Supporting information for

Iron(II) complexes with porphyrin and tetrabenzoporphyrin: CASSCF/MCQDPT2 study of the electronic structures and UV-vis spectra by sTD-DFT

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Cartesian coordinates of $^{1}B_{1g}$ electronic state of FeP optimized PBE0/def2-TZVP level of theory:

N	**1.989715196900**	**0.000000000000**	**0.000000000000**
N	**0.000000000000**	**1.989715196900**	**0.000000000000**
N	**-1.989715196900**	**0.000000000000**	**0.000000000000**
N	**0.000000000000**	**-1.989715196900**	**0.000000000000**
C	**2.403266822600**	**2.403266822600**	**0.000000000000**
C	**-2.403266822600**	**2.403266822600**	**0.000000000000**
C	**-2.403266822600**	**-2.403266822600**	**0.000000000000**
C	**2.403266822600**	**-2.403266822600**	**0.000000000000**
C	**2.816971600100**	**1.086917445400**	**0.000000000000**
C	**-1.086917445400**	**2.816971600100**	**0.000000000000**
C	**-2.816971600100**	**-1.086917445400**	**0.000000000000**

C	1.086917445400	2.816971600100	0.000000000000
C	-2.816971600100	1.086917445400	0.000000000000
C	-1.086917445400	-2.816971600100	0.000000000000
C	2.816971600100	-1.086917445400	0.000000000000
C	1.086917445400	-2.816971600100	0.000000000000
C	4.191046876100	0.676242483400	0.000000000000
C	-0.676242483400	4.191046876100	0.000000000000
C	-4.191046876100	-0.676242483400	0.000000000000
C	0.676242483400	4.191046876100	0.000000000000
C	-4.191046876100	0.676242483400	0.000000000000
C	-0.676242483400	-4.191046876100	0.000000000000
C	4.191046876100	-0.676242483400	0.000000000000
C	0.676242483400	-4.191046876100	0.000000000000
H	3.169276985700	3.169276985700	0.000000000000
H	-3.169276985700	3.169276985700	0.000000000000
H	-3.169276985700	-3.169276985700	0.000000000000
H	3.169276985700	-3.169276985700	0.000000000000
Fe	0.000000000000	0.000000000000	0.000000000000
H	5.034528728000	1.350841842400	0.000000000000
H	-1.350841842400	5.034528728000	0.000000000000
H	-5.034528728000	-1.350841842400	0.000000000000
H	1.350841842400	5.034528728000	0.000000000000
H	-5.034528728000	1.350841842400	0.000000000000
H	-1.350841842400	-5.034528728000	0.000000000000
H	5.034528728000	-1.350841842400	0.000000000000
H	1.350841842400	-5.034528728000	0.000000000000

Cartesian coordinates of $^3A_{2g}$ electronic state of FeP optimized PBE0/def2-TZVP level of theory:

N	1.989807640600	0.000000000000	0.000000000000
N	0.000000000000	1.989807640600	0.000000000000
N	-1.989807640600	0.000000000000	0.000000000000
N	0.000000000000	-1.989807640600	0.000000000000
C	2.404256620600	2.404256620600	0.000000000000
C	-2.404256620600	2.404256620600	0.000000000000
C	-2.404256620600	-2.404256620600	0.000000000000
C	2.404256620600	-2.404256620600	0.000000000000
C	2.816536241800	1.087081515600	0.000000000000
C	-1.087081515600	2.816536241800	0.000000000000
C	-2.816536241800	-1.087081515600	0.000000000000
C	1.087081515600	2.816536241800	0.000000000000
C	-2.816536241800	1.087081515600	0.000000000000
C	-1.087081515600	-2.816536241800	0.000000000000
C	2.816536241800	-1.087081515600	0.000000000000
C	1.087081515600	-2.816536241800	0.000000000000
C	4.188854182100	0.676974418900	0.000000000000
C	-0.676974418900	4.188854182100	0.000000000000
C	-4.188854182100	-0.676974418900	0.000000000000
C	0.676974418900	4.188854182100	0.000000000000
C	-4.188854182100	0.676974418900	0.000000000000
C	-0.676974418900	-4.188854182100	0.000000000000
C	4.188854182100	-0.676974418900	0.000000000000
C	0.676974418900	-4.188854182100	0.000000000000
H	3.170181297800	3.170181297800	0.000000000000
H	-3.170181297800	3.170181297800	0.000000000000
H	-3.170181297800	-3.170181297800	0.000000000000

