Supporting Information

Effects of Imidazole Deprotonation on Vibrational Spectra of High-Spin Iron(II) Porphyrinates

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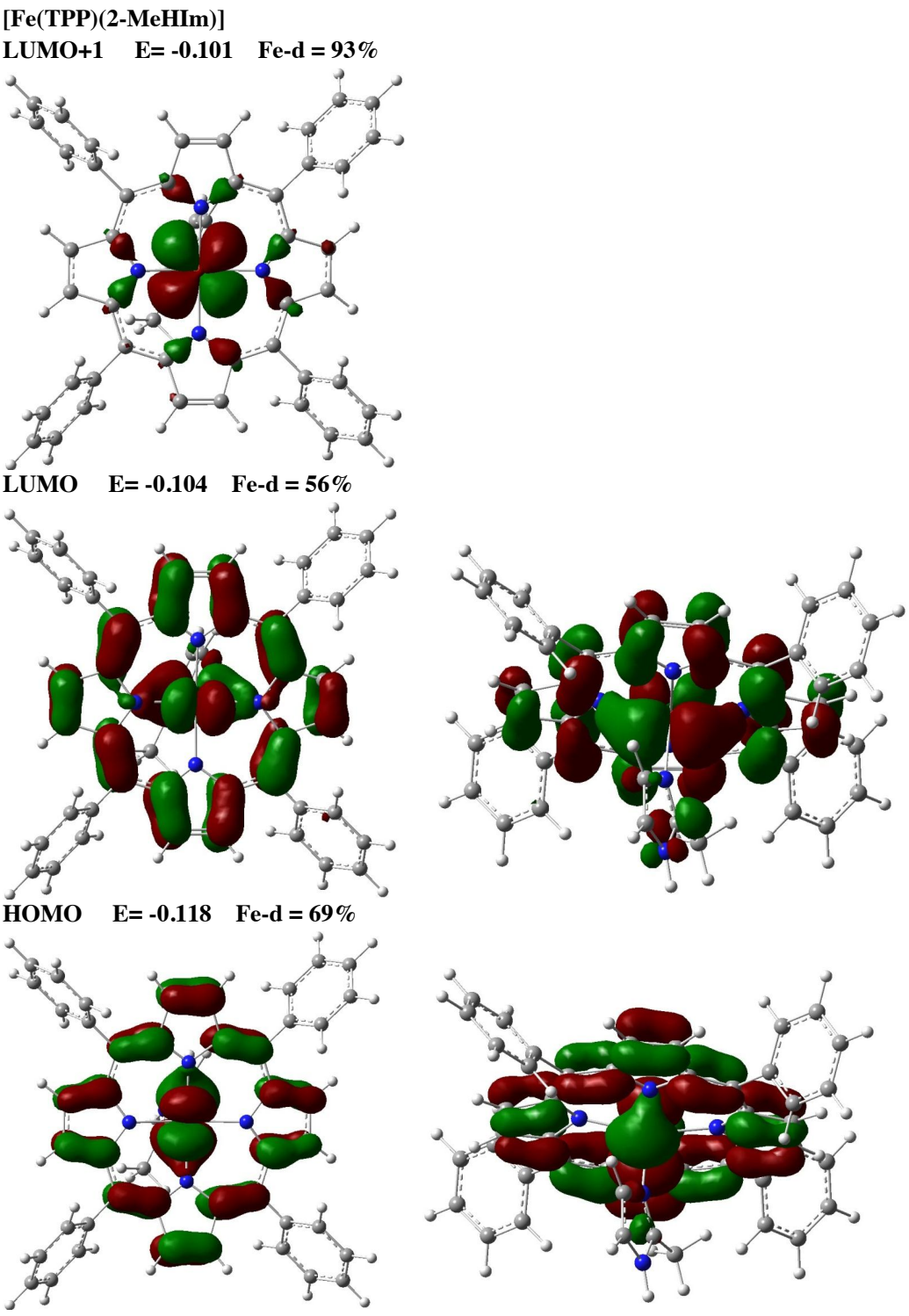

Figure S1. Frontier β-MO's for [Fe(TPP)(2-MeHIm)] calculated with BP86/TZVP.

