FePc

Fe	0.000000000000	0.000000000000	0.000000000000
N	1.940802028486	0.000000000000	0.000000000000
N	0.000000000000	-1.940802028486	0.000000000000
N	-1.940802028486	0.000000000000	0.000000000000
N	0.000000000000	1.940802028486	0.000000000000
C	2.753852895331	-1.113548118046	0.000000000000
C	1.113548118046	-2.753852895331	0.000000000000
C	-1.113548118046	-2.753852895331	0.000000000000
C	-2.753852895331	-1.113548118046	0.000000000000
C	-2.753852895331	1.113548118046	0.000000000000
C	-1.113548118046	2.753852895331	0.000000000000
C	1.113548118046	2.753852895331	0.000000000000
C	2.753852895331	1.113548118046	0.000000000000
C	4.148951379485	0.702824626182	0.000000000000
C	4.148951379485	-0.702824626182	0.000000000000
C	0.702824626182	-4.148951379485	0.000000000000
C	-0.702824626182	-4.148951379485	0.000000000000
C	-4.148951379485	-0.702824626182	0.000000000000
C	-4.148951379485	0.702824626182	0.000000000000
C	-0.702824626182	4.148951379485	0.000000000000
C	0.702824626182	4.148951379485	0.000000000000
N	2.384008348978	-2.384008348978	0.000000000000
N	-2.384008348978	-2.384008348978	0.000000000000
N	-2.384008348978	2.384008348978	0.000000000000
N	2.384008348978	2.384008348978	0.000000000000
C	5.342631859533	1.426416378679	0.000000000000
C	5.342631859533	-1.426416378679	0.000000000000
C	6.534559570139	0.704544163155	0.000000000000
C	6.534559570139	-0.704544163155	0.000000000000
H	7.482772474599	1.235139408462	0.000000000000
H	7.482772474599	-1.235139408462	0.000000000000
H	5.333751083002	2.511757120625	0.000000000000
H	5.333751083002	-2.511757120625	0.000000000000
C	1.426416378679	-5.342631859533	0.000000000000
C	-1.426416378679	-5.342631859533	0.000000000000

C	0.704544163155	-6.534559570139	0.000000000000
C	-0.704544163155	-6.534559570139	0.000000000000
H	1.235139408462	-7.482772474599	0.000000000000
H	-1.235139408462	-7.482772474599	0.000000000000
H	2.511757120625	-5.333751083002	0.000000000000
H	-2.511757120625	-5.333751083002	0.000000000000
C	-5.342631859533	-1.426416378679	0.000000000000
C	-5.342631859533	1.426416378679	0.000000000000
C	-6.534559570139	-0.704544163155	0.000000000000
C	-6.534559570139	0.704544163155	0.000000000000
H	-7.482772474599	-1.235139408462	0.000000000000
H	-7.482772474599	1.235139408462	0.000000000000
H	-5.333751083002	-2.511757120625	0.000000000000
H	-5.333751083002	2.511757120625	0.000000000000
C	-1.426416378679	5.342631859533	0.000000000000
C	1.426416378679	5.342631859533	0.000000000000
C	-0.704544163155	6.534559570139	0.000000000000
C	0.704544163155	6.534559570139	0.000000000000
H	-1.235139408462	7.482772474599	0.000000000000
H	1.235139408462	7.482772474599	0.000000000000
H	-2.511757120625	5.333751083002	0.000000000000
H	2.511757120625	5.333751083002	0.000000000000

$FePc(Py)_2$ (D_{2h})

Fe	0.000000000000	0.000000000000	0.000000000000
N	1.382830984190	1.379678648006	0.000000000000
N	-1.382830984190	1.379678648006	0.000000000000
N	-1.382830984190	-1.379678648006	0.000000000000
N	1.382830984190	-1.379678648006	0.000000000000
C	1.164877606273	2.736239402340	0.000000000000
C	-1.164877606273	2.736239402340	0.000000000000
C	-2.742170100503	1.168221258041	0.000000000000
C	-2.742170100503	-1.168221258040	0.000000000000
C	-1.164877606273	-2.736239402340	0.000000000000
C	1.164877606273	-2.736239402340	0.000000000000
C	2.742170100503	-1.168221258041	0.000000000000

C	2.742170100503	1.168221258040	0.000000000000
C	3.441093064595	2.449143400011	0.000000000000
C	2.443802414839	3.439957502415	0.000000000000
C	-2.443802414839	3.439957502416	0.000000000000
C	-3.441093064595	2.449143400011	0.000000000000
C	-3.441093064595	-2.449143400011	0.000000000000
C	-2.443802414839	-3.439957502415	0.000000000000
C	2.443802414839	-3.439957502416	0.000000000000
C	3.441093064595	-2.449143400011	0.000000000000
N	0.000000000000	3.368848314680	0.000000000000
N	-3.376801902447	0.000000000000	0.000000000000
N	0.000000000000	-3.368848314680	0.000000000000
N	3.376801902447	0.000000000000	0.000000000000
C	4.794813323159	2.787107901456	0.000000000000
C	2.773734264890	4.795375191156	0.000000000000
C	5.125197177198	4.142176785213	0.000000000000
C	4.126681221559	5.134383191084	0.000000000000
H	6.170365986498	4.440363908802	0.000000000000
H	4.418375856694	6.181354336128	0.000000000000
H	5.558600416333	2.015369571484	0.000000000000
H	1.996656590999	5.553544961538	0.000000000000
C	-2.773734264889	4.795375191156	0.000000000000
C	-4.794813323159	2.787107901457	0.000000000000
C	-4.126681221559	5.134383191084	0.000000000000
C	-5.125197177197	4.142176785213	0.000000000000
H	-4.418375856693	6.181354336129	0.000000000000
H	-6.170365986497	4.440363908802	0.000000000000
H	-1.996656590999	5.553544961538	0.000000000000
H	-5.558600416333	2.015369571484	0.000000000000
C	-4.794813323159	-2.787107901456	0.000000000000
C	-2.773734264890	-4.795375191156	0.000000000000
C	-5.125197177198	-4.142176785213	0.000000000000
C	-4.126681221559	-5.134383191084	0.000000000000
H	-6.170365986498	-4.440363908802	0.000000000000
H	-4.418375856694	-6.181354336128	0.000000000000
H	-5.558600416333	-2.015369571484	0.000000000000

H	-1.996656590999	-5.553544961538	0.000000000000
C	2.773734264889	-4.795375191156	0.000000000000
C	4.794813323159	-2.787107901457	0.000000000000
C	4.126681221559	-5.134383191084	0.000000000000
C	5.125197177197	-4.142176785213	0.000000000000
H	4.418375856693	-6.181354336129	0.000000000000
H	6.170365986497	-4.440363908802	0.000000000000
H	1.996656590999	-5.553544961538	0.000000000000
H	5.558600416333	-2.015369571484	0.000000000000
N	0.000000000000	0.000000000000	2.060526867985
C	1.149977894819	0.000000000000	2.765420805889
C	-1.149977894819	0.000000000000	2.765420805889
C	1.193929191761	0.000000000000	4.155811102055
C	-1.193929191761	0.000000000000	4.155811102055
C	0.000000000000	0.000000000000	4.872807826852
H	2.066366893474	0.000000000000	2.192559268390
H	-2.066366893474	0.000000000000	2.192559268390
H	2.156575640792	0.000000000000	4.656722371340
H	-2.156575640792	0.000000000000	4.656722371340
H	0.000000000000	0.000000000000	5.959018503781
N	0.000000000000	0.000000000000	-2.060526867985
C	-1.149977894819	0.000000000000	-2.765420805889
C	1.149977894819	0.000000000000	-2.765420805889
C	-1.193929191761	0.000000000000	-4.155811102055
C	1.193929191761	0.000000000000	-4.155811102055
C	0.000000000000	0.000000000000	-4.872807826852
H	-2.066366893474	0.000000000000	-2.192559268390
H	2.066366893474	0.000000000000	-2.192559268390
H	-2.156575640792	0.000000000000	-4.656722371340
H	2.156575640792	0.000000000000	-4.656722371340
H	0.000000000000	0.000000000000	-5.959018503781

$FePc(Py)_2$ (D_{2d})

Fe	0.000000000000	0.000000000000	0.000000000000
N	1.380510000000	1.380510000000	0.000000000000
N	-1.380510000000	1.380510000000	0.000000000000

