, 0.10338; 267 → 273, -0.10966; 267 → 276, -0.22061; **268** → 274, -0.20655; **268** → 278, -0.14930
76	^{1}B	2.8832	430	0.0018	Fc → π*	262 → 276, -0.34707; 262 → 277, -0.14980; 263 → 275, -0.13786; 264 → 276, -0.11408; 264 → 277, -0.15478; 266 → 276, -0.10301; 266 → 277, 0.49634
78	^{1}B	2.8864	430	0.0304	Fc → π*	262 → 277, 0.30538; 263 → 274, 0.10377; 263 → 278, 0.14912; 264 → 273, -0.11600; 264 → 277, 0.15066; 265 → 275, 0.23820; 266 → 273, -0.17952; 266 → 276, 0.18960; 266 → 277, 0.27919, 267 → 276, 0.17087; **268** → 274, 0.13054; **268** → 278, -0.10377
80	^{1}B	2.8979	428	0.0069	Fc → π*	264 → 277, 0.24518; 266 → 277, 0.16580; **268** → 278, 0.60381
83	^{1}B	2.9104	426	0.0013	Fc → π*	262 → 276; -0.17249; 262 → 277, 0.10355; 263 → 275, -0.11013;

						264 → 277, 0.35608; 265 → 278, 0.49001; 266 → 277, -0.11028; **268** → 279, 0.18814
85	^{1}B	2.9142	425	0.0030	Fc → π*	262 → 277, 0.46807; 263 → 278, -0.46773; 265 → 279, -0.15898
86	^{1}B	2.9176	425	0.0192	Fc → π*	254 → **271**, -0.16734; 265 → 278, -0.23006; 267 → 277, -0.11038; **268** → 279, 0.57586
88	^{1}B	2.9279	423	0.2857	π → π*	254 → **271**, 0.48365; 255 → 272, 0.10214; 256 → **270**, -0.17314; 257 → **271**, 0.10211; 265 → 279, -0.10640; **268** → 279, 0.10787
90	^{1}B	2.9369	422	0.0051	Fc → π*	263 → 278, -0.16912; 263 → 279, 0.48922; 264 → 277, 0.16708; 265 → 278, -0.23539; 265 → 279, 0.30479; **268** → 278, -0.10519
91	^{1}B	2.9391	422	0.0062	Fc → π*	262 → 277, -0.12299; 263 → 278, -0.32046; 263 → 279, -0.31956, 265 → 278, 0.13115; 265 → 279, 0.48041
94	^{1}A	2.9788	416	0.0079	Fc → π*	253 → **270**, 0.28162; 267 → 279, -0.11712; **269** → 280, 0.60426
96	^{1}B	3.0222	410	0.0181	Fc → π*	261 → 274, 0.64973, **268** → 279, -0.11500
97	^{1}B	3.0290	409	0.0121	Fc → π*	261 → 275, 0.67183
99	^{1}A	3.0383	408	0.0083	Fc → π*	253 → **270**, -0.21142; 261 → 276, 0.62680
100	^{1}B	3.0439	407	0.0075	Fc → π*	258 → 273, 0.14131; 259 → 274, 0.18920; 260 → 273, 0.48241; 260 → 276, 0.19650; 261 → 274, 0.10000; 263 → 278, -0.11486

[a] Only transitions with oscillator strengths greater than 0.001 are shown. Gouterman's four-orbital model MOs are shown in bold.

Coordinated for DFT optimized geometries of feropcene-containing porphyrins and reference H_2TPP.