H	**3.170181297800**	**-3.170181297800**	**0.000000000000**
Fe	**0.000000000000**	**0.000000000000**	**0.000000000000**
H	**5.032946132100**	**1.350827150100**	**0.000000000000**
H	**-1.350827150100**	**5.032946132100**	**0.000000000000**
H	**-5.032946132100**	**-1.350827150100**	**0.000000000000**
H	**1.350827150100**	**5.032946132100**	**0.000000000000**
H	**-5.032946132100**	**1.350827150100**	**0.000000000000**
H	**-1.350827150100**	**-5.032946132100**	**0.000000000000**
H	**5.032946132100**	**-1.350827150100**	**0.000000000000**
H	**1.350827150100**	**-5.032946132100**	**0.000000000000**

Cartesian coordinates of $^{5}A_{1g}$ electronic state of FeP optimized PBE0/def2-TZVP level of theory:

N	**2.053997130250**	**0.000000000000**	**0.000000000000**
N	**0.000000000000**	**2.053997130250**	**0.000000000000**
N	**-2.053997130250**	**0.000000000000**	**0.000000000000**
N	**0.000000000000**	**-2.053997130250**	**0.000000000000**
C	**2.416615228928**	**2.416615228928**	**0.000000000000**
C	**-2.416615228928**	**2.416615228928**	**0.000000000000**
C	**-2.416615228928**	**-2.416615228928**	**0.000000000000**
C	**2.416615228928**	**-2.416615228928**	**0.000000000000**
C	**2.859028082406**	**1.097053808028**	**0.000000000000**
C	**-1.097053808028**	**2.859028082406**	**0.000000000000**
C	**-2.859028082406**	**-1.097053808028**	**0.000000000000**
C	**1.097053808028**	**2.859028082406**	**0.000000000000**
C	**-2.859028082406**	**1.097053808028**	**0.000000000000**
C	**-1.097053808028**	**-2.859028082406**	**0.000000000000**
C	**2.859028082406**	**-1.097053808028**	**0.000000000000**
C	**1.097053808028**	**-2.859028082406**	**0.000000000000**

C	4.234697250588	0.678721235699	0.000000000000
C	-0.678721235699	4.234697250588	0.000000000000
C	-4.234697250588	-0.678721235699	0.000000000000
C	0.678721235699	4.234697250588	0.000000000000
C	-4.234697250588	0.678721235699	0.000000000000
C	-0.678721235699	-4.234697250588	0.000000000000
C	4.234697250588	-0.678721235699	0.000000000000
C	0.678721235699	-4.234697250588	0.000000000000
H	3.183134570067	3.183134570067	0.000000000000
H	-3.183134570067	3.183134570067	0.000000000000
H	-3.183134570067	-3.183134570067	0.000000000000
H	3.183134570067	-3.183134570067	0.000000000000
Fe	0.000000000000	0.000000000000	0.000000000000
H	5.086641985290	1.343120820077	0.000000000000
H	-1.343120820077	5.086641985290	0.000000000000
H	-5.086641985290	-1.343120820077	0.000000000000
H	1.343120820077	5.086641985290	0.000000000000
H	-5.086641985290	1.343120820077	0.000000000000
H	-1.343120820077	-5.086641985290	0.000000000000
H	5.086641985290	-1.343120820077	0.000000000000
H	1.343120820077	-5.086641985290	0.000000000000

Cartesian coordinates of $^{1}B_{1g}$ electronic state of FeTBP optimized PBE0/def2-TZVP level of theory:

H	7.583214430456	-1.230402567755	0.000000000000
H	1.230402567755	7.583214430456	0.000000000000
H	-7.583214430456	1.230402567755	0.000000000000
H	-1.230402567755	7.583214430456	0.000000000000
H	-7.583214430456	-1.230402567755	0.000000000000