N	-1.380510000000	-1.380510000000	0.000000000000
N	1.380510000000	-1.380510000000	0.000000000000
C	1.166484000000	2.736951000000	0.063072000000
C	-1.166484000000	2.736951000000	0.063072000000
C	-2.736951000000	1.166484000000	-0.063072000000
C	-2.736951000000	-1.166484000000	-0.063072000000
C	-1.166484000000	-2.736951000000	0.063072000000
C	1.166484000000	-2.736951000000	0.063072000000
C	2.736951000000	-1.166484000000	-0.063072000000
C	2.736951000000	1.166484000000	-0.063072000000
C	3.438582000000	2.446223000000	-0.043476000000
C	2.446223000000	3.438582000000	0.043476000000
C	-2.446223000000	3.438582000000	0.043476000000
C	-3.438582000000	2.446223000000	-0.043476000000
C	-3.438582000000	-2.446223000000	-0.043476000000
C	-2.446223000000	-3.438582000000	0.043476000000
C	2.446223000000	-3.438582000000	0.043476000000
C	3.438582000000	-2.446223000000	-0.043476000000
N	0.000000000000	3.369598000000	0.101663000000
N	-3.369598000000	0.000000000000	-0.101663000000
N	0.000000000000	-3.369598000000	0.101663000000
N	3.369598000000	0.000000000000	-0.101663000000
C	4.792135000000	2.781251000000	-0.086960000000
C	2.781251000000	4.792135000000	0.086960000000
C	5.127828000000	4.134403000000	-0.043070000000
C	4.134403000000	5.127828000000	0.043070000000
H	6.173220000000	4.429921000000	-0.076096000000
H	4.429921000000	6.173220000000	0.076096000000
H	5.551752000000	2.008402000000	-0.153984000000
H	2.008402000000	5.551752000000	0.153984000000
C	-2.781251000000	4.792135000000	0.086960000000
C	-4.792135000000	2.781251000000	-0.086960000000
C	-4.134403000000	5.127828000000	0.043070000000
C	-5.127828000000	4.134403000000	-0.043070000000
H	-4.429921000000	6.173220000000	0.076096000000
H	-6.173220000000	4.429921000000	-0.076096000000

H	-2.008402000000	5.551752000000	0.153984000000
H	-5.551752000000	2.008402000000	-0.153984000000
C	-4.792135000000	-2.781251000000	-0.086960000000
C	-2.781251000000	-4.792135000000	0.086960000000
C	-5.127828000000	-4.134403000000	-0.043070000000
C	-4.134403000000	-5.127828000000	0.043070000000
H	-6.173220000000	-4.429921000000	-0.076096000000
H	-4.429921000000	-6.173220000000	0.076096000000
H	-5.551752000000	-2.008402000000	-0.153984000000
H	-2.008402000000	-5.551752000000	0.153984000000
C	2.781251000000	-4.792135000000	0.086960000000
C	4.792135000000	-2.781251000000	-0.086960000000
C	4.134403000000	-5.127828000000	0.043070000000
C	5.127828000000	-4.134403000000	-0.043070000000
H	4.429921000000	-6.173220000000	0.076096000000
H	6.173220000000	-4.429921000000	-0.076096000000
H	2.008402000000	-5.551752000000	0.153984000000
H	5.551752000000	-2.008402000000	-0.153984000000
N	0.000000000000	0.000000000000	2.054841000000
C	1.150709000000	0.000000000000	2.757728000000
C	-1.150709000000	0.000000000000	2.757728000000
C	1.194602000000	0.000000000000	4.148050000000
C	-1.194602000000	0.000000000000	4.148050000000
C	0.000000000000	0.000000000000	4.864376000000
H	2.065627000000	0.000000000000	2.181388000000
H	-2.065627000000	0.000000000000	2.181388000000
H	2.156819000000	0.000000000000	4.649765000000
H	-2.156819000000	0.000000000000	4.649765000000
H	0.000000000000	0.000000000000	5.950578000000
N	0.000000000000	0.000000000000	-2.054841000000
C	0.000000000000	1.150709000000	-2.757728000000
C	0.000000000000	-1.150709000000	-2.757728000000
C	0.000000000000	1.194602000000	-4.148050000000
C	0.000000000000	-1.194602000000	-4.148050000000
C	0.000000000000	0.000000000000	-4.864376000000
H	0.000000000000	2.065627000000	-2.181388000000

H	0.000000000000	-2.065627000000	-2.181388000000
H	0.000000000000	2.156819000000	-4.649765000000
H	0.000000000000	-2.156819000000	-4.649765000000
H	0.000000000000	0.000000000000	-5.950578000000

FePc(Py)

Fe	0.000000000000	0.000000000000	0.192092782201
N	1.372260866393	1.369981756047	0.370543024662
N	1.372260866393	-1.369981756047	0.370543024662
N	-1.372260866393	-1.369981756047	0.370543024662
N	-1.372260866393	1.369981756047	0.370543024662
C	2.734827756072	1.160410545872	0.393851290302
C	2.734827756072	-1.160410545872	0.393851290302
C	1.163053925976	-2.731990503011	0.434463534278
C	-1.163053925976	-2.731990503011	0.434463534278
C	-2.734827756072	-1.160410545872	0.393851290302
C	-2.734827756072	1.160410545872	0.393851290302
C	-1.163053925976	2.731990503011	0.434463534278
C	1.163053925976	2.731990503011	0.434463534278
C	2.440271669576	3.430194229565	0.489618818856
C	3.433206063631	2.437187604681	0.461870364742
C	3.433206063631	-2.437187604681	0.461870364742
C	2.440271669576	-3.430194229565	0.489618818856
C	-2.440271669576	-3.430194229565	0.489618818856
C	-3.433206063631	-2.437187604681	0.461870364742
C	-3.433206063631	2.437187604681	0.461870364742
C	-2.440271669576	3.430194229565	0.489618818856
N	3.370645568341	0.000000000000	0.384130834255
N	0.000000000000	-3.366699725936	0.446829769229
N	-3.370645568341	0.000000000000	0.384130834255
N	0.000000000000	3.366699725936	0.446829769229
C	2.772953145664	4.783777998450	0.562416130847
C	4.788185420861	2.768541689768	0.506679979938
C	4.126250196214	5.116123533445	0.600781963001
C	5.121959668495	4.120407922325	0.573147297679
H	4.421507001531	6.160592118632	0.655076538625

H	6.167624026485	4.414539480844	0.606215444894
H	1.998693878994	5.544318124801	0.588011767786
H	5.548603728184	1.994023645271	0.488937350688
C	4.788185420861	-2.768541689768	0.506679979938
C	2.772953145664	-4.783777998450	0.562416130847
C	5.121959668495	-4.120407922325	0.573147297679
C	4.126250196214	-5.116123533445	0.600781963001
H	6.167624026485	-4.414539480844	0.606215444894
H	4.421507001531	-6.160592118632	0.655076538625
H	5.548603728184	-1.994023645271	0.488937350688
H	1.998693878994	-5.544318124801	0.588011767786
C	-2.772953145664	-4.783777998450	0.562416130847
C	-4.788185420861	-2.768541689768	0.506679979938
C	-4.126250196214	-5.116123533445	0.600781963001
C	-5.121959668495	-4.120407922325	0.573147297679
H	-4.421507001531	-6.160592118632	0.655076538625
H	-6.167624026485	-4.414539480844	0.606215444894
H	-1.998693878994	-5.544318124801	0.588011767786
H	-5.548603728184	-1.994023645271	0.488937350688
C	-4.788185420861	2.768541689768	0.506679979938
C	-2.772953145664	4.783777998450	0.562416130847
C	-5.121959668495	4.120407922325	0.573147297679
C	-4.126250196214	5.116123533445	0.600781963001
H	-6.167624026485	4.414539480844	0.606215444894
H	-4.421507001531	6.160592118632	0.655076538625
H	-5.548603728184	1.994023645271	0.488937350688
H	-1.998693878994	5.544318124801	0.588011767786
N	0.000000000000	0.000000000000	-1.744128082860
C	0.000000000000	1.156085573630	-2.444423148985
C	0.000000000000	-1.156085573630	-2.444423148985
C	0.000000000000	1.195107207262	-3.833363780112
C	0.000000000000	-1.195107207262	-3.833363780112
C	0.000000000000	0.000000000000	-4.549724732753
H	0.000000000000	2.068487435598	-1.864265670399
H	0.000000000000	-2.068487435598	-1.864265670399
H	0.000000000000	2.157061890877	-4.335279178223

H	0.000000000000	-2.157061890877	-4.335279178223
H	0.000000000000	0.000000000000	-5.635609643302

$FePc(CN^-)_2$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	1.949322000000	0.000000000000
N	-1.949322000000	0.000000000000	0.000000000000
N	0.000000000000	-1.949322000000	0.000000000000
N	1.949322000000	0.000000000000	0.000000000000
C	-1.109424000000	2.751146000000	0.000000000000
C	-2.751146000000	1.109424000000	0.000000000000
C	-2.751146000000	-1.109424000000	0.000000000000
C	-1.109424000000	-2.751146000000	0.000000000000
C	1.109424000000	-2.751146000000	0.000000000000
C	2.751146000000	-1.109424000000	0.000000000000
C	2.751146000000	1.109424000000	0.000000000000
C	1.109424000000	2.751146000000	0.000000000000
C	0.703869000000	4.153823000000	0.000000000000
C	-0.703869000000	4.153823000000	0.000000000000
C	-4.153823000000	0.703869000000	0.000000000000
C	-4.153823000000	-0.703869000000	0.000000000000
C	-0.703869000000	-4.153823000000	0.000000000000
C	0.703869000000	-4.153823000000	0.000000000000
C	4.153823000000	-0.703869000000	0.000000000000
C	4.153823000000	0.703869000000	0.000000000000
N	-2.384047000000	2.384047000000	0.000000000000
N	-2.384047000000	-2.384047000000	0.000000000000
N	2.384047000000	-2.384047000000	0.000000000000
N	2.384047000000	2.384047000000	0.000000000000
C	1.421160000000	5.349717000000	0.000000000000
C	-1.421160000000	5.349717000000	0.000000000000
C	0.703801000000	6.548144000000	0.000000000000
C	-0.703801000000	6.548144000000	0.000000000000
H	1.238292000000	7.496897000000	0.000000000000
H	-1.238292000000	7.496897000000	0.000000000000
H	2.507750000000	5.335901000000	0.000000000000