H_2TPP:
Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

N	-1.49941	1.48606	-0.02909
N	-1.43603	-1.44908	0.01211
N	1.43603	1.44908	0.01211
N	1.49941	-1.48606	-0.02909
C	-2.85047	1.23044	0.02896
C	-1.25595	2.83953	0.02654
C	-2.7897	-1.2697	-0.04871
C	-1.24464	-2.80102	-0.05035
C	1.24464	2.80102	-0.05035
C	2.7897	1.2697	-0.04871
C	1.25595	-2.83953	0.02654
C	2.85047	-1.23044	0.02896
C	-3.46781	-0.03176	-0.00676
C	-3.49946	2.5044	0.14162
C	-2.53558	3.47714	0.1395
C	-3.47983	-2.54941	-0.18171
C	-0.00071	-3.46806	-0.00995
C	-2.51825	-3.50246	-0.18269
C	0.00071	3.46806	-0.00995
C	2.51825	3.50246	-0.18269
C	3.47983	2.54941	-0.18171
C	2.53558	-3.47714	0.1395
C	3.46781	0.03176	-0.00676
C	3.49946	-2.5044	0.14162
H	-4.56697	2.64182	0.22595
H	-2.68256	4.54354	0.22164
H	-4.54722	-2.68498	-0.27986
H	-2.64437	-4.57091	-0.28195
H	2.64437	4.57091	-0.28195
H	4.54722	2.68498	-0.27986
H	2.68256	-4.54354	0.22164
H	4.56697	-2.64182	0.22595
H	-0.77853	0.77205	-0.05614
H	0.77853	-0.77205	-0.05614
C	4.96588	0.04394	0.00493
C	5.66995	0.57555	1.09728
C	5.69882	-0.47656	-1.07359
C	7.06503	0.58654	1.11064
H	5.11439	0.97502	1.941
C	7.09413	-0.46418	-1.0616

H	5.16632	-0.8824	-1.92924
C	7.78183	0.06699	0.03101
H	7.59175	0.99818	1.96764
H	7.64333	-0.86548	-1.90936
H	8.86849	0.07647	0.04093
C	-0.00071	4.96616	-0.00148
C	0.52143	5.67728	1.09086
C	-0.52522	5.69213	-1.08279
C	0.51916	7.07242	1.10168
H	0.9238	5.12705	1.93669
C	-0.52616	7.08751	-1.0733
H	-0.9234	5.15427	-1.93869
C	-0.00447	7.78226	0.01943
H	0.92347	7.60459	1.9588
H	-0.9304	7.63132	-1.92315
H	-0.00546	8.86897	0.02738
C	-4.96588	-0.04394	0.00493
C	-5.69882	0.47656	-1.07359
C	-5.66995	-0.57555	1.09728
C	-7.09413	0.46418	-1.0616
H	-5.16632	0.8824	-1.92924
C	-7.06503	-0.58654	1.11064
H	-5.11439	-0.97502	1.941
C	-7.78183	-0.06699	0.03101
H	-7.64333	0.86548	-1.90936
H	-7.59175	-0.99818	1.96764
H	-8.86849	-0.07647	0.04093
C	0.00071	-4.96616	-0.00148
C	-0.52143	-5.67728	1.09086
C	0.52522	-5.69213	-1.08279
C	-0.51916	-7.07242	1.10168
H	-0.9238	-5.12705	1.93669
C	0.52616	-7.08751	-1.0733
H	0.9234	-5.15427	-1.93869
C	0.00447	-7.78226	0.01943
H	-0.92347	-7.60459	1.9588
H	0.9304	-7.63132	-1.92315
H	0.00546	-8.86897	0.02738

H_2FcPh_3P:
Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	5.584485	-0.626015	0.535311
2	6	0	6.161887	1.285784	1.141212
3	6	0	5.116285	0.800686	1.983810
4	6	0	7.263086	0.382383	1.238414
5	6	0	6.897483	-0.660517	2.142113
6	1	0	6.126990	2.179785	0.532012
7	1	0	4.139186	1.249787	2.103509
8	1	0	8.202987	0.464581	0.707915
9	1	0	7.509581	-1.512018	2.410714
10	6	0	5.570582	-0.401715	2.602411
11	1	0	5.000380	-1.020614	3.283209
12	6	0	4.904789	-0.643913	-1.448691
13	6	0	6.067887	-1.455415	-1.308189
14	6	0	4.442584	-2.286713	0.096308
15	6	0	5.780984	-2.477615	-0.354990
16	1	0	4.801991	0.199887	-2.117291
17	1	0	7.007988	-1.306916	-1.823787
18	1	0	3.932081	-2.884212	0.839407
19	1	0	6.467082	-3.239716	-0.008189
20	6	0	3.867786	-1.162312	-0.596892
21	7	0	0.153585	-1.759906	-0.367599
22	7	0	-2.712514	-1.048602	-0.002703
23	7	0	0.752690	1.057493	-0.467297
24	7	0	-2.110710	1.780997	-0.065602
25	6	0	-0.435517	-2.999205	-0.494100
26	6	0	1.510785	-1.835608	-0.590597
27	6	0	-2.818317	-2.409601	0.015196
28	6	0	-3.957714	-0.581700	0.313795
29	6	0	2.042589	0.598891	-0.499295
30	6	0	0.843692	2.420593	-0.519297
31	6	0	-3.470410	1.857199	0.132496
32	6	0	-1.577608	3.032497	-0.274101
33	6	0	-1.785817	-3.327703	-0.275402
34	6	0	0.609483	-3.905207	-0.866798
35	6	0	1.784984	-3.205008	-0.920196
36	6	0	-4.167518	-2.823099	0.392694
37	6	0	-4.340512	0.776301	0.357494
38	6	0	-4.874616	-1.684198	0.586693
39	6	0	2.433287	-0.763709	-0.536695