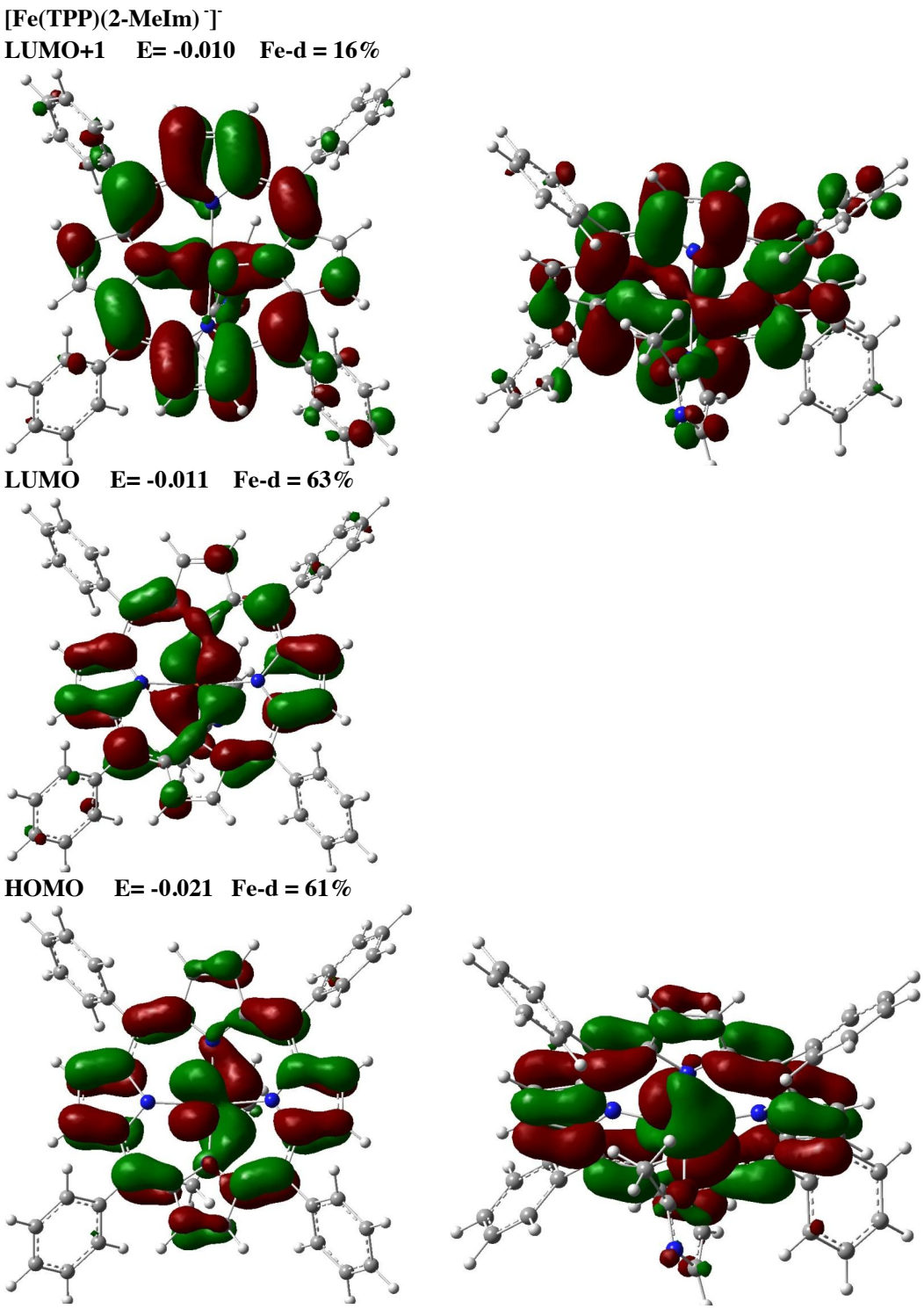

Figure S2. Frontier β-MO's for $[Fe(TPP)(2\text{-}MeIm^{-})]^{-}$ calculated with BP86/TZVP.