H	-2.507750000000	5.335901000000	0.000000000000
C	-5.349717000000	1.421160000000	0.000000000000
C	-5.349717000000	-1.421160000000	0.000000000000
C	-6.548144000000	0.703801000000	0.000000000000
C	-6.548144000000	-0.703801000000	0.000000000000
H	-7.496897000000	1.238292000000	0.000000000000
H	-7.496897000000	-1.238292000000	0.000000000000
H	-5.335901000000	2.507750000000	0.000000000000
H	-5.335901000000	-2.507750000000	0.000000000000
C	-1.421160000000	-5.349717000000	0.000000000000
C	1.421160000000	-5.349717000000	0.000000000000
C	-0.703801000000	-6.548144000000	0.000000000000
C	0.703801000000	-6.548144000000	0.000000000000
H	-1.238292000000	-7.496897000000	0.000000000000
H	1.238292000000	-7.496897000000	0.000000000000
H	-2.507750000000	-5.335901000000	0.000000000000
H	2.507750000000	-5.335901000000	0.000000000000
C	5.349717000000	-1.421160000000	0.000000000000
C	5.349717000000	1.421160000000	0.000000000000
C	6.548144000000	-0.703801000000	0.000000000000
C	6.548144000000	0.703801000000	0.000000000000
H	7.496897000000	-1.238292000000	0.000000000000
H	7.496897000000	1.238292000000	0.000000000000
H	5.335901000000	-2.507750000000	0.000000000000
H	5.335901000000	2.507750000000	0.000000000000
C	0.000000000000	0.000000000000	1.993148000000
C	0.000000000000	0.000000000000	-1.993148000000
N	0.000000000000	0.000000000000	3.165628000000
N	0.000000000000	0.000000000000	-3.165628000000

FePc(CN^-)

Fe	0.	0.	0.09977
N	0.	1.93124	-0.05854
N	1.93124	0.	-0.05854
N	0.	-1.93124	-0.05854
N	-1.93124	0.	-0.05854

C	1.11012	2.7473	-0.0838
C	2.7473	1.11012	-0.0838
C	2.7473	-1.11012	-0.0838
C	1.11012	-2.7473	-0.0838
C	-1.11012	-2.7473	-0.0838
C	-2.7473	-1.11012	-0.0838
C	-2.7473	1.11012	-0.0838
C	-1.11012	2.7473	-0.0838
C	-0.70222	4.14533	-0.12966
C	0.70222	4.14533	-0.12966
C	4.14533	0.70222	-0.12966
C	4.14533	-0.70222	-0.12966
C	0.70222	-4.14533	-0.12966
C	-0.70222	-4.14533	-0.12966
C	-4.14533	-0.70222	-0.12966
C	-4.14533	0.70222	-0.12966
N	2.38092	2.38092	-0.08862
N	2.38092	-2.38092	-0.08862
N	-2.38092	-2.38092	-0.08862
N	-2.38092	2.38092	-0.08862
C	-1.42334	5.33934	-0.17347
C	1.42334	5.33934	-0.17347
C	-0.70422	6.53352	-0.21406
C	0.70422	6.53352	-0.21406
H	-1.23643	7.48157	-0.24485
H	1.23643	7.48157	-0.24485
H	-2.50928	5.32722	-0.17219
H	2.50928	5.32722	-0.17219
C	5.33934	1.42334	-0.17347
C	5.33934	-1.42334	-0.17347
C	6.53352	0.70422	-0.21406
C	6.53352	-0.70422	-0.21406
H	7.48157	1.23643	-0.24485
H	7.48157	-1.23643	-0.24485
H	5.32722	2.50928	-0.17219
H	5.32722	-2.50928	-0.17219

C	1.42334	-5.33934	-0.17347
C	-1.42334	-5.33934	-0.17347
C	0.70422	-6.53352	-0.21406
C	-0.70422	-6.53352	-0.21406
H	1.23643	-7.48157	-0.24485
H	-1.23643	-7.48157	-0.24485
H	2.50928	-5.32722	-0.17219
H	-2.50928	-5.32722	-0.17219
C	-5.33934	-1.42334	-0.17347
C	-5.33934	1.42334	-0.17347
C	-6.53352	-0.70422	-0.21406
C	-6.53352	0.70422	-0.21406
H	-7.48157	-1.23643	-0.24485
H	-7.48157	1.23643	-0.24485
H	-5.32722	-2.50928	-0.17219
H	-5.32722	2.50928	-0.17219
C	0.00000	0.00000	1.96258
N	0.00000	0.00000	3.13346

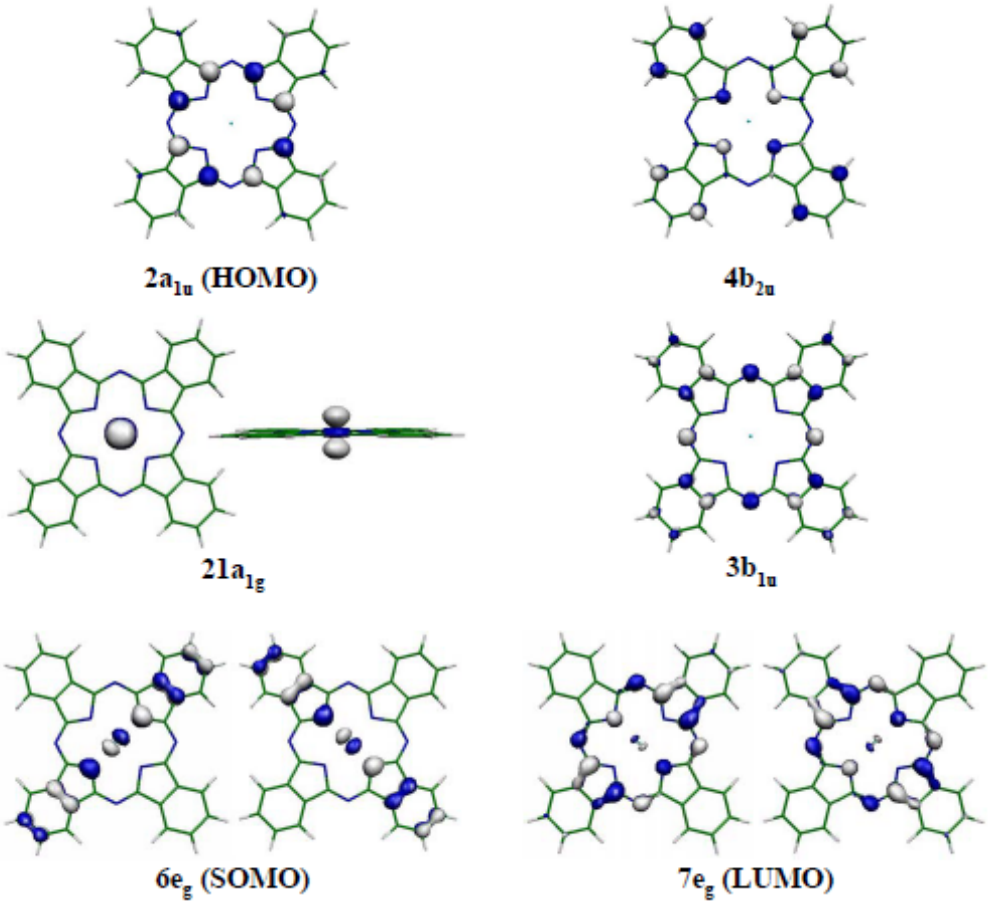

Fig. S-1 Several molecular orbitals near the HOMO and LUMO of FePc. The orbital symmetries are labeled under the D_{4h} symmetry.

