Nuclear Resonance Vibrational Spectroscopy applied to [Fe(OEP)(NO)]: The Vibrational Assignments of Five-Coordinate Ferrous Heme Nitrosyls and Implications for Electronic Structure

Nicolai Lehnert,*[1] Mary Grace I. Galinato,[1] Florian Paulat,[1] George Richter-Addo,[2] Wolfgang Sturhahn,[3] Nan Xu,[2] Jiyong Zhao[3]

[1] Department of Chemistry, University of Michigan, Ann Arbor, MI 48109, USA
[2] Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK 73019, USA
[3] Argonne National Laboratory, APS/XFD, 431/D003, Argonne, IL 60439

E-mail: lehnertn@umich.edu

Supporting Information

Complete ref. 28:

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, Gaussian, Inc.: Pittsburgh, PA, 2003.

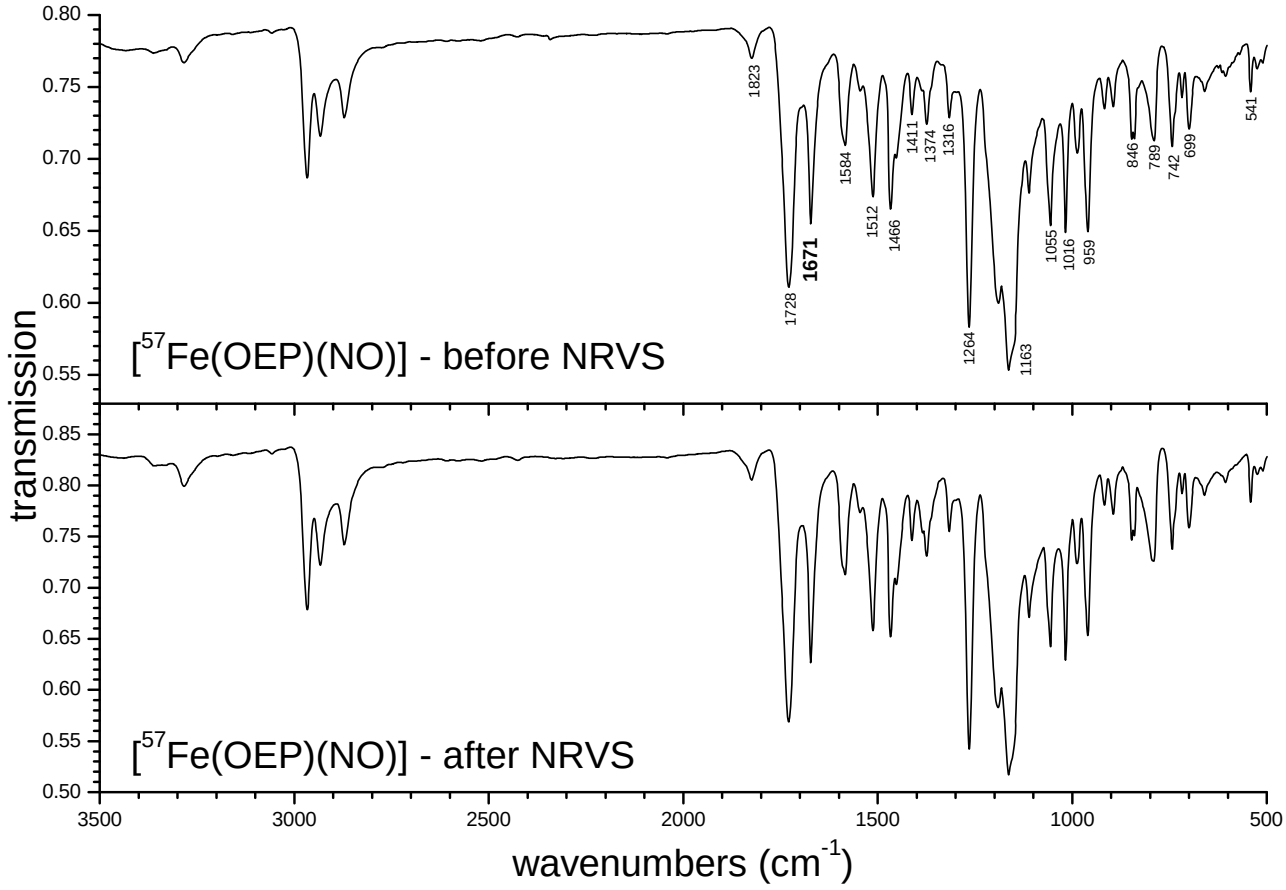

Figure S1. IR spectra of [^{57}Fe(OEP)(NO)] (**1**) taken before (top) and after (bottom) the NRVS measurements. The spectra show no noticeable decomposition of the compound due to the exposure of the sample to the x-ray beam.