H	1.230402567755	-7.583214430456	0.000000000000
H	7.583214430456	1.230402567755	0.000000000000
H	-1.230402567755	-7.583214430456	0.000000000000
N	2.037745897275	0.000000000000	0.000000000000
N	0.000000000000	2.037745897275	0.000000000000
N	-2.037745897275	0.000000000000	0.000000000000
N	0.000000000000	-2.037745897275	0.000000000000
C	2.421702261999	-2.421702261999	0.000000000000
C	2.421702261999	2.421702261999	0.000000000000
C	-2.421702261999	2.421702261999	0.000000000000
C	-2.421702261999	-2.421702261999	0.000000000000
C	2.850641774499	-1.102092856524	0.000000000000
C	1.102092856524	2.850641774499	0.000000000000
C	-2.850641774499	1.102092856524	0.000000000000
C	-1.102092856524	2.850641774499	0.000000000000
C	-2.850641774499	-1.102092856524	0.000000000000
C	1.102092856524	-2.850641774499	0.000000000000
C	2.850641774499	1.102092856524	0.000000000000
C	-1.102092856524	-2.850641774499	0.000000000000
C	4.248610901064	-0.700369041067	0.000000000000
C	0.700369041067	4.248610901064	0.000000000000
C	-4.248610901064	0.700369041067	0.000000000000
C	-0.700369041067	4.248610901064	0.000000000000
C	-4.248610901064	-0.700369041067	0.000000000000
C	0.700369041067	-4.248610901064	0.000000000000
C	4.248610901064	0.700369041067	0.000000000000
C	-0.700369041067	-4.248610901064	0.000000000000

C	1.412081598246	-5.453096409046	0.000000000000
C	5.453096409046	1.412081598246	0.000000000000
C	-1.412081598246	5.453096409046	0.000000000000
C	-5.453096409046	1.412081598246	0.000000000000
C	-1.412081598246	-5.453096409046	0.000000000000
C	5.453096409046	-1.412081598246	0.000000000000
C	1.412081598246	5.453096409046	0.000000000000
C	-5.453096409046	-1.412081598246	0.000000000000
C	6.636938775304	-0.701056230907	0.000000000000
C	0.701056230907	6.636938775304	0.000000000000
C	-6.636938775304	0.701056230907	0.000000000000
C	-0.701056230907	6.636938775304	0.000000000000
C	-6.636938775304	-0.701056230907	0.000000000000
C	0.701056230907	-6.636938775304	0.000000000000
C	6.636938775304	0.701056230907	0.000000000000
C	-0.701056230907	-6.636938775304	0.000000000000
H	5.466499591810	-2.496453662866	0.000000000000
H	2.496453662866	5.466499591810	0.000000000000
H	-5.466499591810	2.496453662866	0.000000000000
H	-2.496453662866	5.466499591810	0.000000000000
H	-5.466499591810	-2.496453662866	0.000000000000
H	2.496453662866	-5.466499591810	0.000000000000
H	5.466499591810	2.496453662866	0.000000000000
H	-2.496453662866	-5.466499591810	0.000000000000
H	3.185843186359	-3.185843186359	0.000000000000
H	3.185843186359	3.185843186359	0.000000000000
H	-3.185843186359	3.185843186359	0.000000000000

H	**-3.185843186359**	**-3.185843186359**	**0.000000000000**
Fe	**0.000000000000**	**0.000000000000**	**0.000000000000**

Cartesian coordinates of $^3A_{2g}$ electronic state of FeTBP optimized PBE0/def2-TZVP level of theory:

H	**7.537066849999**	**-1.230788456558**	**0.000000000000**
H	**1.230788456558**	**7.537066849999**	**0.000000000000**
H	**-7.537066849999**	**1.230788456558**	**0.000000000000**
H	**-1.230788456558**	**7.537066849999**	**0.000000000000**
H	**-7.537066849999**	**-1.230788456558**	**0.000000000000**
H	**1.230788456558**	**-7.537066849999**	**0.000000000000**
H	**7.537066849999**	**1.230788456558**	**0.000000000000**
H	**-1.230788456558**	**-7.537066849999**	**0.000000000000**
N	**2.014138009110**	**0.000000000000**	**0.000000000000**
N	**0.000000000000**	**2.014138009110**	**0.000000000000**
N	**-2.014138009110**	**0.000000000000**	**0.000000000000**
N	**0.000000000000**	**-2.014138009110**	**0.000000000000**
C	**2.407703170723**	**-2.407703170723**	**0.000000000000**
C	**2.407703170723**	**2.407703170723**	**0.000000000000**
C	**-2.407703170723**	**2.407703170723**	**0.000000000000**
C	**-2.407703170723**	**-2.407703170723**	**0.000000000000**
C	**2.827469089642**	**-1.098460447888**	**0.000000000000**
C	**1.098460447888**	**2.827469089642**	**0.000000000000**
C	**-2.827469089642**	**1.098460447888**	**0.000000000000**
C	**-1.098460447888**	**2.827469089642**	**0.000000000000**
C	**-2.827469089642**	**-1.098460447888**	**0.000000000000**
C	**1.098460447888**	**-2.827469089642**	**0.000000000000**
C	**2.827469089642**	**1.098460447888**	**0.000000000000**
C	**-1.098460447888**	**-2.827469089642**	**0.000000000000**