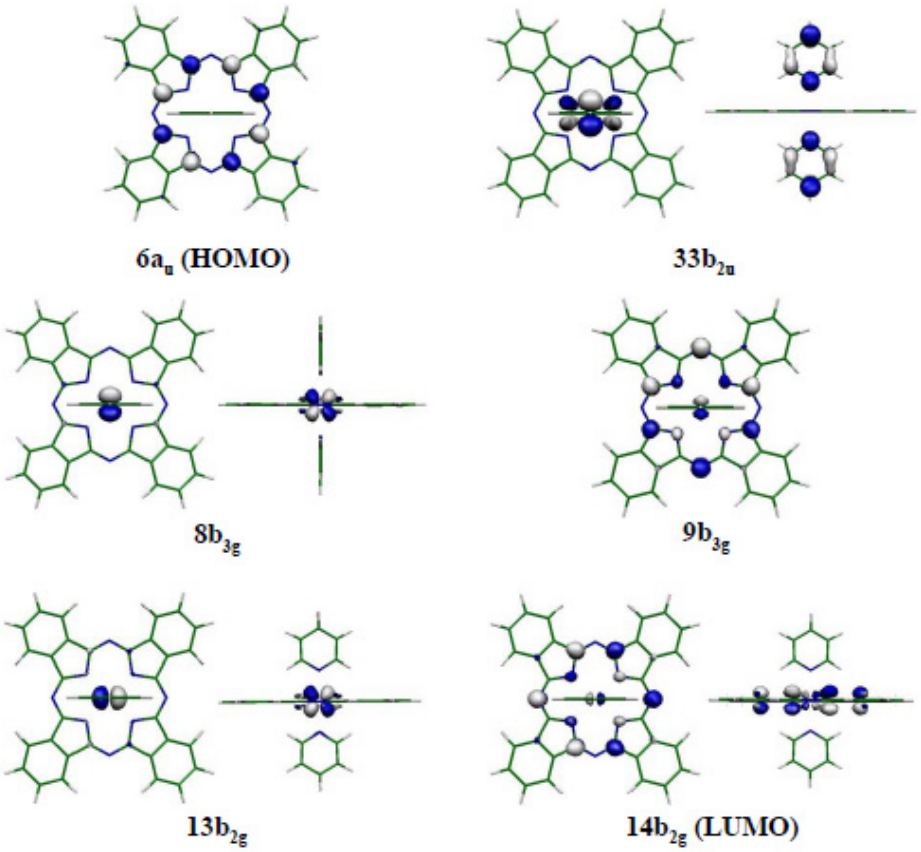

Fig. S-2 Several molecular orbitals near the HOMO and LUMO of $FePc(Py)_2$. The orbital symmetries are labeled under the D_{2h} symmetry.

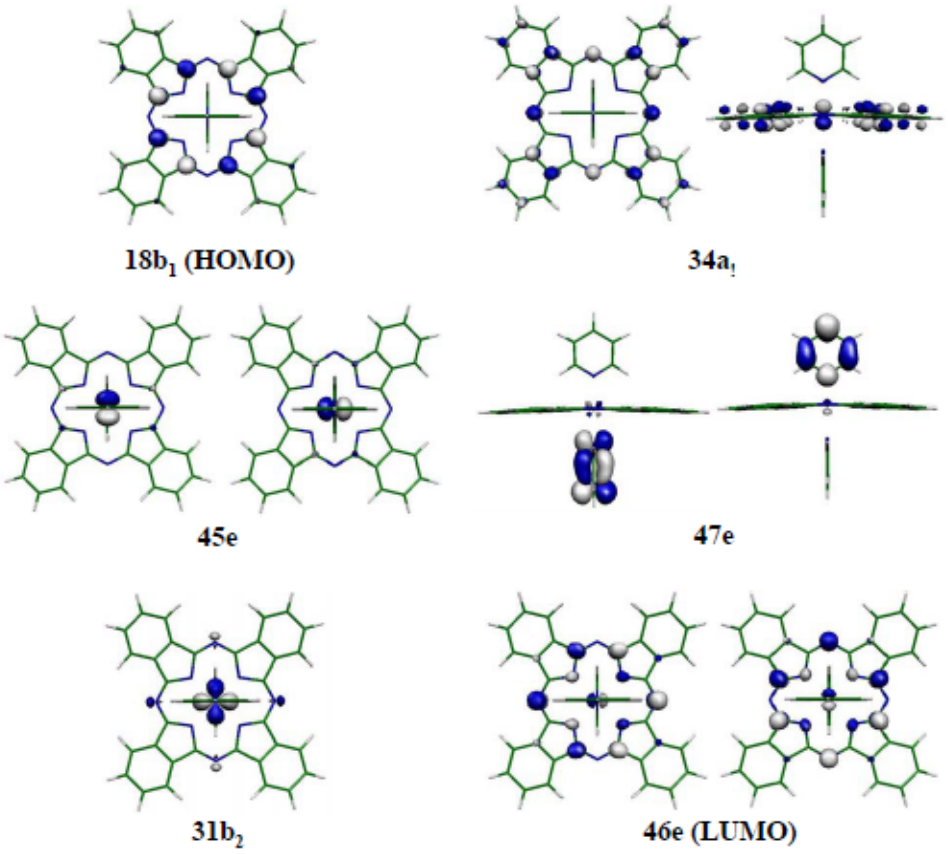

Fig. S-3 Several molecular orbitals near the HOMO and LUMO of $FePc(Py)_2$. The orbital symmetries are labeled under the D_{2d} symmetry.

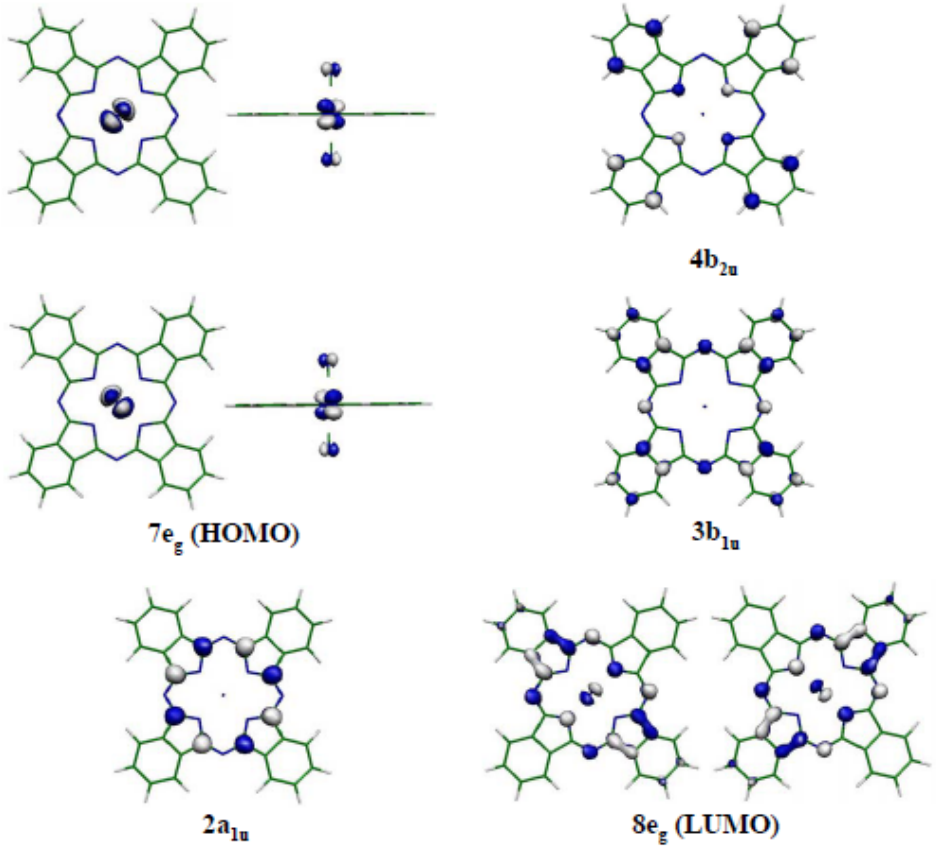

Fig. S-4 Several molecular orbitals near the HOMO and LUMO of $FePc(CN^{-})_2$. The orbital symmetries are labeled under the D_{4h} symmetry.

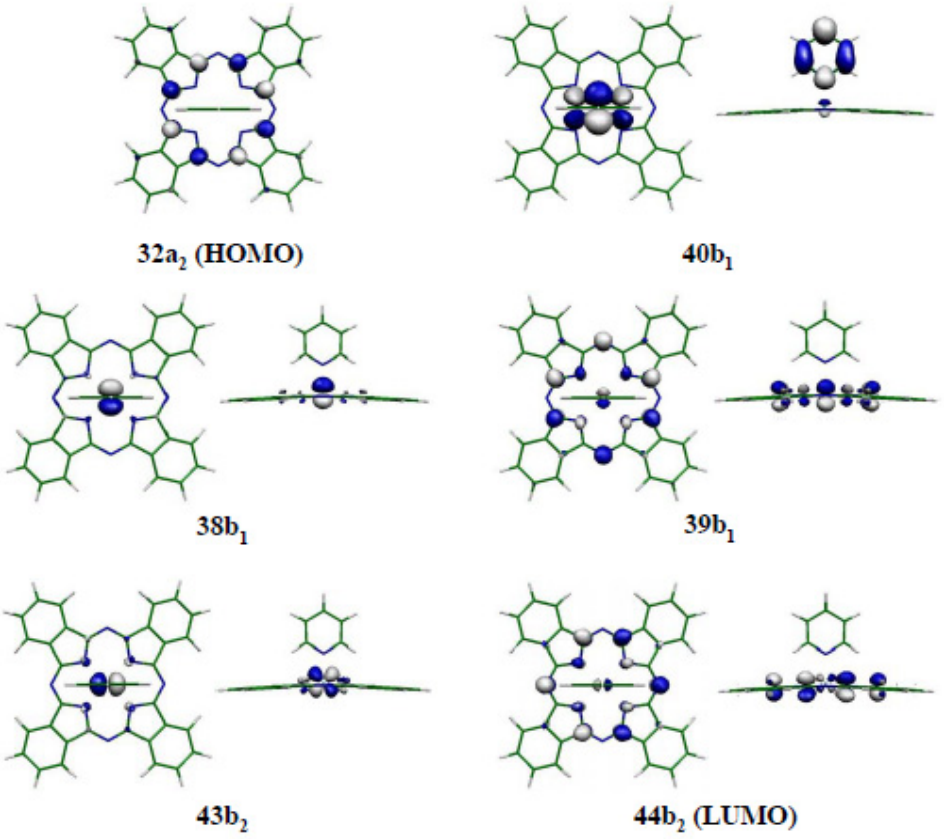

Fig. S-5 Several molecular orbitals near the HOMO and LUMO of FePc(Py). The orbital symmetries are labeled under the C_{2v} symmetry.