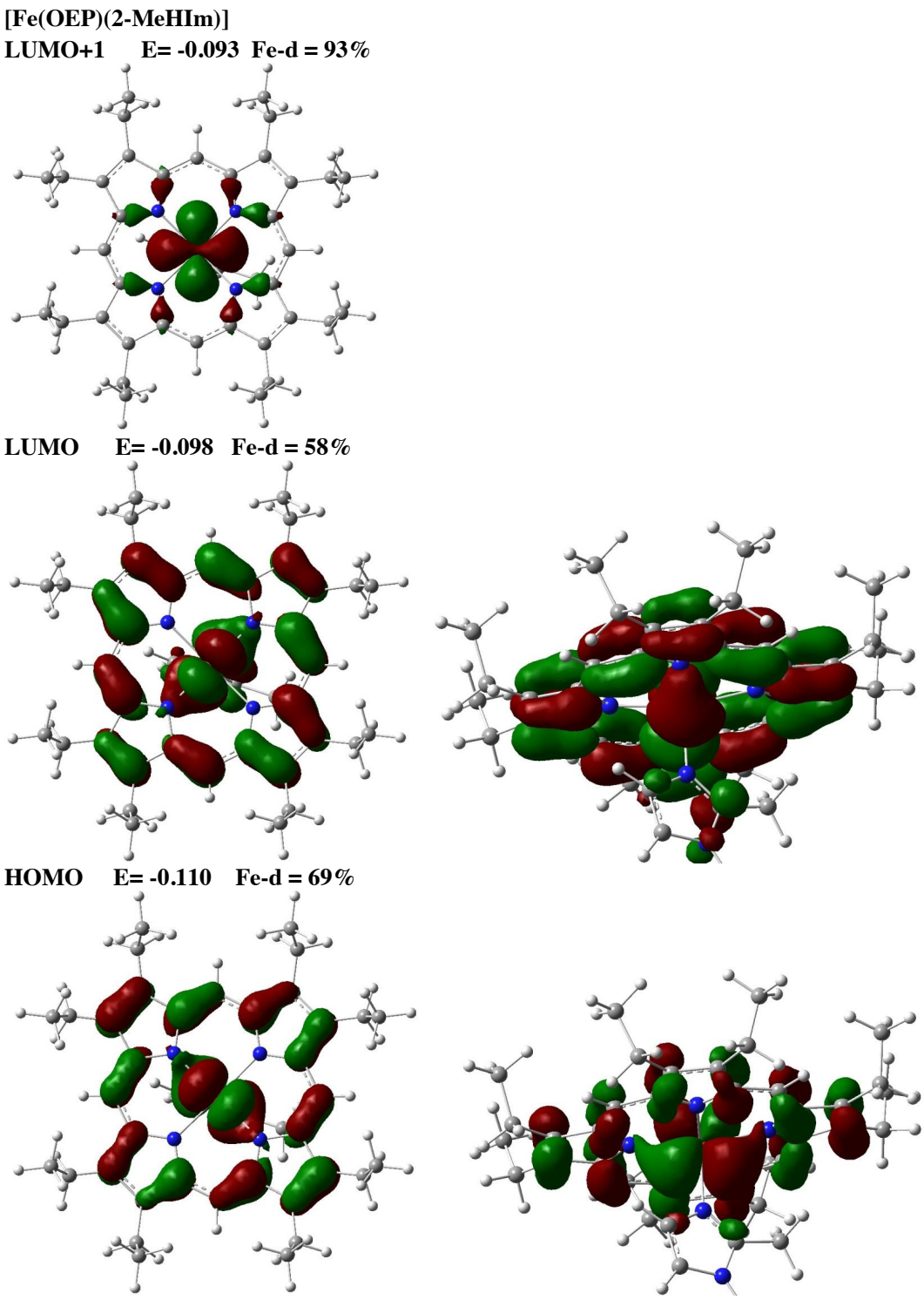

Figure S3. Frontier β-MO's for [Fe(OEP)(2-MeHIm)] calculated with BP86/TZVP.