40	6	0	2.981591	1.714090	-0.547293
41	6	0	2.237793	2.844991	-0.575494
42	6	0	-3.819508	3.244100	0.033196
43	6	0	-0.223407	3.345595	-0.478498
44	6	0	-2.676006	3.954298	-0.221502
45	1	0	0.463881	-4.953106	-1.081099
46	1	0	2.752484	-3.588710	-1.202495
47	1	0	-4.505820	-3.842099	0.513293
48	1	0	-5.905917	-1.587997	0.894391
49	1	0	4.055791	1.634888	-0.548092
50	1	0	2.587994	3.866490	-0.606294
51	1	0	-4.823107	3.630602	0.127294
52	1	0	-2.587504	5.020298	-0.366502
53	6	0	0.103196	4.799194	-0.650597
54	6	0	0.560999	5.284694	-1.885997
55	6	0	-0.041205	5.704794	0.412602
56	6	0	0.863701	6.636693	-2.054196
57	1	0	0.672899	4.593894	-2.716897
58	6	0	0.262598	7.056994	0.245503
59	1	0	-0.385707	5.340094	1.376402
60	6	0	0.715401	7.527393	-0.988896
61	1	0	1.212103	6.994193	-3.019695
62	1	0	0.149897	7.741494	1.082203
63	1	0	0.951602	8.579993	-1.119395
64	6	0	-2.139620	-4.781102	-0.351703
65	6	0	-1.609923	-5.702903	0.566297
66	6	0	-3.014319	-5.254001	-1.343905
67	6	0	-1.944525	-7.055903	0.495197
68	1	0	-0.941123	-5.349205	1.345999
69	6	0	-3.346921	-6.607300	-1.417306
70	1	0	-3.426716	-4.552300	-2.063205
71	6	0	-2.813424	-7.512901	-0.497805
72	1	0	-1.529827	-7.751804	1.219897
73	1	0	-4.020820	-6.954199	-2.196307
74	1	0	-3.073525	-8.566501	-0.554206
75	1	0	-0.341414	-0.893705	-0.182599
76	1	0	-1.594011	0.908597	-0.114001
77	6	0	-5.772412	1.111603	0.635592
78	6	0	-6.131513	1.814703	1.797491
79	6	0	-6.788211	0.736205	-0.258910
80	6	0	-7.465713	2.129705	2.059189
81	1	0	-5.357014	2.103602	2.502393
82	6	0	-8.122311	1.052007	0.001788
83	1	0	-6.523211	0.200104	-1.165710
84	6	0	-8.465712	1.749607	1.161888
85	1	0	-7.723514	2.667905	2.967589