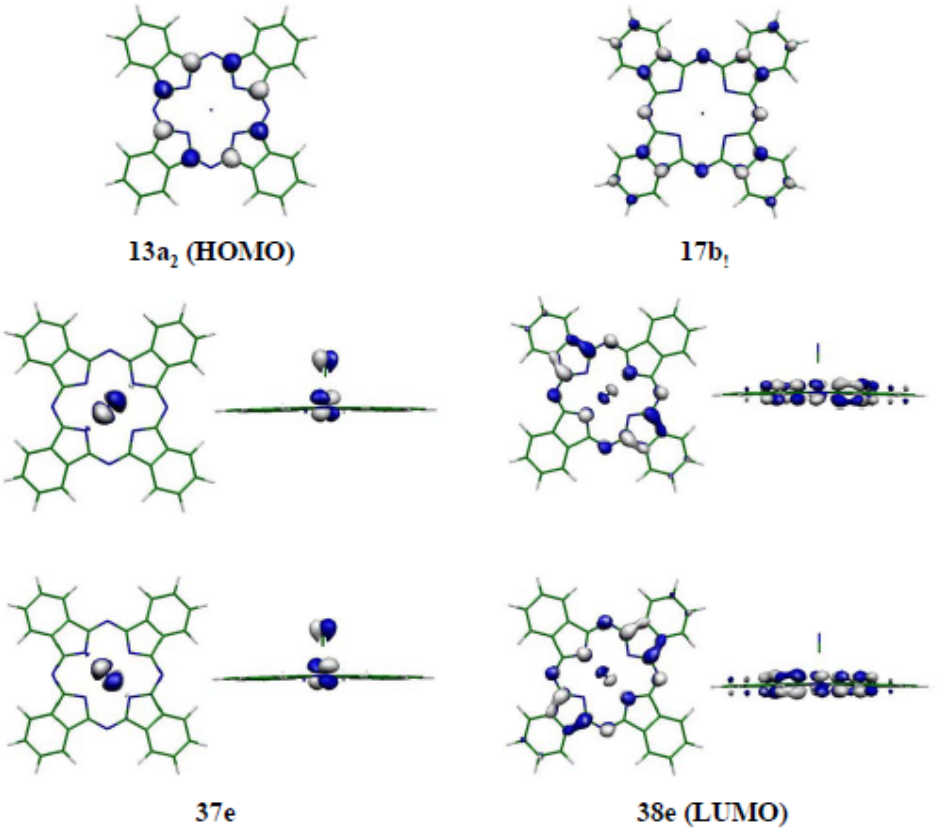

Fig. S-6 Several molecular orbitals near the HOMO and LUMO of FePc(CN^-). The orbital symmetries are labeled under the C_{4v} symmetry.

Table S-1 B3LYP-optimized and X-ray observed bond lengths in Å of FePc, $FePc(Py)_2$, FePc(Py), $FePc(CN^-)_2$, and $FePc(CN^-)$

	FePc D_{4h}	FePc D_{4h}	$FePc(Py)_2$ D_{2h}	$FePc(Py)_2$ D_{2d}	$FePc(Py)_2$ D_{2h}	FePc(Py) C_{2v}	$FePc(CN^-)_2$ D_{4h}	$FePc(CN^-)_2$ D_{4h}	$FePc(CN^-)$ C_{4v}
	Calc.[b]	Expt.[c]	Calc.	Calc.	Expt.[d]	Calc.	Calc.	Expt.[e]	Calc.
a	1.941 (1.939)	1.927	1.953, 1.953	1.952, 1.952	1.935	1.947, 1.947	1.949	1.942	1.938
b	1.379 (1.380)	1.378	1.376, 1.374	1.375, 1.375	1.372	1.379, 1.379	1.369	1.373	1.378
c	1.323 (1.323)	1.322	1.326, 1.329	1.328, 1.328	1.328	1.323, 1.325	1.326	1.323	1.323
d	1.454 (1.455)	1.45	1.459, 1.460	1.460, 1.460	1.454	1.457, 1.457	1.460	1.459	1.457
e	1.396 (1.396)	1.395	1.395	1.395	1.392	1.396	1.395	1.387	1.396
f	1.406 (1.404)	1.392	1.406	1.406	1.400	1.405	1.408	1.390	1.404
g	1.393 (1.394)	1.39	1.395	1.395	1.386	1.394	1.397	1.388	1.395
h	1.409 (1.409)	1.394	1.408	1.408	1.387	1.408	1.408	1.389	1.408
Fe–N[a]	–	–	2.061	2.055	2.040	1.936	–	–	–
Fe–C[a]	–	–	–		–	–	1.993	1.981	1.863

[a] Atomic distance between the central metal and axial ligand.

[b] Atomic distances of FePc with a singlet spin state are in parentheses (ref 22).

[c] Ref 11.

[d] The value are experimental distances for $FePc(4Me\text{-}Py)_2$ (ref 16).

[e] Ref 17.

Table S-2 Orbital energies in eV and characters of FePc, $FePc(Py)_2$, FePc(Py), $FePc(CN^-)_2$, and $FePc(CN^-)$

FePc				$FePc(Py)_2$				FePc(Py)		$FePc(CN^-)_2$		$FePc(CN^-)$	
α		β		D_{2h}		D_{2d}		C_{2v}		D_{4h}		C_{4v}	
$7a_{2u}$	−0.653	$7a_{2u}$	−0.019	$20b_{1u}$	−0.704	$19b_1$	−0.619	$33a_2$	−0.512	$9e_g$	4.493	39e	2.018
$4b_{2u}$	−0.908	$7e_g$	−0.851	$10b_{3g}$	−1.099	$16a_2$	−0.664	$54a_1$	−0.803	$12a_{2u}$	4.480	$19b_2$	1.695
$3b_{1u}$	−1.067	$4b_{2u}$	−0.902	$33b_{2u}$	−1.269	$34a_1$	−0.699	$40b_1$	−0.951	$4b_{2u}$	4.252	$32a_1$	1.607
$7e_g$	−2.702	$3b_{1u}$	−1.059	$9b_{3g}$	−2.200	47e	−1.195	$39b_1$	−2.537	$3b_{1u}$	4.135	$17b_1$	1.604
–	–	$6e_g$	−2.939	$14b_{2g}$	−2.218	46e	−2.201	$44b_2$	−2.537	$8e_g$	2.997	38e	0.237
$2a_{1u}$	−4.986	$2a_{1u}$	−4.901	$6a_u$	−4.591	$18b_1$	−4.583	$32a_2$	−4.726	$7e_g$	0.632	$13a_2$	−2.195
$21a_{1g}$	−6.392	$21a_{1g}$	−5.455	$8b_{3g}$	−5.059	45e	−5.094	$38b_1$	−5.336	$2a_{1u}$	0.487	37e	−2.303
$6e_g$	−6.397	–	–	$13b_{2g}$	−5.159	$31b_2$	−5.396	$43b_2$	−5.437	$14b_{2g}$	0.047	$16b_1$	−2.801
$14b_{2g}$	−6.680	$14b_{2g}$	−5.778	$45a_g$	−5.424	$30b_2$	−6.254	$53a_1$	−5.692	$11a_{1u}$	−0.156	36e	−4.002
$3b_{2u}$	−6.774	$3b_{2u}$	−6.776	$19b_{1u}$	−6.254	$15a_2$	−6.403	$31a_2$	−6.559	$6e_g$	−1.071	$31a_1$	−4.008
$6a_{2u}$	−6.803	$6a_{2u}$	−6.806	$5a_u$	−6.406	$29b_2$	−6.523	$52a_1$	−6.598	$31e_u$	−1.237	$18b_2$	−4.141