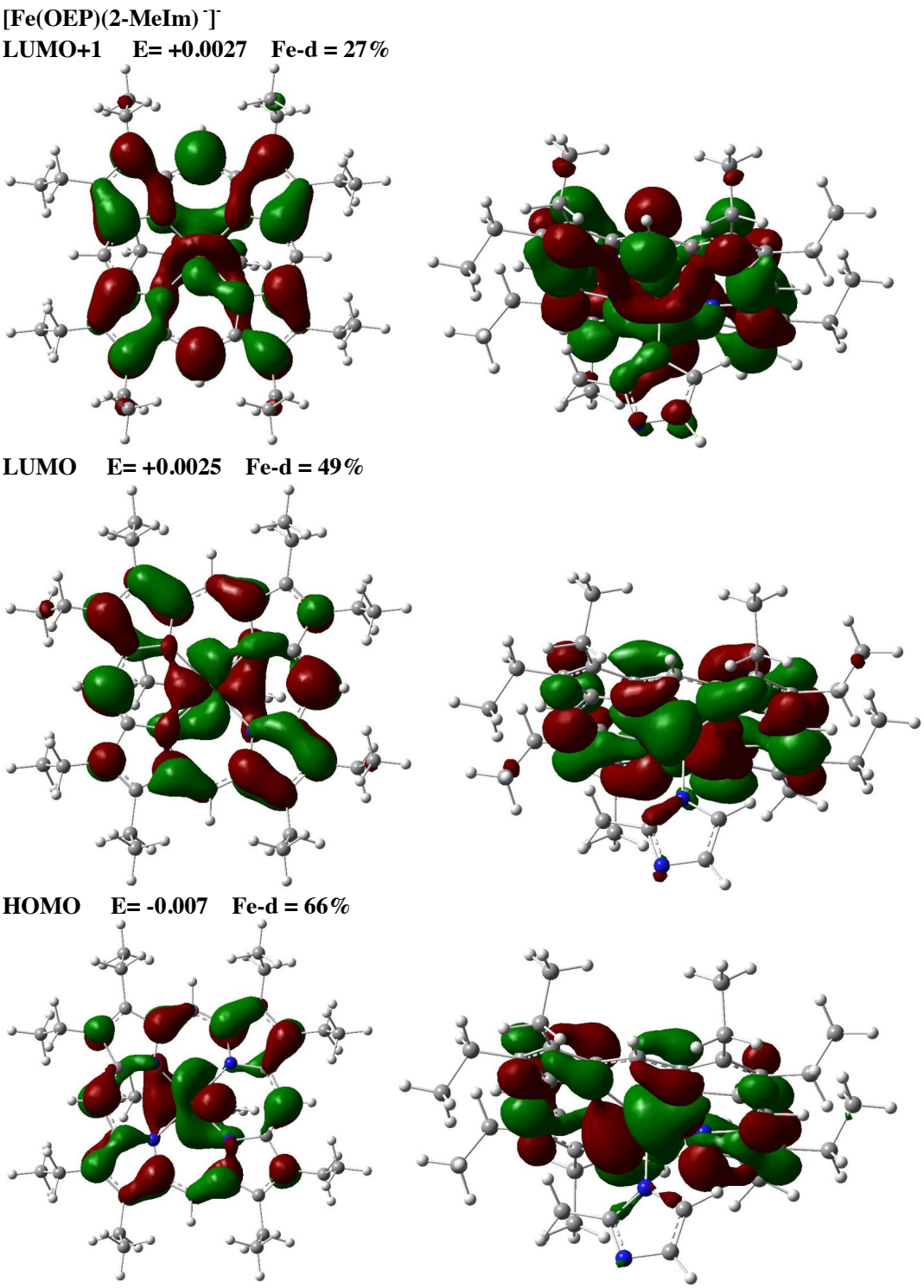

Figure S4. Frontier β-MO's for $[Fe(OEP)(2\text{-}MeIm^{-})]^{-}$ calculated with BP86/TZVP.