86	1	0	-8.893110	0.756608	-0.705313
87	1	0	-9.504712	1.994909	1.364986

***cis*-$H_2Fc_2Ph_2P$**:

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-4.246182	-3.800600	-1.004767
2	6	0	-2.976319	-5.378382	-0.597516
3	6	0	-2.223204	-4.208307	-0.905173
4	6	0	-3.773918	-5.093219	0.550952
5	6	0	-3.505036	-3.752216	0.952932
6	1	0	-2.970339	-6.304819	-1.157356
7	1	0	-1.533031	-4.092380	-1.729927
8	1	0	-4.474244	-5.767699	1.026916
9	1	0	-3.935622	-3.255135	1.811444
10	6	0	-2.520563	-3.189837	0.067061
11	6	0	-5.355527	-4.401057	-2.654221
12	6	0	-6.223017	-4.155158	-1.547460
13	6	0	-5.098371	-2.193975	-2.025443
14	6	0	-6.064422	-2.790322	-1.159491
15	1	0	-5.227707	-5.347689	-3.163560
16	1	0	-6.874644	-4.879677	-1.076106
17	1	0	-4.738648	-1.175176	-1.970488
18	1	0	-6.585321	-2.297742	-0.348428
19	6	0	-4.660573	-3.189097	-2.949020
20	1	0	-3.916102	-3.053627	-3.722919
21	7	0	-0.518904	3.058284	0.132282
22	7	0	-1.993501	0.556969	0.549188
23	7	0	1.930563	1.615955	-0.505745
24	6	0	-1.656803	3.589345	0.671037
25	6	0	0.277766	4.126873	-0.163212
26	6	0	-2.954697	1.467839	0.924971
27	6	0	-2.526635	-0.711089	0.457218
28	6	0	2.303572	2.877483	-0.914327
29	6	0	2.935768	0.706487	-0.737576
30	6	0	-0.389040	-1.931427	0.044852
31	6	0	1.718871	-1.392357	-0.148674

32	6	0	-2.805754	2.861343	1.044983
33	6	0	-1.558762	5.042773	0.767131
34	6	0	-0.361003	5.379129	0.230209
35	6	0	-4.168413	0.726567	1.096013
36	6	0	-1.805775	-1.887863	0.170213
37	6	0	-3.914981	-0.584901	0.791908
38	6	0	1.567806	4.062421	-0.734668
39	6	0	3.605142	2.744822	-1.495814
40	6	0	3.993602	1.436043	-1.376424
41	6	0	0.371246	-3.171979	0.163919
42	6	0	2.908176	-0.676422	-0.434170
43	6	0	1.677987	-2.831935	0.065939
44	26	0	5.274484	-2.688838	0.764703
45	6	0	6.452617	-3.271872	2.372724
46	6	0	5.363528	-2.470492	2.831623
47	6	0	5.911763	-4.422176	1.723107
48	6	0	4.488251	-4.332248	1.782656
49	1	0	7.504153	-3.036126	2.476425
50	1	0	5.443456	-1.522209	3.347299
51	1	0	6.480646	-5.214990	1.254502
52	1	0	3.790358	-5.053685	1.377707
53	6	0	4.149911	-3.125332	2.466411
54	1	0	3.148595	-2.756203	2.644326
55	6	0	5.475484	-0.808149	-0.061485
56	6	0	6.544009	-1.649140	-0.487849
57	6	0	4.559227	-2.585180	-1.203415
58	6	0	5.974348	-2.752536	-1.191137
59	1	0	5.573770	0.100885	0.516204
60	1	0	7.595688	-1.495850	-0.282573
61	1	0	3.849710	-3.246453	-1.681629
62	1	0	6.516551	-3.582252	-1.626537
63	6	0	4.228125	-1.361246	-0.523523
64	1	0	-2.303371	5.701020	1.190929
65	1	0	0.069823	6.365456	0.134382
66	1	0	-5.113324	1.159032	1.388857
67	1	0	-4.620841	-1.398237	0.796089
68	1	0	4.159265	3.551727	-1.951140
69	1	0	4.912274	0.999011	-1.735005
70	1	0	-0.037519	-4.153663	0.350543
71	1	0	2.532598	-3.482854	0.141484
72	1	0	-1.040307	0.793779	0.292503
73	1	0	1.019302	1.390505	-0.121192
74	7	0	0.451425	-0.867544	-0.120645
75	6	0	2.221103	5.340906	-1.153553
76	6	0	1.644825	6.139341	-2.155975
77	6	0	3.415741	5.778156	-0.557047