Table S-3 Symmetry-allowed TD-B3LYP excited states of FePc with the same spin multiplicity as the ground state

	state	main configuration ($\|C\| \geq 0.30$)	E^a	f^b	p^c
FePc	$1E_u$	$-0.72(2a_{1u}\rightarrow 7e_g)(\alpha)+0.91(2a_{1u}\rightarrow 6e_g)(\beta)$	1.05	0.006	$x+y$
		$-0.72(2a_{1u}\rightarrow 7e_g)(\alpha)+0.91(2a_{1u}\rightarrow 6e_g)(\beta)$			
	$2E_u$	$-0.32(2a_{1u}\rightarrow 7e_g)(\alpha)+0.65(2a_{1u}\rightarrow 7e_g)(\alpha)+0.42(2a_{1u}\rightarrow 6e_g)(\beta)$	2.01	0.342	$x+y$
		$+0.32(2a_{1u}\rightarrow 7e_g)(\alpha)+0.65(2a_{1u}\rightarrow 7e_g)(\alpha)+0.42(2a_{1u}\rightarrow 6e_g)(\beta)$			
	$3E_u$	$-0.47(6a_{2u}\rightarrow 7e_g)(\alpha)-0.34(3b_{2u}\rightarrow 7e_g)(\alpha)+0.59(6a_{2u}\rightarrow 6e_g)(\beta)+0.50(3b_{2u}\rightarrow 6e_g)(\beta)$	2.87	0.002	$x+y$
		$-0.47(6a_{2u}\rightarrow 7e_g)(\alpha)+0.34(3b_{2u}\rightarrow 7e_g)(\alpha)+0.59(6a_{2u}\rightarrow 6e_g)(\beta)-0.50(3b_{2u}\rightarrow 6e_g)(\beta)$			
	$4E_u$	$-0.30(5a_{2u}\rightarrow 7e_g)(\alpha)+0.31(6a_{2u}\rightarrow 7e_g)(\alpha)-0.44(5a_{2u}\rightarrow 6e_g)(\beta)-0.36(6a_{2u}\rightarrow 6e_g)(\beta)+0.53(3b_{2u}\rightarrow 6e_g)(\beta)$	3.08	0.007	$x+y$
		$+0.30(5a_{2u}\rightarrow 7e_g)(\alpha)-0.31(6a_{2u}\rightarrow 7e_g)(\alpha)-0.44(5a_{2u}\rightarrow 6e_g)(\beta)+0.36(6a_{2u}\rightarrow 6e_g)(\beta)+0.53(3b_{2u}\rightarrow 6e_g)(\beta)$			
	$5E_u$	$-0.31(2a_{1u}\rightarrow 8e_g)(\alpha)+0.39(3b_{2u}\rightarrow 6e_g)(\beta)+0.62(2a_{1u}\rightarrow 7e_g)(\beta)$	3.26	0.031	$x+y$
		$-0.31(2a_{1u}\rightarrow 8e_g)(\alpha)+0.39(3b_{2u}\rightarrow 6e_g)(\beta)+0.62(2a_{1u}\rightarrow 7e_g)(\beta)$			
	$6E_u$	$-0.37(5a_{2u}\rightarrow 7e_g)(\alpha)+0.52(5a_{2u}\rightarrow 6e_g)(\beta)+0.32(6a_{2u}\rightarrow 6e_g)(\beta)-0.33(3b_{2u}\rightarrow 6e_g)(\beta)+0.30(2a_{1u}\rightarrow 7e_g)(\beta)$	3.34	0.018	$x+y$
		$-0.37(5a_{2u}\rightarrow 7e_g)(\alpha)+0.52(5a_{2u}\rightarrow 6e_g)(\beta)+0.32(6a_{2u}\rightarrow 6e_g)(\beta)+0.33(3b_{2u}\rightarrow 6e_g)(\beta)-0.30(2a_{1u}\rightarrow 7e_g)(\beta)$			
	$7E_u$	$+0.67(3b_{2u}\rightarrow 7e_g)(\alpha)+0.46(3b_{2u}\rightarrow 7e_g)(\alpha)$	3.40	0.002	$x+y$
		$+0.67(3b_{2u}\rightarrow 7e_g)(\alpha)-0.46(3b_{2u}\rightarrow 7e_g)(\alpha)$			
	$8E_u$	$+0.79(2b_{1u}\rightarrow 6e_g)(\beta)-0.42(2a_{1u}\rightarrow 7e_g)(\beta)$	3.43	0.009	$x+y$
		$+0.79(2b_{1u}\rightarrow 6e_g)(\beta)+0.42(2a_{1u}\rightarrow 7e_g)(\beta)$			
	$1A_{1u}$	$-0.36(30e_u\rightarrow 7e_g)(\alpha)-0.36(30e_u\rightarrow 7e_g)(\alpha)+0.55(30e_u\rightarrow 6e_g)(\beta)+0.55(30e_u\rightarrow 6e_g)(\beta)+0.31(14b_{2g}\rightarrow 3b_{1u})(\beta)$	3.60	0.0001	z
	$9E_u$	$+0.42(5a_{2u}\rightarrow 7e_g)(\alpha)+0.62(6a_{2u}\rightarrow 7e_g)(\alpha)+0.38(6a_{2u}\rightarrow 6e_g)(\beta)$	3.68	0.272	$x+y$
		$+0.42(5a_{2u}\rightarrow 7e_g)(\alpha)+0.62(6a_{2u}\rightarrow 7e_g)(\alpha)+0.38(6a_{2u}\rightarrow 6e_g)(\beta)$			
	$10E_u$	$-0.40(2b_{1u}\rightarrow 7e_g)(\alpha)+0.53(2a_{1u}\rightarrow 8e_g)(\alpha)-0.35(1a_{1u}\rightarrow 6e_g)(\beta)$	3.69	0.026	$x+y$
		$+0.40(2b_{1u}\rightarrow 7e_g)(\alpha)+0.53(2a_{1u}\rightarrow 8e_g)(\alpha)-0.35(1a_{1u}\rightarrow 6e_g)(\beta)$			
	$11E_u$	$+0.43(5a_{2u}\rightarrow 7e_g)(\alpha)+0.43(2b_{1u}\rightarrow 7e_g)(\alpha)-0.30(1a_{1u}\rightarrow 6e_g)(\beta)$	3.78	0.470	$x+y$
		$+0.43(5a_{2u}\rightarrow 7e_g)(\alpha)+0.43(2b_{1u}\rightarrow 7e_g)(\alpha)+0.30(1a_{1u}\rightarrow 6e_g)(\beta)$			
	$12E_u$	$-0.45(5a_{2u}\rightarrow 7e_g)(\alpha)+0.52(2b_{1u}\rightarrow 7e_g)(\alpha)-0.34(5a_{2u}\rightarrow 6e_g)(\beta)+0.35(2b_{1u}\rightarrow 6e_g)(\beta)$	3.79	0.028	$x+y$
		$-0.45(5a_{2u}\rightarrow 7e_g)(\alpha)+0.52(2b_{1u}\rightarrow 7e_g)(\alpha)-0.34(5a_{2u}\rightarrow 6e_g)(\beta)+0.35(2b_{1u}\rightarrow 6e_g)(\beta)$			
	$13E_u$	$-0.38(1a_{1u}\rightarrow 7e_g)(\alpha)+0.49(2a_{1u}\rightarrow 8e_g)(\alpha)+0.58(1a_{1u}\rightarrow 6e_g)(\beta)$	3.93	0.051	$x+y$
		$-0.38(1a_{1u}\rightarrow 7e_g)(\alpha)+0.49(2a_{1u}\rightarrow 8e_g)(\alpha)+0.58(1a_{1u}\rightarrow 6e_g)(\beta)$			
	$2A_{1u}$	$+0.56(30e_u\rightarrow 7e_g)(\alpha)+0.56(30e_u\rightarrow 7e_g)(\alpha)+0.31(30e_u\rightarrow 6e_g)(\beta)+0.31(30e_u\rightarrow 6e_g)(\beta)+0.30(14b_{2g}\rightarrow 3b_{1u})(\beta)$	3.96	0.003	z
	$3A_{1u}$	$-0.30(30e_u\rightarrow 6e_g)(\beta)-0.30(30e_u\rightarrow 6e_g)(\beta)+0.90(14b_{2g}\rightarrow 3b_{1u})(\beta)$	4.06	0.0001	z
	$14E_u$	$-0.35(2a_{1u}\rightarrow 8e_g)(\alpha)+0.79(2a_{1u}\rightarrow 8e_g)(\beta)$	4.15	0.003	$x+y$
		$-0.35(2a_{1u}\rightarrow 8e_g)(\alpha)+0.79(2a_{1u}\rightarrow 8e_g)(\beta)$			
	$4A_{1u}$	$+0.99(21a_{1g}\rightarrow 7a_{2u})(\beta)$	4.19	0.004	z
	$15E_u$	$+0.69(1a_{1u}\rightarrow 7e_g)(\alpha)+0.39(1a_{1u}\rightarrow 7e_g)(\alpha)+0.37(1a_{1u}\rightarrow 6e_g)(\beta)$	4.30	0.046	$x+y$
		$+0.69(1a_{1u}\rightarrow 7e_g)(\alpha)-0.39(1a_{1u}\rightarrow 7e_g)(\alpha)+0.37(1a_{1u}\rightarrow 6e_g)(\beta)$			

[a] E: excitation energy in eV.

[b] f: oscillator strength.

[c] p: polarization of the electrical dipole. The x and y axes directed toward two of four inner nitrogen atoms of the Pc ring.