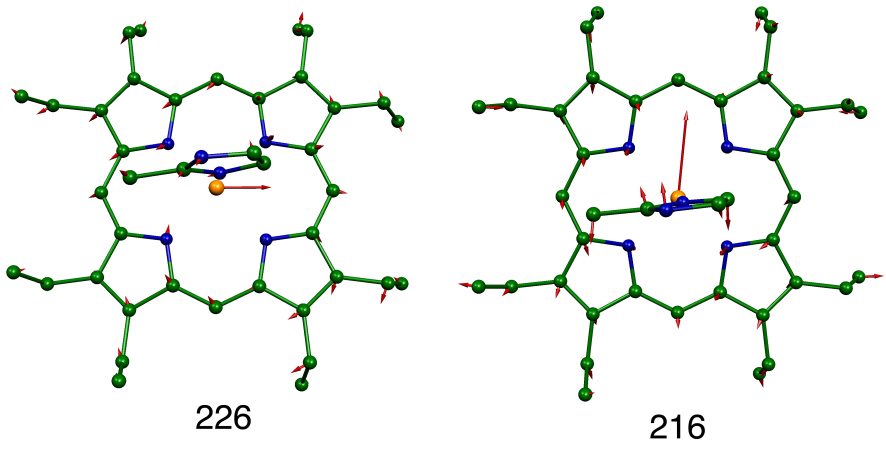

Figure S5. Two DFT-predicted in-plane Fe modes contributing to the experimental feature at 224 cm^{-1} in [K(222)][Fe(OEP)(2-MeIm$^-$)].

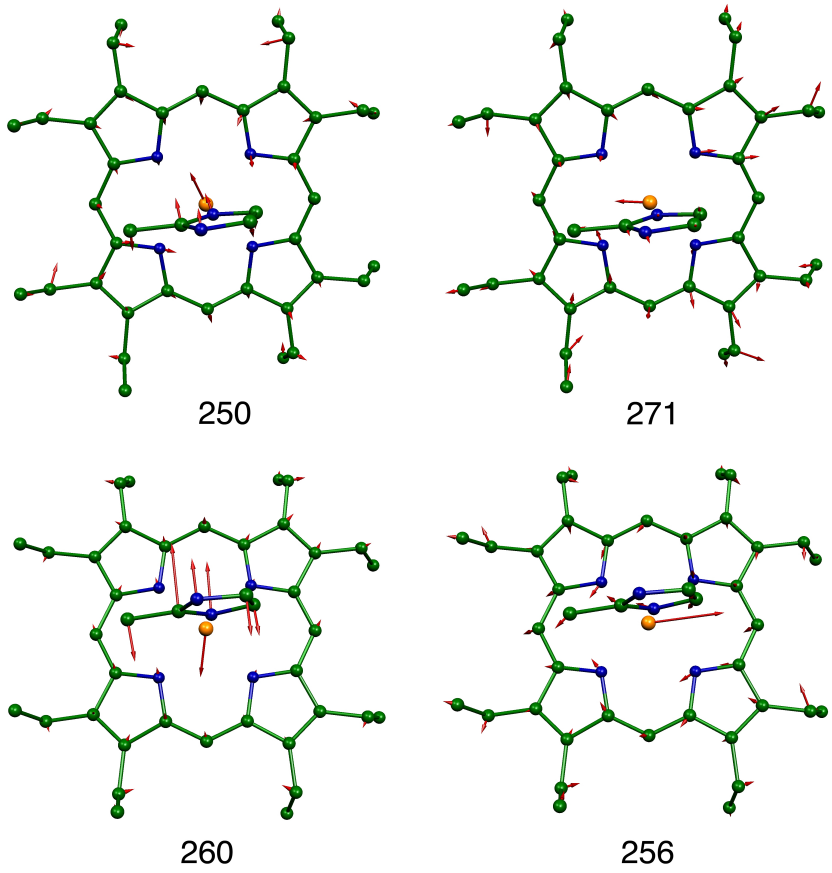

Figure S6. Other modes with significant in-plane Fe motion from the BP86 calculations on [K(222)][Fe(OEP)(2-MeIm$^-$)] with observed experimental features at 244 and 266 cm^{-1}. .

