Differential Sensing of Protein Influences by NO and CO Vibrations in Heme Adducts

- Supporting Information -

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Table S1. Key structural parameters and S^2 values calculated by the different DFT functionals in this study, with selected structural information from experiments and other computations for comparison

	Fe-NO(Å)	N-O (Å)	Fe-N-O (deg)	Fe-L (Å)	Fe-Np(Å)	S^2	Ref
			Five-coordinate				
Experimental							
Fe(TPP)(NO)	1.717(7)	1.122(12)	149.2(6)		2.001(3)		1
Fe(TpivPP)(NO)	1.716(15)	1.197(9)	143.8		1.981(26)		2
<Fe(Por)(NO)>	1.728(5)	1.168(1)	143.4(9)		2.008(3)		3
Functional, basis (calc.)							
B3LYP, VTZ	1.709	1.173	140.4		2.0725/2.0037	0.84	t.w.
B3PW91, VTZ	1.780	1.173	142.0		2.018/2.0023	1.42	t.w.
B3P86, VTZ	1.761	1.172	141.2		2.0133/1.9959	1.31	t.w.
BLYP, VTZ	1.716	1.196	142.5		2.0436/2.0154	0.77	t.w.
BPW91, VTZ	1.699	1.189	143.6		2.0296/2.001	0.77	t.w.
BP86, VTZ	1.699	1.191	143.2		2.0279/1.9995	0.77	t.w.
PW91/STO-TZP	1.704	1.182	144.8		2.025/2.002		4
BP86, TZVP	1.700	1.180	146.0				5
			Six-coordinate				
Experimental							
(N-MeIm)Fe(TPP)(NO)	1.750(2)	1.182(3)	137.7(2)	2.173(2)	2.008(13)		3
(Py)Fe(TpivPP)(NO)	1.742(5)	1.194(9)	133.4(5)	2.260(5)	2.009(2)		3
<(L)Fe(Por)(NO)>	1.752(4)	1.174(6)	138.5(11)		2.007		3
Functional, basis (calc.)							
B3LYP, VTZ	1.782	1.174	139.6	2.123	2.0299/2.02	0.86	t.w.
B3PW91, VTZ	1.763	1.171	140.0	2.099	2.0196/2.0075	0.86	t.w.
B3P86, VTZ	1.757	1.171	139.6	2.080	2.0149/2.0027	0.85	t.w.
BLYP, VTZ	1.749	1.199	139.3	2.236	2.0456/2.0263	0.77	t.w.
BPW91, VTZ	1.735	1.192	139.8	2.186	2.0315/2.0105	0.77	t.w.
BP86, VTZ	1.735	1.194	139.4	2.161	2.0304/2.0101	0.76	t.w.
PW91/STO-TZP	1.741	1.186	140.1	2.173	2.027/2.008		4
BP86, TZVP	1.730	1.190	140.0	2.180			5

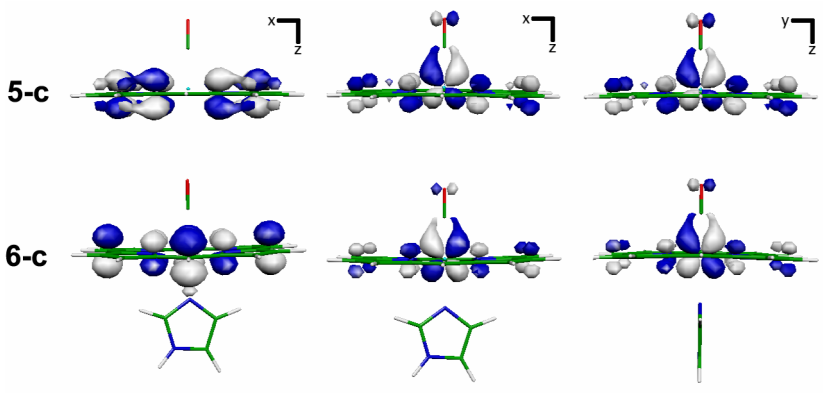

Figure S1. Three highest HOMOs of Fe(II)P(CO) and (ImH)Fe(II)P(CO), which correspond to the selected HOMOs of Fe(II)P(NO) and (ImH)Fe(II)P(NO) in Figure 9 in the main article.

Complete Reference 15:

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