Table S-4 Symmetry-allowed TD-B3LYP excited states of $FePc(Py)_2$ (D_{2h}) with the same spin multiplicity as the ground state

	state	main configuration ($\|C\| \geq 0.30$)	E^a	f^b	p^c
$FePc(Py)_2$ D_{2h}	$1B_{3u}$	$+0.62(6a_u \rightarrow 9b_{3g})$	2.17	0.319	x
	$1B_{2u}$	$+0.62(6a_u \rightarrow 14b_{2g})$	2.19	0.372	y
	$2B_{3u}$	$+0.70(6a_u \rightarrow 10b_{3g})$	2.92	0.006	x
	$1B_{1u}$	$+0.69(8b_{3g} \rightarrow 33b_{2u})$	3.11	0.131	z
	$2B_{1u}$	$+0.71(6a_u \rightarrow 28b_{1g})$	3.42	0.004	z
	$3B_{3u}$	$-0.40(5a_u \rightarrow 9b_{3g})+0.46(19b_{1u} \rightarrow 14b_{2g})$	3.49	0.053	x
	$2B_{2u}$	$+0.44(5a_u \rightarrow 14b_{2g})-0.41(19b_{1u} \rightarrow 9b_{3g})$	3.49	0.039	y
	$4B_{3u}$	$+0.40(5a_u \rightarrow 14b_{2g})+0.47(8b_{3g} \rightarrow 7a_u)$	3.66	0.009	x
	$3B_{2u}$	$+0.50(5a_u \rightarrow 14b_{2g})+0.34(19b_{1u} \rightarrow 9b_{3g})$	3.69	0.021	y
	$5B_{3u}$	$+0.31(18b_{1u} \rightarrow 14b_{2g})+0.38(5a_u \rightarrow 9b_{3g})+0.43(8b_{3g} \rightarrow 7a_u)$	3.74	0.008	x
	$4B_{2u}$	$+0.61(8b_{3g} \rightarrow 20b_{1u})$	3.74	0.029	y
	$5B_{2u}$	$+0.49(18b_{1u} \rightarrow 9b_{3g})-0.43(13b_{2g} \rightarrow 7a_u)$	3.80	0.001	y
	$6B_{3u}$	$+0.41(18b_{1u} \rightarrow 14b_{2g})+0.56(13b_{2g} \rightarrow 20b_{1u})$	3.83	0.013	x
	$7B_{3u}$	$-0.32(18b_{1u} \rightarrow 14b_{2g})+0.31(13b_{2g} \rightarrow 20b_{1u})+0.43(8b_{3g} \rightarrow 8a_u)$	3.85	0.187	x
	$6B_{2u}$	$+0.62(6a_u \rightarrow 15b_{2g})$	3.90	0.0002	y
	$8B_{3u}$	$+0.35(17b_{1u} \rightarrow 14b_{2g})+0.58(6a_u \rightarrow 11b_{3g})$	3.91	0.015	x
	$7B_{2u}$	$+0.35(18b_{1u} \rightarrow 9b_{3g})+0.32(13b_{2g} \rightarrow 7a_u)+0.37(13b_{2g} \rightarrow 8a_u)$	3.92	0.335	y
	$3B_{1u}$	$+0.33(32b_{2u} \rightarrow 9b_{3g})+0.58(45a_g \rightarrow 20b_{1u})$	3.96	0.002	z
	$8B_{2u}$	$+0.58(17b_{1u} \rightarrow 9b_{3g})$	3.98	0.004	y

[a] E: excitation energy in eV.

[b] f: oscillator strength.

[c] p: polarization of the electrical dipole. The x and y axes directed toward two of four inner nitrogen atoms of the Pc ring.

Table S-5 Symmetry-allowed TD-B3LYP excited states of $FePc(Py)_2$ (D_{2d}) with the same spin multiplicity as the ground state

	state	main configuration ($\|C\| \geq 0.30$)	E^a	f^b	p^c
$FePc(Py)_2$	$1B_2$	$+0.49(45e\rightarrow46e)+0.49(45e\rightarrow46e)$	1.94	0.001	z
D_{2d}	1E	$+0.64(31b_2\rightarrow46e)$	2.10	0.008	$x+y$
		$+0.64(31b_2\rightarrow46e)$			
	2E	$+0.59(18b_1\rightarrow46e)$	2.18	0.320	$x+y$
		$+0.59(18b_1\rightarrow46e)$			
	3E	$+0.54(45e\rightarrow35a_1)$	2.20	0.017	$x+y$
		$+0.54(45e\rightarrow35a_1)$			
	4E	$+0.68(18b_1\rightarrow47e)$	2.82	0.003	$x+y$
		$+0.68(18b_1\rightarrow47e)$			
	$2B_2$	$+0.48(31b_2\rightarrow35a_1)$	2.94	0.032	z
	$3B_2$	$+0.42(45e\rightarrow47e)+0.42(45e\rightarrow47e)$	3.27	0.097	z
	5E	$+0.67(31b_2\rightarrow47e)$	3.28	0.0001	$x+y$
		$+0.67(31b_2\rightarrow47e)$			
	$4B_2$	$+0.69(18b_1\rightarrow16a_2)$	3.40	0.002	z
	6E	$-0.42(15a_2\rightarrow46e)+0.43(30b_2\rightarrow46e)$	3.49	0.045	$x+y$
		$-0.42(15a_2\rightarrow46e)+0.43(30b_2\rightarrow46e)$			
	$5B_2$	$+0.68(18b_1\rightarrow17a_2)$	3.63	0.0003	z
	7E	$-0.32(15a_2\rightarrow46e)+0.35(45e\rightarrow16a_2)$	3.67	0.014	$x+y$
		$+0.32(15a_2\rightarrow46e)+0.35(45e\rightarrow16a_2)$			
	8E	$+0.36(15a_2\rightarrow46e)+0.31(45e\rightarrow34a_1)+0.42(45e\rightarrow16a_2)$	3.74	0.001	$x+y$
		$-0.36(15a_2\rightarrow46e)-0.31(45e\rightarrow34a_1)+0.42(45e\rightarrow16a_2)$			
	9E	$-0.38(29b_2\rightarrow46e)+0.56(45e\rightarrow34a_1)$	3.79	0.011	$x+y$
		$-0.38(29b_2\rightarrow46e)+0.56(45e\rightarrow34a_1)$			
	10E	$+0.35(28b_2\rightarrow46e)+0.49(45e\rightarrow19b_1)$	3.81	0.005	$x+y$
		$+0.35(28b_2\rightarrow46e)+0.49(45e\rightarrow19b_1)$			
	$6B_2$	$+0.45(43e\rightarrow46e)+0.45(43e\rightarrow46e)$	3.85	0.0001	z
	11E	$+0.37(29b_2\rightarrow46e)-0.33(45e\rightarrow17a_2)$	3.86	0.191	$x+y$
		$+0.37(29b_2\rightarrow46e)+0.33(45e\rightarrow17a_2)$			
	12E	$+0.45(28b_2\rightarrow46e)+0.38(18b_1\rightarrow48e)$	3.90	0.013	$x+y$
		$+0.45(28b_2\rightarrow46e)+0.38(18b_1\rightarrow48e)$			
	13E	$-0.31(33a_1\rightarrow46e)+0.46(18b_1\rightarrow48e)$	3.90	0.042	$x+y$
		$+0.31(33a_1\rightarrow46e)+0.46(18b_1\rightarrow48e)$			
	$7B_2$	$+0.59(31b_2\rightarrow34a_1)$	3.95	0.002	z

[a] E: excitation energy in eV.

[b] f: oscillator strength.

[c] p: polarization of the electrical dipole. The x and y axes directed toward two of four inner nitrogen atoms of the Pc ring.

Table S-6 Symmetry-allowed TD-B3LYP excited states of FePc(Py) with the same spin multiplicity as the ground state