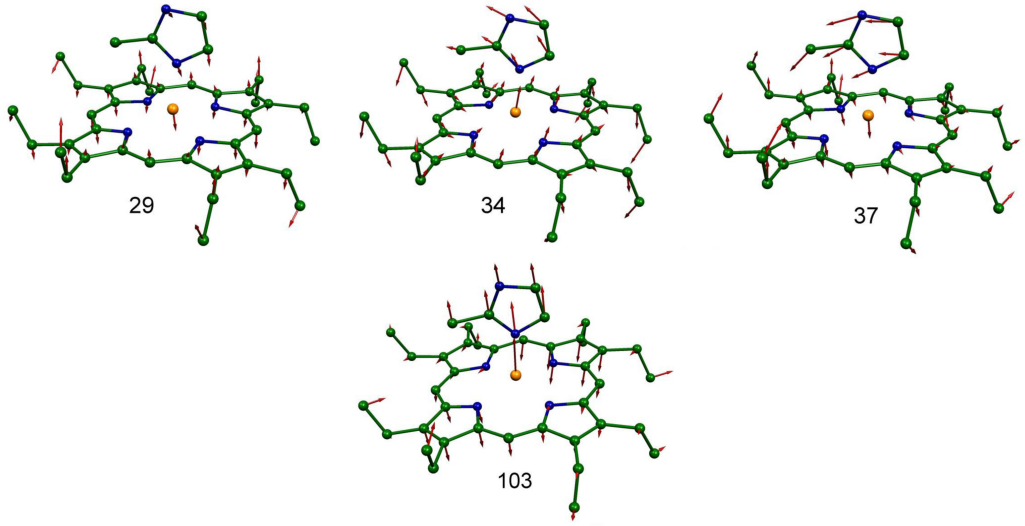

Figure S7. The low-frequency out-of-plane Fe modes, predicted at 103 cm^{-1}, contributing to the experimental feature at 115 and 125 cm^{-1} in [K(222)][Fe(OEP)(2-MeIm$^-$)].

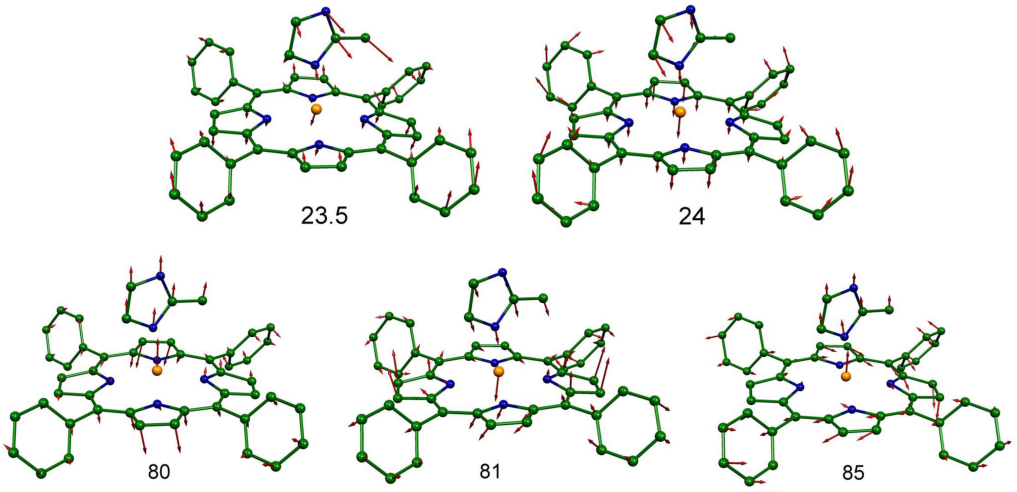

Figure S8. The low-frequency out-of-plane Fe modes, predicted at 80, 81, and 85 cm^{-1}, contributing to the experimental feature at 103 cm^{-1} in [K(222)][Fe(TPP)(2-MeIm$^-$)].

Table S1. Predicted frequencies and e^2_{Fe} values for Two Calculated Imidazolate Derivatives.[a]