78	6	0	2.246019	7.334555	-2.551895
79	1	0	0.724261	5.810431	-2.629482
80	6	0	4.016194	6.974539	-0.951259
81	1	0	3.864470	5.179338	0.230361
82	6	0	3.434105	7.756394	-1.951243
83	1	0	1.787287	7.934263	-3.333705
84	1	0	4.936038	7.298627	-0.471441
85	1	0	3.901862	8.687772	-2.258962
86	6	0	-3.994440	3.613799	1.560096
87	6	0	-4.423126	3.449334	2.887229
88	6	0	-4.711861	4.489683	0.729148
89	6	0	-5.533099	4.143656	3.371130
90	1	0	-3.873558	2.778564	3.541852
91	6	0	-5.822807	5.182786	1.211855
92	1	0	-4.396501	4.617828	-0.302397
93	6	0	-6.236725	5.012669	2.534769
94	1	0	-5.844890	4.008009	4.403477
95	1	0	-6.367659	5.852659	0.551737
96	1	0	-7.101294	5.553112	2.910831

***trans*-$H_2Fc_2Ph_2P$**:

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

Fe	-0.98138	6.24126	1.24261
C	0.80558	7.03695	0.58096
C	0.9223	5.62454	0.73347
C	-0.21742	7.28685	-0.38205
C	-0.72374	6.03008	-0.82498
H	1.36822	7.78478	1.12483
H	1.59649	5.11043	1.40539
H	-0.56318	8.25876	-0.71033
H	-1.4914	5.88767	-1.57341
C	-0.00884	4.97762	-0.15431
C	-1.35198	7.14723	3.07533
C	-2.4113	7.43993	2.16427
C	-2.30393	5.14629	2.42403
C	-3.00042	6.20294	1.76307
H	-0.69745	7.87171	3.54311
H	-2.70596	8.42505	1.82584
H	-2.49393	4.0884	2.30189
H	-3.82719	6.08929	1.07391
C	-1.28573	5.7297	3.23528
H	-0.57423	5.19064	3.8475
Fe	0.98138	-6.24126	1.24261

C	3.00042	-6.20294	1.76307
C	2.30393	-5.14629	2.42403
C	2.4113	-7.43993	2.16427
C	1.35198	-7.14723	3.07533
H	3.82719	-6.08929	1.07391
H	2.49393	-4.0884	2.30189
H	2.70596	-8.42505	1.82584
H	0.69745	-7.87171	3.54311
C	1.28573	-5.7297	3.23528
H	0.57423	-5.19064	3.8475
C	0.72374	-6.03008	-0.82498
C	0.21742	-7.28685	-0.38205
C	-0.9223	-5.62454	0.73347
C	-0.80558	-7.03695	0.58096
H	1.4914	-5.88767	-1.57341
H	0.56318	-8.25876	-0.71033
H	-1.59649	-5.11043	1.40539
H	-1.36822	-7.78478	1.12483
C	0.00884	-4.97762	-0.15431
N	-1.43104	-1.53617	-0.67653
N	-1.41103	1.46078	-0.71458
N	1.41103	-1.46078	-0.71458
N	1.43104	1.53617	-0.67653
C	-2.76078	-1.28068	-0.9279
C	-1.19772	-2.89001	-0.59385
C	-2.74953	1.23012	-0.86144
C	-1.28573	2.81081	-0.5255
C	1.28573	-2.81081	-0.5255
C	2.74953	-1.23012	-0.86144
C	1.19772	2.89001	-0.59385
C	2.76078	1.28068	-0.9279
C	-3.38146	-0.02292	-1.01634
C	-3.40109	-2.55809	-1.04226
C	-2.46124	-3.53001	-0.8234
C	-3.50309	2.47519	-0.76459
C	-0.05899	3.5103	-0.40504
C	-2.59506	3.45301	-0.53327
C	0.05899	-3.5103	-0.40504
C	2.59506	-3.45301	-0.53327
C	3.50309	-2.47519	-0.76459
C	2.46124	3.53001	-0.8234
C	3.38146	0.02292	-1.01634
C	3.40109	2.55809	-1.04226
H	-4.44673	-2.70121	-1.26888
H	-2.6128	-4.59743	-0.86053
H	-4.57677	2.57242	-0.83588