C	4.212621318865	-0.698332199576	0.000000000000
C	0.698332199576	4.212621318865	0.000000000000
C	-4.212621318865	0.698332199576	0.000000000000
C	-0.698332199576	4.212621318865	0.000000000000
C	-4.212621318865	-0.698332199576	0.000000000000
C	0.698332199576	-4.212621318865	0.000000000000
C	4.212621318865	0.698332199576	0.000000000000
C	-0.698332199576	-4.212621318865	0.000000000000
C	1.412854965236	-5.408707134036	0.000000000000
C	5.408707134036	1.412854965236	0.000000000000
C	-1.412854965236	5.408707134036	0.000000000000
C	-5.408707134036	1.412854965236	0.000000000000
C	-1.412854965236	-5.408707134036	0.000000000000
C	5.408707134036	-1.412854965236	0.000000000000
C	1.412854965236	5.408707134036	0.000000000000
C	-5.408707134036	-1.412854965236	0.000000000000
C	6.591356542896	-0.701088891303	0.000000000000
C	0.701088891303	6.591356542896	0.000000000000
C	-6.591356542896	0.701088891303	0.000000000000
C	-0.701088891303	6.591356542896	0.000000000000
C	-6.591356542896	-0.701088891303	0.000000000000
C	0.701088891303	-6.591356542896	0.000000000000
C	6.591356542896	0.701088891303	0.000000000000
C	-0.701088891303	-6.591356542896	0.000000000000
H	5.421319436531	-2.496911739859	0.000000000000
H	2.496911739859	5.421319436531	0.000000000000
H	-5.421319436531	2.496911739859	0.000000000000

H	**-2.496911739859**	**5.421319436531**	**0.000000000000**
H	**-5.421319436531**	**-2.496911739859**	**0.000000000000**
H	**2.496911739859**	**-5.421319436531**	**0.000000000000**
H	**5.421319436531**	**2.496911739859**	**0.000000000000**
H	**-2.496911739859**	**-5.421319436531**	**0.000000000000**
H	**3.173191677651**	**-3.173191677651**	**0.000000000000**
H	**3.173191677651**	**3.173191677651**	**0.000000000000**
H	**-3.173191677651**	**3.173191677651**	**0.000000000000**
H	**-3.173191677651**	**-3.173191677651**	**0.000000000000**
Fe	**0.000000000000**	**0.000000000000**	**0.000000000000**

Cartesian coordinates of $^{5}A_{1g}$ electronic state of FeTBP optimized PBE0/def2-TZVP level of theory:

H	**7.583474329142**	**-1.230327026961**	**0.000000000000**
H	**1.230327026961**	**7.583474329142**	**0.000000000000**
H	**-7.583474329142**	**1.230327026961**	**0.000000000000**
H	**-1.230327026961**	**7.583474329142**	**0.000000000000**
H	**-7.583474329142**	**-1.230327026961**	**0.000000000000**
H	**1.230327026961**	**-7.583474329142**	**0.000000000000**
H	**7.583474329142**	**1.230327026961**	**0.000000000000**
H	**-1.230327026961**	**-7.583474329142**	**0.000000000000**
N	**2.076759555258**	**0.000000000000**	**0.000000000000**
N	**0.000000000000**	**2.076759555258**	**0.000000000000**
N	**-2.076759555258**	**0.000000000000**	**0.000000000000**
N	**0.000000000000**	**-2.076759555258**	**0.000000000000**
C	**2.419407961118**	**-2.419407961118**	**0.000000000000**
C	**2.419407961118**	**2.419407961118**	**0.000000000000**
C	**-2.419407961118**	**2.419407961118**	**0.000000000000**
C	**-2.419407961118**	**-2.419407961118**	**0.000000000000**