K(222) [Fe(OEP)(2MeIm)$^-$]				K(222) [Fe(TPP)(2MeIm)$^-$]			
frequency	e^2_{IP}	e^2_{OP}	e^2_{total}	frequency	e^2_{IP}	e^2_{OP}	e^2_{total}
29.1	0.001	0.026	0.027	21.3	0.002	0.008	0.009
34.4	0.001	0.059	0.059	23.5	0.000	0.019	0.020
36.6	0.001	0.028	0.028	24.2	0.000	0.038	0.038
102.2	0.002	0.017	0.020	50.6	0.012	0.001	0.013
103.1	0.003	0.120	0.123	52.5	0.015	0.000	0.015
115.5	0.014	0.001	0.015	53.7	0.011	0.000	0.011
128.6	0.032	0.020	0.052	79.7	0.000	0.094	0.094
132.5	0.006	0.005	0.010	80.5	0.001	0.050	0.050
154.5	0.030	0.002	0.032	85.0	0.000	0.048	0.048
158.1	0.038	0.002	0.040	114.4	0.017	0.000	0.017
175.4	0.012	0.000	0.012	131.5	0.042	0.009	0.051
185.5	0.056	0.000	0.057	161.1	0.010	0.002	0.012
192.0	0.012	0.000	0.012	163.8	0.003	0.010	0.014
193.7	0.017	0.000	0.017	176.9	0.101	0.006	0.107
197.8	0.011	0.000	0.011	201.2	0.032	0.005	0.038
200.8	0.012	0.000	0.012	206.9	0.107	0.010	0.117
203.6	0.010	0.000	0.010	209.7	0.301	0.025	0.326
207.1	0.036	0.001	0.037	211.9	0.312	0.034	0.346
211.9	0.081	0.000	0.081	214.6	0.073	0.002	0.075
216.0	0.358	0.003	0.361	218.5	0.132	0.001	0.134
219.6	0.041	0.006	0.047	225.3	0.059	0.009	0.068
226.0	0.229	0.008	0.237	229.9	0.033	0.006	0.039
233.0	0.059	0.001	0.060	241.6	0.003	0.032	0.035
242.6	0.007	0.007	0.014	257.7	0.036	0.097	0.133
247.7	0.085	0.324	0.409	259.6	0.017	0.347	0.364
250.0	0.092	0.023	0.115	271.6	0.226	0.029	0.255
255.9	0.262	0.119	0.381	273.7	0.187	0.000	0.187
259.6	0.099	0.019	0.119	381.1	0.002	0.015	0.017
264.2	0.010	0.075	0.084	389.5	0.022	0.000	0.022
270.6	0.059	0.000	0.059	391.6	0.024	0.000	0.024
280.5	0.010	0.001	0.011	427.6	0.011	0.001	0.011
299.0	0.010	0.001	0.011				
325.2	0.011	0.002	0.013				
338.1	0.006	0.005	0.011				

a. All predicted frequencies are expressed in cm^{-1}

Table S2. Cartesian coordinates of the calculated structures and energies

[Fe(OEP)(2MeIm$^-$)]$^-$				[Fe(TPP)(2MeIm$^-$)]$^-$			
Fe	0.015199	-0.015002	0.222481	Fe	0.012942	-0.009073	0.134660
N	-1.705727	-1.013176	-0.519914	N	-0.771678	-1.904087	-0.332700
N	-0.967490	1.785192	-0.404225	N	-1.891498	0.802550	-0.274134
N	1.822469	1.062364	0.027436	N	0.802674	1.909415	-0.415252
N	1.100735	-1.779455	-0.169842	N	1.929150	-0.765265	-0.362955
C	-1.844349	-2.388712	-0.600771	C	1.188393	-0.002446	4.180886
C	-2.946284	-0.480576	-0.804437	H	1.905661	0.041685	5.004590
C	-2.311598	1.948129	-0.671693	N	0.191918	-0.041734	2.171232
C	-0.431536	3.057330	-0.314363	N	-0.173485	-0.117031	4.423795
C	1.985313	2.432636	0.018470	C	-0.728540	-0.135849	3.198194
C	3.087351	0.516755	0.119650	C	1.422595	0.038501	2.817348
C	2.465970	-1.927020	-0.050320	H	2.348925	0.127687	2.249149
C	0.576853	-3.044771	-0.326481	C	-2.210094	-0.254145	2.982687
C	-3.233131	-2.740989	-0.903159	H	-2.698509	-0.372483	3.964281
C	-3.920597	-1.548185	-1.040775	H	-2.470091	-1.125241	2.352292
C	-2.648586	3.365833	-0.747481	H	-2.632029	0.639200	2.484398
C	-1.470323	4.060063	-0.515905	C	-3.191469	-1.323506	-0.479640
C	3.401766	2.777891	0.134229	C	-1.321678	3.223907	-0.325138
C	4.092785	1.580285	0.201596	C	3.238318	1.344141	-0.463832
C	2.829060	-3.338766	-0.126285	C	1.359192	-3.196027	-0.340333
C	1.641861	-4.038986	-0.303211	C	-0.058948	-3.090883	-0.319941
C	-3.225111	0.892492	-0.864036	C	-2.110460	-2.247625	-0.403976
H	-4.259899	1.176128	-1.086653	C	-3.065344	0.085891	-0.466156
C	0.930385	3.348004	-0.100955	C	-2.227740	2.141774	-0.399118
H	1.196991	4.410549	-0.056609	C	0.095288	3.095325	-0.287996
C	3.374652	-0.859183	0.105178	C	2.144012	2.250922	-0.370356
H	4.432270	-1.134048	0.192578	C	3.117116	-0.063690	-0.489347
C	-0.795526	-3.314905	-0.491415	C	2.264042	-2.112323	-0.407346
H	-1.071415	-4.371280	-0.591217	C	-0.972203	-4.211637	-0.364602
C	-3.772816	-4.142669	-1.018623	H	-0.684387	-5.263049	-0.366707
H	-3.064293	-4.773278	-1.592121	C	-2.246366	-3.688939	-0.406623
H	-4.711724	-4.131616	-1.606459	H	-3.188543	-4.236396	-0.428881
C	-4.043699	-4.811342	0.349383	C	-4.167227	1.004711	-0.715282
H	-3.122089	-4.853984	0.955695	H	-5.195119	0.711762	-0.929204
H	-4.425213	-5.842341	0.223029	C	-3.650042	2.272588	-0.674004
H	-4.789228	-4.235022	0.925507	H	-4.172834	3.212151	-0.854579
C	-5.380542	-1.340445	-1.349922	C	1.013822	4.203291	-0.128967
H	-5.787140	-2.239505	-1.853564	H	0.729249	5.243655	0.028093
H	-5.494821	-0.509469	-2.074588	C	2.284816	3.680684	-0.184946
C	-6.237670	-1.034870	-0.098981	H	3.229226	4.216131	-0.087904
H	-6.195885	-1.873254	0.618787	C	4.229867	-0.993133	-0.627888
H	-7.296818	-0.863451	-0.369925	H	5.273105	-0.712654	-0.773702
H	-5.862767	-0.137079	0.422480	C	3.706125	-2.256090	-0.550281
C	-4.024378	3.932030	-0.991898	H	4.243628	-3.203205	-0.597245
H	-4.543920	3.339983	-1.771645	C	-4.571276	-1.889266	-0.622080
H	-3.938783	4.957428	-1.401528	C	-5.557537	-1.649092	0.362886
C	-4.904327	3.970080	0.279598	H	-5.289903	-1.052003	1.241441
H	-5.022327	2.958349	0.705364	C	-6.853314	-2.172346	0.231289
H	-5.910942	4.374599	0.060586	H	-7.598455	-1.977365	1.012057