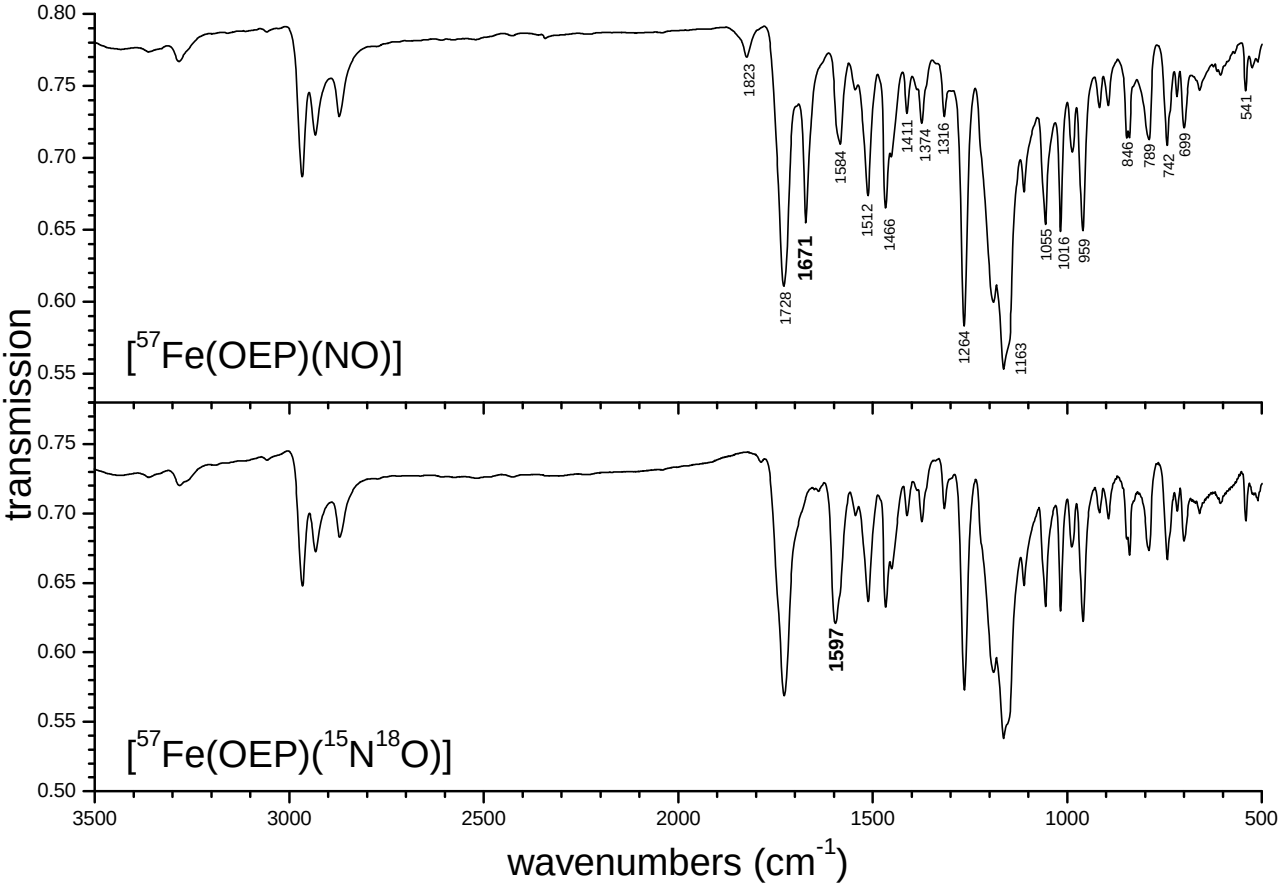

Figure S2. IR spectra of [^{57}Fe(OEP)(NO)] (**1**) with natural abundance (top) and $^{15}N^{18}O$ labeled (bottom) nitric oxide. The spectra show the N-O stretch ν(N-O) of **1** at 1671 cm^{-1} which shifts to 1597 cm^{-1} in the isotopically labeled compound.