H	-2.78486	4.5026	-0.38131
H	2.78486	-4.5026	-0.38131
H	4.57677	-2.57242	-0.83588
H	2.6128	4.59743	-0.86053
H	4.44673	2.70121	-1.26888
C	4.86094	0.02815	-1.26478
C	5.37715	-0.43637	-2.48499
C	5.75951	0.48882	-0.28931
C	6.7522	-0.43768	-2.72436
H	4.69092	-0.79292	-3.248
C	7.13503	0.48578	-0.52709
H	5.37312	0.84137	0.66301
C	7.63559	0.02351	-1.74607
H	7.13245	-0.79702	-3.67703
H	7.81539	0.84023	0.24286
H	8.70634	0.02148	-1.93169
C	-4.86094	-0.02815	-1.26478
C	-5.75951	-0.48882	-0.28931
C	-5.37715	0.43637	-2.48499
C	-7.13503	-0.48578	-0.52709
H	-5.37312	-0.84137	0.66301
C	-6.7522	0.43768	-2.72436
H	-4.69092	0.79292	-3.248
C	-7.63559	-0.02351	-1.74607
H	-7.81539	-0.84023	0.24286
H	-7.13245	0.79702	-3.67703
H	-8.70634	-0.02148	-1.93169
H	-0.69522	-0.83895	-0.62065
H	0.69522	0.83895	-0.62065

H_2Fc_3PhP:
Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.472180	5.923569	1.147907
2	6	0	-1.265290	6.466039	-0.695662
3	6	0	-0.478998	5.287407	-0.848434
4	6	0	-2.307949	6.184529	0.237051
5	6	0	-2.156149	4.833252	0.662465

6	1	0	-1.088386	7.412357	-1.190780
7	1	0	0.371316	5.178475	-1.507360
8	1	0	-3.058508	6.881615	0.587016
9	1	0	-2.777596	4.320379	1.384063
10	6	0	-1.033211	4.246649	-0.023525
11	6	0	1.449227	6.429511	1.785173
12	6	0	0.578468	7.555115	1.899766
13	6	0	-0.269995	5.855971	3.216183
14	6	0	-0.483895	7.200505	2.784866
15	1	0	2.347965	6.381352	1.183781
16	1	0	0.694488	8.504328	1.392429
17	1	0	-0.912713	5.289245	3.877455
18	1	0	-1.318994	7.831885	3.060404
19	6	0	0.924158	5.379651	2.597886
20	1	0	1.341920	4.386581	2.698652
21	26	0	-6.086478	-1.690695	-1.535820
22	6	0	-6.611135	-3.177229	-0.197776
23	6	0	-5.193042	-3.063427	-0.274342
24	6	0	-7.125730	-1.923507	0.249180
25	6	0	-6.024763	-1.041850	0.452003
26	1	0	-7.194791	-4.049484	-0.462761
27	1	0	-4.508280	-3.834823	-0.599272
28	1	0	-8.169462	-1.675715	0.394521
29	1	0	-6.091258	-0.025863	0.816165
30	6	0	-4.804569	-1.744474	0.151872
31	6	0	-6.850669	-2.296018	-3.369767
32	6	0	-7.432929	-1.049864	-2.987942
33	6	0	-5.146589	-0.753949	-3.143731
34	6	0	-6.379338	-0.096261	-2.849705
35	1	0	-7.384827	-3.223062	-3.534663
36	1	0	-8.485917	-0.864141	-2.819194
37	1	0	-4.161714	-0.308015	-3.099001
38	1	0	-6.498279	0.942478	-2.569059
39	6	0	-5.437809	-2.112940	-3.465794
40	1	0	-4.712087	-2.875579	-3.716875
41	26	0	6.060242	-0.728783	-1.849582
42	6	0	6.399877	-2.784246	-1.917164
43	6	0	5.166097	-2.470497	-2.564091
44	6	0	7.445007	-2.088880	-2.597365
45	6	0	6.856689	-1.346996	-3.665589
46	1	0	6.524687	-3.434041	-1.060514
47	1	0	4.185931	-2.818089	-2.265712
48	1	0	8.495956	-2.107696	-2.338687
49	1	0	7.383243	-0.699937	-4.355514
50	6	0	5.448540	-1.583041	-3.644877
51	1	0	4.719866	-1.149220	-4.317485