H	-4.439484	4.601273	1.057851
C	-1.262827	5.553726	-0.533021
H	-0.548978	5.845586	0.262208
H	-2.213516	6.063862	-0.284097
C	-0.748365	6.083715	-1.891831
H	0.208905	5.603591	-2.161134
H	-0.592136	7.178988	-1.864901
H	-1.469184	5.856772	-2.697761
C	3.960033	4.177416	0.133351
H	4.956544	4.180729	0.617008
H	3.320368	4.836188	0.753681
C	4.086538	4.790615	-1.280730
H	4.765718	4.188018	-1.910098
H	4.480724	5.823687	-1.237301
H	3.104426	4.815358	-1.784788
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H	5.796720	0.530412	0.989624
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H	1.155502	-7.063126	-2.019902
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N	-0.095520	-0.131235	2.263623
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N	-0.787428	-0.165132	4.438536
C	0.586043	-0.357883	4.388485
H	1.169514	-0.494678	5.302933
C	1.017379	-0.337803	3.072616
H	2.011795	-0.454881	2.639532
C	-2.574671	0.182440	2.722965
H	-2.968313	-0.663953	2.128596
H	-2.686740	1.088382	2.099038
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E= -3146.39116338 Hartree

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C	-6.224215	-3.197933	-1.875653
H	-6.479568	-3.797334	-2.758060
C	-4.929179	-2.673482	-1.743651
H	-4.177737	-2.859363	-2.519049
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C	-2.806180	4.999026	0.697398
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C	-2.111701	6.840599	-1.298159
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C	-1.562468	5.549488	-1.311141
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H	7.600768	1.945366	1.185201
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C	6.278067	3.342801	-1.645604
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H	2.230312	-7.314558	1.737732
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H	3.622775	-6.810091	-2.334842
C	2.590419	-5.115430	-1.461971
H	2.679974	-4.496159	-2.361585

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