C	2.868321155479	-1.108183191879	0.000000000000
C	1.108183191879	2.868321155479	0.000000000000
C	-2.868321155479	1.108183191879	0.000000000000
C	-1.108183191879	2.868321155479	0.000000000000
C	-2.868321155479	-1.108183191879	0.000000000000
C	1.108183191879	-2.868321155479	0.000000000000
C	2.868321155479	1.108183191879	0.000000000000
C	-1.108183191879	-2.868321155479	0.000000000000
C	4.256812338570	-0.701202271286	0.000000000000
C	0.701202271286	4.256812338570	0.000000000000
C	-4.256812338570	0.701202271286	0.000000000000
C	-0.701202271286	4.256812338570	0.000000000000
C	-4.256812338570	-0.701202271286	0.000000000000
C	0.701202271286	-4.256812338570	0.000000000000
C	4.256812338570	0.701202271286	0.000000000000
C	-0.701202271286	-4.256812338570	0.000000000000
C	1.412162296771	-5.454055801842	0.000000000000
C	5.454055801842	1.412162296771	0.000000000000
C	-1.412162296771	5.454055801842	0.000000000000
C	-5.454055801842	1.412162296771	0.000000000000
C	-1.412162296771	-5.454055801842	0.000000000000
C	5.454055801842	-1.412162296771	0.000000000000
C	1.412162296771	5.454055801842	0.000000000000
C	-5.454055801842	-1.412162296771	0.000000000000
C	6.637823475208	-0.700477030903	0.000000000000
C	0.700477030903	6.637823475208	0.000000000000
C	-6.637823475208	0.700477030903	0.000000000000

C	**-0.700477030903**	**6.637823475208**	**0.000000000000**
C	**-6.637823475208**	**-0.700477030903**	**0.000000000000**
C	**0.700477030903**	**-6.637823475208**	**0.000000000000**
C	**6.637823475208**	**0.700477030903**	**0.000000000000**
C	**-0.700477030903**	**-6.637823475208**	**0.000000000000**
H	**5.466529304425**	**-2.496380959362**	**0.000000000000**
H	**2.496380959362**	**5.466529304425**	**0.000000000000**
H	**-5.466529304425**	**2.496380959362**	**0.000000000000**
H	**-2.496380959362**	**5.466529304425**	**0.000000000000**
H	**-5.466529304425**	**-2.496380959362**	**0.000000000000**
H	**2.496380959362**	**-5.466529304425**	**0.000000000000**
H	**5.466529304425**	**2.496380959362**	**0.000000000000**
H	**-2.496380959362**	**-5.466529304425**	**0.000000000000**
H	**3.185560752343**	**-3.185560752343**	**0.000000000000**
H	**3.185560752343**	**3.185560752343**	**0.000000000000**
H	**-3.185560752343**	**3.185560752343**	**0.000000000000**
H	**-3.185560752343**	**-3.185560752343**	**0.000000000000**
Fe	**0.000000000000**	**0.000000000000**	**0.000000000000**

Table S1. The relative energies (kJ/mol) of excited states and contributions (in %) of electronic configurations to the wave functions from MCQDPT2 calculations.

State	Contributions	ΔE , kJ/mol	State	Contributions	ΔE, kJ/mol
	FeP			FeTBP	
$^1B_{1g}$	89[$(e_g)^2(b_{2g})^2(a_{1g})^2(b_{1g})^0$]	107.5	$^1B_{1g}$	88[$(e_g)^2(b_{2g})^2(a_{1g})^2(b_{1g})^0$]	
	+7[$(e_g)^2(b_{2g})^2(a_{1g})^1(b_{1g})^1$]			+8[$(e_g)^2(b_{2g})^2(a_{1g})^1(b_{1g})^1$]	119.0
$^1B_{2g}$	86[$(e_g)^2(b_{2g})^2(a_{1g})^2(b_{1g})^0$]	107.5	$^1B_{2g}$	85[$(e_g)^2(b_{2g})^2(a_{1g})^2(b_{1g})^0$]	
	+6[$(e_g)^2(b_{2g})^1(a_{1g})^2(b_{1g})^1$]			+8[$(e_g)^2(b_{2g})^1(a_{1g})^2(b_{1g})^1$]	120.6
^1E_g	91[$(e_g)^3(b_{2g})^2(a_{1g})^1(b_{1g})^0$]	116.2	$^1A_{1g}$	86[$(e_g)^4(b_{2g})^2(a_{1g})^0(b_{1g})^0$]	
				+10[$(e_g)^2(b_{2g})^2(a_{1g})^2(b_{1g})^0$]	120.6
$^1A_{1g}$	86[$(e_g)^4(b_{2g})^2(a_{1g})^0(b_{1g})^0$]	117.1	^1E_g	91[$(e_g)^3(b_{2g})^2(a_{1g})^1(b_{1g})^0$]	
	+10[$(e_g)^2(b_{2g})^2(a_{1g})^2(b_{1g})^0$]				123.1
$^1A_{1g}$	57[$(e_g)^2(b_{2g})^2(a_{1g})^2(b_{1g})^0$]	186.1	$^1A_{1g}$	54[$(e_g)^2(b_{2g})^2(a_{1g})^2(b_{1g})^0$]	
	+25[$(e_g)^2(b_{2g})^2(a_{1g})^1(b_{1g})^1$]			+28[$(e_g)^2(b_{2g})^2(a_{1g})^1(b_{1g})^1$]	
	+10[$(e_g)^4(b_{2g})^0(a_{1g})^2(b_{1g})^0$]			+9[$(e_g)^4(b_{2g})^0(a_{1g})^2(b_{1g})^0$]	
	+6[$(e_g)^4(b_{2g})^2(a_{1g})^0(b_{1g})^0$]			+5[$(e_g)^4(b_{2g})^2(a_{1g})^0(b_{1g})^0$]	194.6