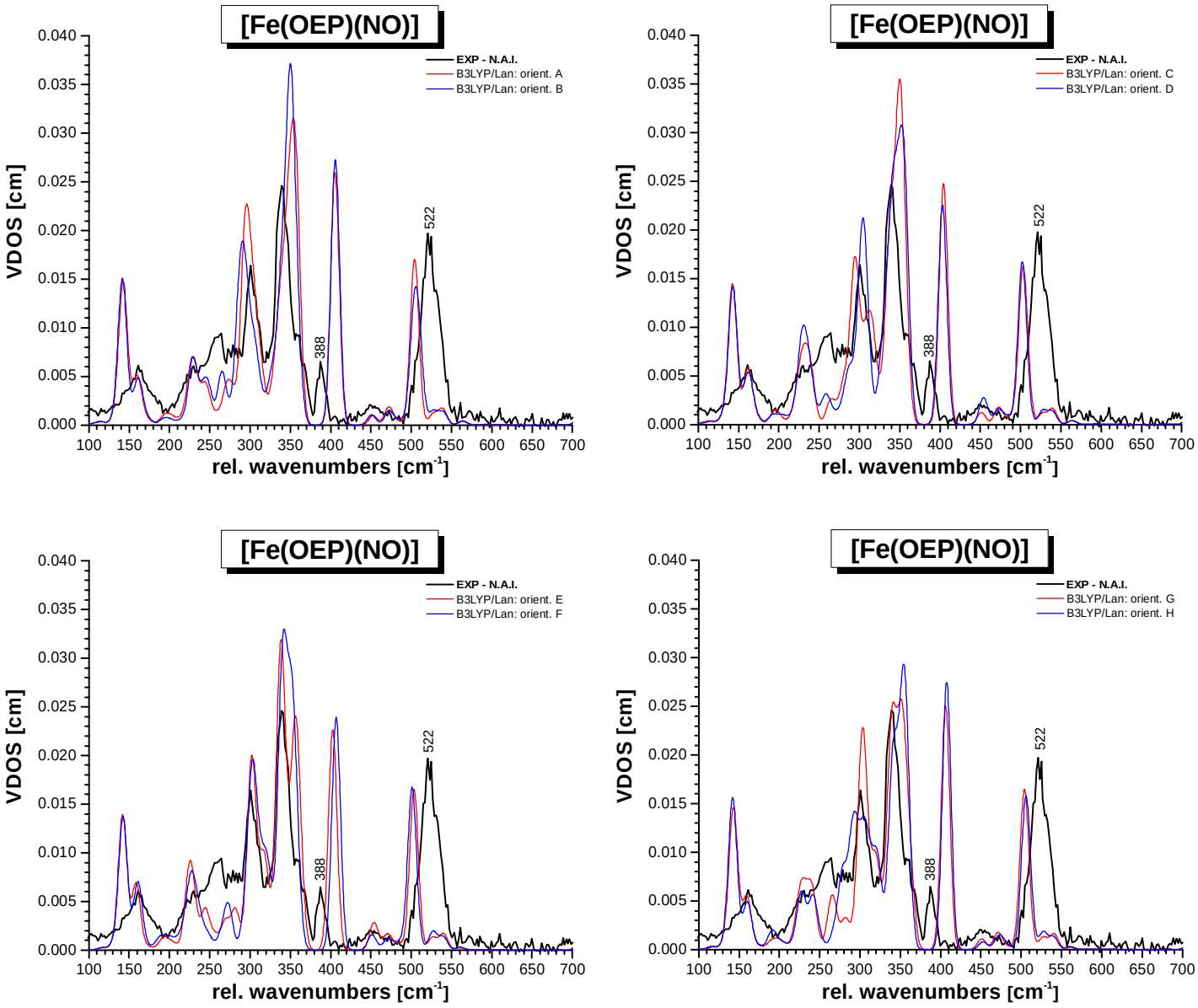

Figure S3. Calculated NRVS spectra of [Fe(OEP)(NO)] (**1**) for form **I** (5/3 structure) according to Figure 1 using B3LYP/LanL2DZ.