52	6	0	5.993477	-0.039231	0.123262
53	6	0	7.068393	0.573952	-0.584374
54	6	0	5.106561	1.097736	-1.673035
55	6	0	6.519484	1.281146	-1.695695
56	1	0	6.087737	-0.621573	1.029788
57	1	0	8.117742	0.500160	-0.328575
58	1	0	4.399431	1.493068	-2.389792
59	1	0	7.078052	1.831180	-2.442095
60	6	0	4.756341	0.295504	-0.530857
61	7	0	1.109621	1.076227	0.047448
62	7	0	-1.773791	0.568495	0.233198
63	7	0	1.745370	-1.611821	0.818039
64	7	0	-1.152436	-2.118202	0.989892
65	6	0	0.681698	2.379066	0.056474
66	6	0	2.466547	1.129460	-0.092769
67	6	0	-1.771258	1.915045	-0.043158
68	6	0	-3.021392	0.019062	0.020488
69	6	0	3.005710	-1.249820	0.395629
70	6	0	1.748761	-2.880976	1.347341
71	6	0	-2.512424	-2.223915	0.962598
72	6	0	-0.708728	-3.219163	1.670858
73	6	0	-0.669018	2.803489	0.031337
74	6	0	1.818426	3.287242	-0.019071
75	6	0	2.923704	2.514265	-0.144443
76	6	0	-3.096662	2.230523	-0.489077
77	6	0	-3.401887	-1.298702	0.351047
78	6	0	-3.843061	1.080900	-0.473523
79	6	0	3.362655	0.024535	-0.089070
80	6	0	3.853032	-2.375891	0.656555
81	6	0	3.098969	-3.351525	1.255575
82	6	0	-2.953149	-3.402892	1.703423
83	6	0	0.639890	-3.604450	1.824861
84	6	0	-1.830881	-4.009440	2.161705
85	1	0	1.772995	4.362523	0.028452
86	1	0	3.950382	2.843145	-0.207765
87	1	0	-3.417343	3.204709	-0.823640
88	1	0	-4.869342	0.968821	-0.780441
89	1	0	4.902193	-2.423117	0.417067
90	1	0	3.430892	-4.325265	1.583188
91	1	0	-3.977696	-3.688942	1.890058
92	1	0	-1.762191	-4.894747	2.777221
93	6	0	0.940023	-4.912188	2.489139
94	6	0	0.514666	-6.126501	1.925228
95	6	0	1.666474	-4.952051	3.690871
96	6	0	0.803126	-7.342523	2.545924
97	1	0	-0.037924	-6.110438	0.990277

98	6	0	1.952749	-6.167758	4.313607
99	1	0	1.996624	-4.019989	4.140984
100	6	0	1.521954	-7.367255	3.743081
101	1	0	0.469755	-8.271489	2.090682
102	1	0	2.509094	-6.176543	5.247286
103	1	0	1.745439	-8.314236	4.227120
104	1	0	-0.965749	0.021779	0.511942
105	1	0	0.923720	-1.029915	0.687848

H_2TFcP:

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

Fe	3.74521	4.71479	-2.43237
C	4.97379	5.14721	-0.84459
C	3.71409	4.68293	-0.3675
C	5.54346	4.12315	-1.6582
C	4.62809	3.03186	-1.68699
H	5.41351	6.11325	-0.63188
H	3.05463	5.221	0.29958
H	6.4865	4.17711	-2.18666
H	4.75872	2.10644	-2.23163
C	3.48912	3.35143	-0.86647
C	2.35572	6.0532	-3.15871
C	3.66719	6.40731	-3.59695
C	3.20565	4.27996	-4.36878
C	4.19151	5.31183	-4.34628
H	1.6935	6.67595	-2.57114
H	4.17752	7.33916	-3.39009
H	3.3067	3.31305	-4.84443
H	5.17284	5.26453	-4.80068
C	2.07189	4.73731	-3.63447
H	1.16667	4.17566	-3.44616
Fe	4.65747	-3.76734	2.44705
C	4.06547	-5.57301	1.68851
C	2.9792	-4.65157	1.68717
C	5.10654	-5.02078	0.88446
C	4.65817	-3.76435	0.38371
H	4.10459	-6.50975	2.22928
H	2.04261	-4.76878	2.21527
H	6.07271	-5.4697	0.69257
H	5.21093	-3.11969	-0.28587
C	3.31988	-3.52572	0.85891