$^1B_{2g}$	71[$(e_g)^4(b_{2g})^1(a_{1g})^1(b_{1g})^0$]	220.2	$^1B_{2g}$	67[$(e_g)^4(b_{2g})^1(a_{1g})^1(b_{1g})^0$]	
	+26[$(e_g)^2(b_{2g})^2(a_{1g})^1(b_{1g})^1$]			+30[$(e_g)^2(b_{2g})^2(a_{1g})^1(b_{1g})^1$]	224.1
^1E_g	58[$(e_g)^3(b_{2g})^1(a_{1g})^2(b_{1g})^0$]	232.6	^1E_g	52[$(e_g)^3(b_{2g})^1(a_{1g})^2(b_{1g})^0$]	
	+29[$(e_g)^1(b_{2g})^2(a_{1g})^2(b_{1g})^1$]			+32[$(e_g)^1(b_{2g})^2(a_{1g})^2(b_{1g})^1$]	
	+6[$(e_g)^3(b_{2g})^1(a_{1g})^1(b_{1g})^1$]			+7[$(e_g)^3(b_{2g})^1(a_{1g})^1(b_{1g})^1$]	239.2
$^1A_{1g}$	77[$(e_g)^2(b_{2g})^1(a_{1g})^2(b_{1g})^1$]	363.3	$^1B_{1g}$	79[$(e_g)^2(b_{2g})^1(a_{1g})^2(b_{1g})^1$]	
	+9[$(e_g)^4(b_{2g})^0(a_{1g})^2(b_{1g})^0$]			+15[$(e_g)^2(b_{2g})^2(a_{1g})^1(b_{1g})^1$]	
	+5[$(e_g)^0(b_{2g})^2(a_{1g})^2(b_{1g})^2$]				348.1
$^1B_{1g}$	80[$(e_g)^2(b_{2g})^1(a_{1g})^2(b_{1g})^1$]	367.5	$^1A_{1g}$	77[$(e_g)^2(b_{2g})^1(a_{1g})^2(b_{1g})^1$]	
	+15[$(e_g)^2(b_{2g})^2(a_{1g})^1(b_{1g})^1$]			+8[$(e_g)^4(b_{2g})^0(a_{1g})^2(b_{1g})^0$]	
				+6[$(e_g)^0(b_{2g})^2(a_{1g})^2(b_{1g})^2$]	351.1
$^1B_{2g}$	79[$(e_g)^2(b_{2g})^1(a_{1g})^2(b_{1g})^1$]	381.2	^1E_g	89[$(e_g)^3(b_{2g})^1(a_{1g})^1(b_{1g})^1$]	
	+10[$(e_g)^2(b_{2g})^2(a_{1g})^1(b_{1g})^1$]			+7[$(e_g)^3(b_{2g})^2(a_{1g})^0(b_{1g})^1$]	
	+6[$(e_g)^4(b_{2g})^1(a_{1g})^1(b_{1g})^0$]				357.7
^1E_g	88[$(e_g)^3(b_{2g})^1(a_{1g})^1(b_{1g})^1$]	382.5			
	+10[$(e_g)^3(b_{2g})^2(a_{1g})^0(b_{1g})^1$]				
$^3A_{2g}$	96[$(e_g)^2(b_{2g})^2(a_{1g})^2(b_{1g})^0$]	0	$^3A_{2g}$	96[$(e_g)^2(b_{2g})^2(a_{1g})^2(b_{1g})^0$]	0
^3E_g	86[$(e_g)^3(b_{2g})^2(a_{1g})^1(b_{1g})^0$]	15.8	^3E_g	84[$(e_g)^3(b_{2g})^2(a_{1g})^1(b_{1g})^0$]	
	+12[$(e_g)^3(b_{2g})^1(a_{1g})^2(b_{1g})^0$]			+11[$(e_g)^3(b_{2g})^1(a_{1g})^2(b_{1g})^0$]	11.1
$^3B_{2g}$	86[$(e_g)^4(b_{2g})^1(a_{1g})^1(b_{1g})^0$]	79.8	$^3B_{2g}$	85[$(e_g)^4(b_{2g})^1(a_{1g})^1(b_{1g})^0$]	
	+12[$(e_g)^2(b_{2g})^2(a_{1g})^1(b_{1g})^1$]			+13[$(e_g)^2(b_{2g})^2(a_{1g})^1(b_{1g})^1$]	71.5