	state	main configuration ($\|C\| \geq 0.30$)	E^a	f^b	p^c
FePc(Py)	$1B_1$	$+0.61(38b_1 \rightarrow 54a_1)$	1.21	0.0003	*x*
	$1B_2$	$+0.60(43b_2 \rightarrow 54a_1)$	1.21	0.0004	*y*
	$1A_1$	$+0.50(53a_1 \rightarrow 54a_1)$	1.71	0.0004	*z*
	$2B_2$	$+0.62(32a_2 \rightarrow 39b_1)$	2.16	0.364	*y*
	$2B_1$	$+0.61(32a_2 \rightarrow 44b_2)$	2.16	0.387	*x*
	$3B_1$	$+0.68(53a_1 \rightarrow 39b_1)$	2.24	0.002	*x*
	$2A_1$	$+0.40(43b_2 \rightarrow 44b_2)+0.48(38b_1 \rightarrow 39b_1)$	2.25	0.0008	*z*
	$3B_2$	$+0.71(32a_2 \rightarrow 40b_1)$	2.64	0.0007	*y*
	$3A_1$	$+0.47(43b_2 \rightarrow 44b_2)-0.39(38b_1 \rightarrow 39b_1)$	2.65	0.040	*z*
	$4A_1$	$+0.67(32a_2 \rightarrow 33a_2)$	3.27	0.001	*z*
	$5A_1$	$+0.60(38b_1 \rightarrow 40b_1)$	3.29	0.056	*z*
	$6A_1$	$+0.68(32a_2 \rightarrow 34a_2)$	3.55	0.0001	*z*
	$4B_1$	$+0.65(31a_2 \rightarrow 44b_2)$	3.55	0.003	*x*
	$4B_2$	$+0.61(31a_2 \rightarrow 39b_1)$	3.56	0.003	*y*
	$5B_2$	$+0.51(38b_1 \rightarrow 35a_2)$	3.57	0.002	*y*
	$5B_1$	$+0.52(43b_2 \rightarrow 35a_2)$	3.65	0.0001	*x*
	$6B_2$	$+0.68(38b_1 \rightarrow 33a_2)$	3.68	0.001	*y*
	$6B_1$	$-0.30(52a_1 \rightarrow 39b_1)+0.62(43b_2 \rightarrow 33a_2)$	3.77	0.033	*x*
	$7B_2$	$+0.58(52a_1 \rightarrow 44b_2)$	3.80	0.241	*y*
	$7B_1$	$+0.32(50a_1 \rightarrow 39b_1)+0.50(52a_1 \rightarrow 39b_1)$	3.82	0.154	*x*
	$7A_1$	$+0.30(36b_1 \rightarrow 39b_1)-0.38(42b_2 \rightarrow 44b_2)+0.48(37b_1 \rightarrow 39b_1)$	3.83	0.0002	*z*
	$8B_2$	$+0.56(51a_1 \rightarrow 44b_2)$	3.85	0.027	*y*
	$8B_1$	$+0.36(51a_1 \rightarrow 39b_1)+0.44(38b_1 \rightarrow 55a_1)$	3.85	0.006	*x*
	$9B_1$	$-0.37(51a_1 \rightarrow 39b_1)+0.42(38b_1 \rightarrow 55a_1)$	3.89	0.052	*x*
	$9B_2$	$+0.64(49a_1 \rightarrow 44b_2)$	3.90	0.001	*y*
	$10B_1$	$+0.60(49a_1 \rightarrow 39b_1)$	3.91	0.015	*x*
	$10B_2$	$+0.57(32a_2 \rightarrow 41b_1)$	3.92	0.008	*y*
	$11B_1$	$+0.54(32a_2 \rightarrow 45b_2)$	3.92	0.049	*x*
	$11B_2$	$+0.51(43b_2 \rightarrow 55a_1)$	3.95	0.001	*y*
	$12B_2$	$+0.42(50a_1 \rightarrow 39b_1)$	4.01	0.063	*x*
	$13B_2$	$+0.33(50a_1 \rightarrow 44b_2)+0.39(43b_2 \rightarrow 55a_1)$	4.01	0.002	*y*
	$8A_1$	$-0.39(35b_1 \rightarrow 39b_1)+0.40(53a_1 \rightarrow 55a_1)$	4.03	0.002	*z*
	$9A_1$	$+0.50(41b_2 \rightarrow 44b_2)-0.31(36b_1 \rightarrow 39b_1)$	4.09	0.001	*z*

[a] *E*: excitation energy in eV.

[b] *f*: oscillator strength.

[c] *p*: polarization of the electrical dipole. The x and y axes directed toward two of four inner nitrogen atoms of the Pc ring.

Table S-7 Symmetry-allowed TD-B3LYP excited states of $FePc(CN^-)_2$ with the same spin multiplicity as the ground state

	state	main configuration ($\|C\| \geq 0.30$)	E^a	f^b	p^c
$FePc(CN^-)_2$	$1E_u$	$+0.36(11a_{2u}\rightarrow 8e_g)+0.57(2a_{1u}\rightarrow 8e_g)$	2.17	0.203	$x+y$
		$-0.36(11a_{2u}\rightarrow 8e_g)+0.57(2a_{1u}\rightarrow 8e_g)$			
	$2E_u$	$+0.56(11a_{2u}\rightarrow 8e_g)$	2.60	0.117	$x+y$
		$+0.56(11a_{2u}\rightarrow 8e_g)$			
	$3E_u$	$+0.61(7e_g\rightarrow 3b_{1u})-0.34(7e_g\rightarrow 4b_{2u})$	2.91	0.018	$x+y$
		$+0.61(7e_g\rightarrow 3b_{1u})+0.34(7e_g\rightarrow 4b_{2u})$			
	$4E_u$	$+0.56(7e_g\rightarrow 4b_{2u})$	3.07	0.250	$x+y$
		$+0.56(7e_g\rightarrow 4b_{2u})$			
	$5E_u$	$+0.66(7e_g\rightarrow 12a_{2u})$	3.33	0.192	$x+y$
		$+0.66(7e_g\rightarrow 12a_{2u})$			
	$1A_{2u}$	$+0.70(14b_{2g}\rightarrow 3b_{1u})$	3.42	0.0002	z
	$6E_u$	$+0.66(2a_{1u}\rightarrow 9e_g)$	3.50	0.045	$x+y$
		$+0.66(2a_{1u}\rightarrow 9e_g)$			
	$7E_u$	$+0.63(3b_{2u}\rightarrow 8e_g)$	3.95	0.022	$x+y$
		$+0.63(3b_{2u}\rightarrow 8e_g)$			
	$8E_u$	$+0.61(11a_{2u}\rightarrow 9e_g)$	4.10	0.018	$x+y$
		$+0.61(11a_{2u}\rightarrow 9e_g)$			
	$9E_u$	$+0.52(10a_{2u}\rightarrow 8e_g)$	4.14	0.518	$x+y$
		$+0.52(10a_{2u}\rightarrow 8e_g)$			
	$2A_{2u}$	$+0.48(30e_u\rightarrow 8e_g)+0.48(30e_u\rightarrow 8e_g)$	4.21	0.003	z

[a] *E*: excitation energy in eV.

[b] *f*: oscillator strength.

[c] *p*: polarization of the electrical dipole. The x and y axes directed toward two of four inner nitrogen atoms of the Pc ring.

Table S-8 Symmetry-allowed TD-B3LYP excited states of $FePc(CN^-)$ with the same spin multiplicity as the ground state

	state	main configuration ($\|C\| \geq 0.30$)	E^a	f^b	p^c
$FePc(CN^-)$	1E	$+0.52(37e\rightarrow32a_1)+0.37(37e\rightarrow33a_1)$	1.70	0.001	*x*
		$+0.52(37e\rightarrow32a_1)+0.37(37e\rightarrow33a_1)$			*y*
	2E	$+0.62(13a_2\rightarrow38e)$	2.21	0.358	*x*
		$+0.62(13a_2\rightarrow38e)$			*y*
	$1A_1$	$+0.42(37e\rightarrow38e)+0.42(37e\rightarrow38e)$	2.38	0.011	*z*
	3E	$+0.44(37e\rightarrow17b_1)-0.43(37e\rightarrow19b_2)$	3.31	0.072	*y*
		$+0.44(37e\rightarrow17b_1)+0.43(37e\rightarrow19b_2)$			*x*
	4E	$+0.49(37e\rightarrow20b_2)$	3.61	0.015	*x*
		$+0.49(37e\rightarrow20b_2)$			*y*
	$2A_1$	$+0.47(36e\rightarrow38e)+0.47(36e\rightarrow38e)$	3.63	0.0001	*z*
	5E	$+0.34(18b_2\rightarrow38e)+0.47(13a_2\rightarrow39e)$	3.67	0.009	*y*
		$+0.34(18b_2\rightarrow38e)+0.47(13a_2\rightarrow39e)$			*x*
	$3A_1$	$+0.69(16b_1\rightarrow17b_1)$	3.71	0.001	*z*
	6E	$-0.36(18b_2\rightarrow38e)+0.48(13a_2\rightarrow39e)$	3.77	0.109	*x*
		$-0.36(18b_2\rightarrow38e)+0.48(13a_2\rightarrow39e)$			*y*
	7E	$+0.33(18b_2\rightarrow38e)-0.33(37e\rightarrow32a_1)+0.45(37e\rightarrow33a_1)$	3.82	0.023	*y*
		$-0.33(18b_2\rightarrow38e)-0.33(37e\rightarrow32a_1)+0.45(37e\rightarrow33a_1)$			*x*
	$4A_1$	$+0.44(37e\rightarrow39e)+0.44(37e\rightarrow39e)$	3.85	0.004	*z*
	8E	$+0.35(30a_1\rightarrow38e)-0.34(18b_2\rightarrow38e)+0.32(31a_1\rightarrow38e)$	3.92	0.208	*y*
		$+0.35(30a_1\rightarrow38e)+0.34(18b_2\rightarrow38e)+0.32(31a_1\rightarrow38e)$			*x*
	9E	$+0.61(14b_1\rightarrow38e)$	3.94	0.045	*y*
		$+0.61(14b_1\rightarrow38e)$			*x*
	10E	$+0.54(30a_1\rightarrow38e)-0.36(31a_1\rightarrow38e)$	4.08	0.549	*y*
		$+0.54(30a_1\rightarrow38e)-0.36(31a_1\rightarrow38e)$			*x*
	$5A_1$	$-0.45(35e\rightarrow38e)+0.45(35e\rightarrow38e)$	4.17	0.001	*z*
	$6A_1$	$+0.46(34e\rightarrow38e)+0.46(34e\rightarrow38e)$	4.21	0.005	*z*
	11E	$+0.67(15b_1\rightarrow38e)$	4.23	0.109	*y*
		$+0.67(15b_1\rightarrow38e)$			*x*
	12E	$+0.67(29a_1\rightarrow38e)$	4.32	0.039	*x*
		$+0.67(29a_1\rightarrow38e)$			*y*

[a] *E*: excitation energy in eV.

[b] *f*: oscillator strength.

[c] *p*: polarization of the electrical dipole. The x and y axes directed toward two of four inner nitrogen atoms of the Pc ring.