C	5.22406	-4.18945	4.375
C	6.33279	-3.67992	3.63493
C	4.66868	-2.07767	3.62518
C	5.99037	-2.37318	3.17318
H	5.16603	-5.16402	4.84247
H	7.26586	-4.1962	3.44944
H	4.11334	-1.17245	3.41863
H	6.62597	-1.72118	2.58773
C	4.1959	-3.19945	4.36832
H	3.22136	-3.28978	4.83028
Fe	-4.65747	3.76734	2.44705
C	-5.99037	2.37318	3.17318
C	-4.66868	2.07767	3.62518
C	-6.33279	3.67992	3.63493
C	-5.22406	4.18945	4.375
H	-6.62597	1.72118	2.58773
H	-4.11334	1.17245	3.41863
H	-7.26586	4.1962	3.44944
H	-5.16603	5.16402	4.84247
C	-4.1959	3.19945	4.36832
H	-3.22136	3.28978	4.83028
C	-4.65817	3.76435	0.38371
C	-5.10654	5.02078	0.88446
C	-2.9792	4.65157	1.68717
C	-4.06547	5.57301	1.68851
H	-5.21093	3.11969	-0.28587
H	-6.07271	5.4697	0.69257
H	-2.04261	4.76878	2.21527
H	-4.10459	6.50975	2.22928
C	-3.31988	3.52572	0.85891
N	0.01706	2.00083	-0.00798
N	2.08019	-0.03038	-0.01299
N	-2.08019	0.03038	-0.01299
N	-0.01706	-2.00083	-0.00798
C	1.05822	2.79769	-0.40743
C	-1.05822	2.83035	0.12461
C	2.85759	1.09359	-0.15784
C	2.83698	-1.11097	0.38567
C	-2.83698	1.11097	0.38567
C	-2.85759	-1.09359	-0.15784
C	1.05822	-2.83035	0.12461
C	-1.05822	-2.79769	-0.40743
C	2.411	2.39279	-0.50249
C	0.60521	4.16769	-0.59876
C	-0.70082	4.19725	-0.23908
C	4.19151	0.70203	0.1907

C	2.37888	-2.44078	0.47875
C	4.17187	-0.62147	0.54706
C	-2.37888	2.44078	0.47875
C	-4.17187	0.62147	0.54706
C	-4.19151	-0.70203	0.1907
C	0.70082	-4.19725	-0.23908
C	-2.411	-2.39279	-0.50249
C	-0.60521	-4.16769	-0.59876
Fe	-3.74521	-4.71479	-2.43237
C	-4.19151	-5.31183	-4.34628
C	-3.20565	-4.27996	-4.36878
C	-3.66719	-6.40731	-3.59695
C	-2.35572	-6.0532	-3.15871
H	-5.17284	-5.26453	-4.80068
H	-3.3067	-3.31305	-4.84443
H	-4.17752	-7.33916	-3.39009
H	-1.6935	-6.67595	-2.57114
C	-2.07189	-4.73731	-3.63447
H	-1.16667	-4.17566	-3.44616
C	-4.62809	-3.03186	-1.68699
C	-5.54346	-4.12315	-1.6582
C	-3.71409	-4.68293	-0.3675
C	-4.97379	-5.14721	-0.84459
H	-4.75872	-2.10644	-2.23163
H	-6.4865	-4.17711	-2.18666
H	-3.05463	-5.221	0.29958
H	-5.41351	-6.11325	-0.63188
C	-3.48912	-3.35143	-0.86647
H	1.20783	4.98047	-0.96788
H	-1.37157	5.0434	-0.26858
H	5.04219	1.36576	0.21052
H	4.99947	-1.21494	0.89688
H	-4.99947	1.21494	0.89688
H	-5.04219	-1.36576	0.21052
H	1.37157	-5.0434	-0.26858
H	-1.20783	-4.98047	-0.96788
H	1.07067	-0.05697	-0.11225
H	-1.07067	0.05697	-0.11225