^3E_g	52[$(e_g)^3(b_{2g})^1(a_{1g})^2(b_{1g})^0$]	137.7	^3E_g	49[$(e_g)^3(b_{2g})^1(a_{1g})^2(b_{1g})^0$]	
	+27[$(e_g)^3(b_{2g})^1(a_{1g})^1(b_{1g})^1$]			+30[$(e_g)^3(b_{2g})^1(a_{1g})^1(b_{1g})^1$]	
	+11[$(e_g)^1(b_{2g})^2(a_{1g})^2(b_{1g})^1$]			+11[$(e_g)^1(b_{2g})^2(a_{1g})^2(b_{1g})^1$]	
				+5[$(e_g)^3(b_{2g})^2(a_{1g})^1(b_{1g})^0$]	132.6
$^3B_{1g}$	91[$(e_g)^2(b_{2g})^1(a_{1g})^2(b_{1g})^1$]	264.1	$^3B_{1g}$	90[$(e_g)^2(b_{2g})^1(a_{1g})^2(b_{1g})^1$]	
	+8[$(e_g)^2(b_{2g})^2(a_{1g})^1(b_{1g})^1$]			+9[$(e_g)^2(b_{2g})^2(a_{1g})^1(b_{1g})^1$]	249.1
$^3B_{1g}$	59[$(e_g)^2(b_{2g})^1(a_{1g})^2(b_{1g})^1$]	275.7	^3E_g	74[$(e_g)^3(b_{2g})^1(a_{1g})^1(b_{1g})^1$]	
	+27[$(e_g)^2(b_{2g})^2(a_{1g})^1(b_{1g})^1$]			+23[$(e_g)^3(b_{2g})^2(a_{1g})^0(b_{1g})^1$]	
	+13[$(e_g)^4(b_{2g})^0(a_{1g})^1(b_{1g})^1$]				258.6
^3E_g	86[$(e_g)^3(b_{2g})^1(a_{1g})^1(b_{1g})^1$]	275.8	$^3B_{1g}$	57[$(e_g)^2(b_{2g})^1(a_{1g})^2(b_{1g})^1$]	
	+8[$(e_g)^1(b_{2g})^2(a_{1g})^2(b_{1g})^1$]			+27[$(e_g)^2(b_{2g})^2(a_{1g})^1(b_{1g})^1$]	
				+14[$(e_g)^4(b_{2g})^0(a_{1g})^1(b_{1g})^1$]	259.7
$^3B_{2g}$	53[$(e_g)^2(b_{2g})^2(a_{1g})^1(b_{1g})^1$]	282.1	$^3B_{2g}$	53[$(e_g)^2(b_{2g})^2(a_{1g})^1(b_{1g})^1$]	
	+44[$(e_g)^2(b_{2g})^1(a_{1g})^2(b_{1g})^1$]			+45[$(e_g)^2(b_{2g})^1(a_{1g})^2(b_{1g})^1$]	266.1
$^3A_{2g}$	60[$(e_g)^2(b_{2g})^2(a_{1g})^1(b_{1g})^1$]	284.0	$^3A_{2g}$	64[$(e_g)^2(b_{2g})^2(a_{1g})^1(b_{1g})^1$]	
	+35[$(e_g)^4(b_{2g})^1(a_{1g})^0(b_{1g})^1$]			+29[$(e_g)^4(b_{2g})^1(a_{1g})^0(b_{1g})^1$]	
				+6[$(e_g)^2(b_{2g})^1(a_{1g})^2(b_{1g})^1$]	267.0
$^5A_{1g}$	100[$(e_g)^2(b_{2g})^1(a_{1g})^2(b_{1g})^1$]	23.9	$^5A_{1g}$	100[$(e_g)^2(b_{2g})^1(a_{1g})^2(b_{1g})^1$]	8.5
^5E_g	98[$(e_g)^3(b_{2g})^1(a_{1g})^1(b_{1g})^1$]	46.0	^5E_g	100[$(e_g)^3(b_{2g})^1(a_{1g})^1(b_{1g})^1$]	26.7
$^5B_{2g}$	100[$(e_g)^2(b_{2g})^2(a_{1g})^1(b_{1g})^1$]	59.8	$^5B_{2g}$	100[$(e_g)^2(b_{2g})^2(a_{1g})^1(b_{1g})^1$]	42.8
$^5B_{1g}$	100[$(e_g)^2(b_{2g})^1(a_{1g})^1(b_{1g})^2$]	290.6	$^5B_{1g}$	100[$(e_g)^2(b_{2g})^1(a_{1g})^1(b_{1g})^2$]	261.8

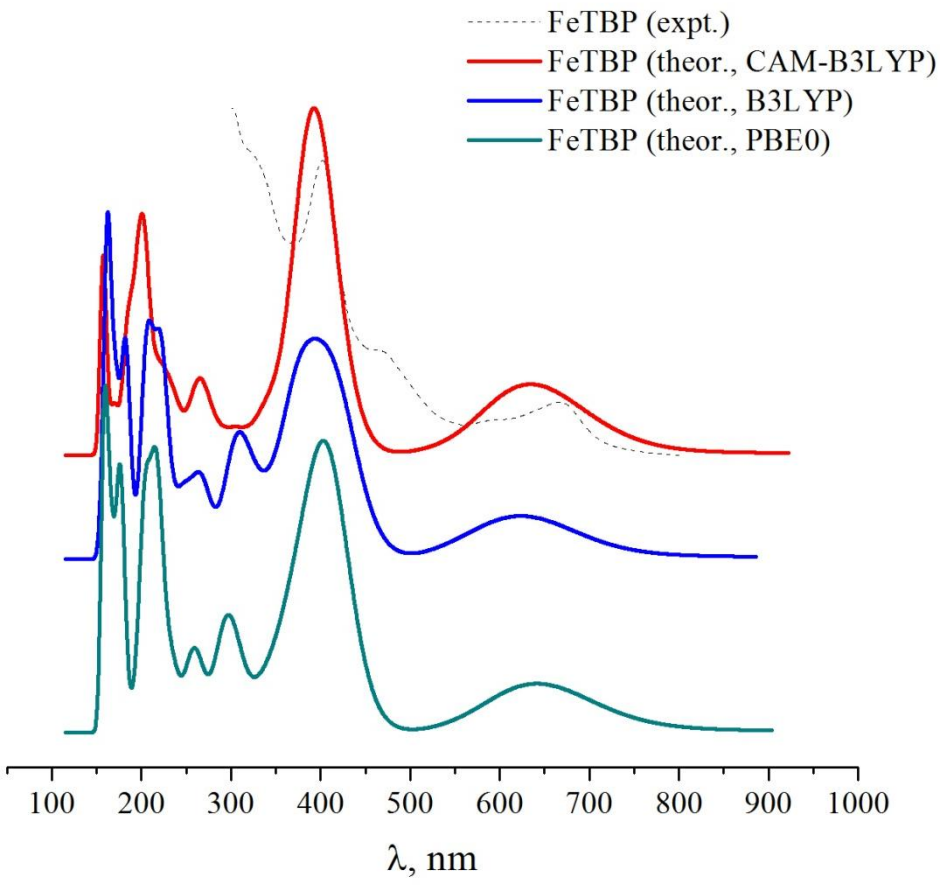


Figure S1. Normalized theoretical (sTDDFT) and experimental electronic absorption spectra of FeTBP in the DMF solvent. Gaussian broadening function with FWHM = 0.4 eV was used for the model spectra.