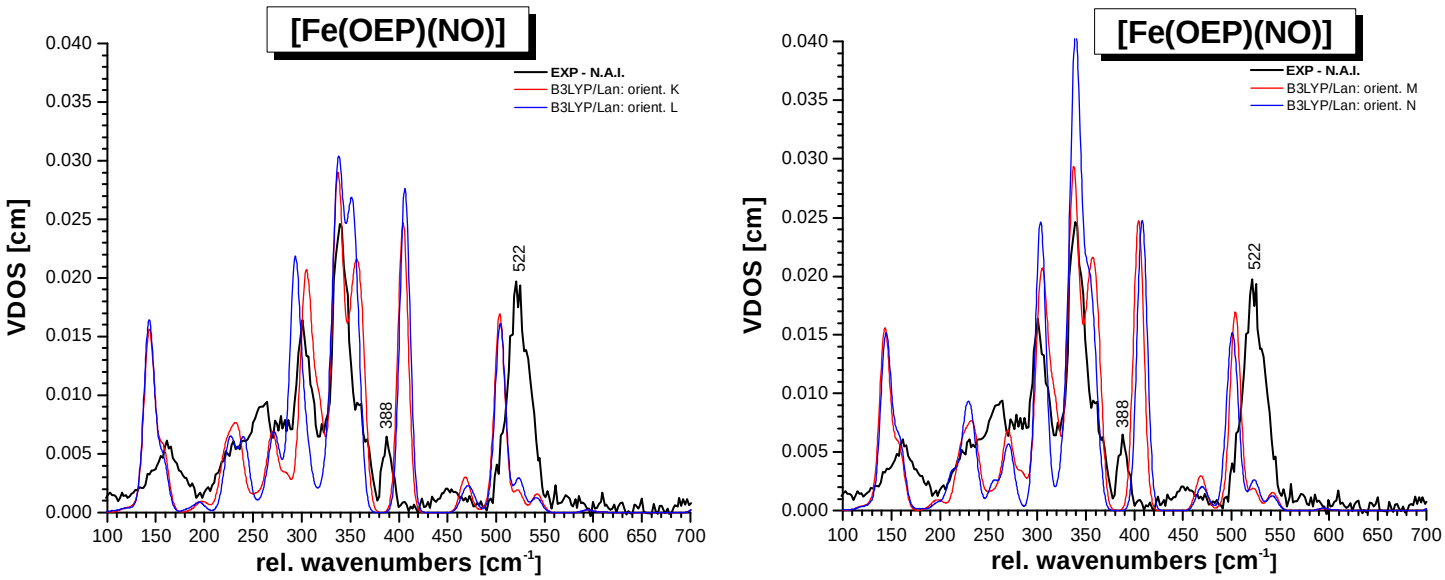

Figure S4. Calculated NRVS spectra of [Fe(OEP)(NO)] (**1**) for form **II** (4/4 structure) according to Figure 2 using B3LYP/LanL2DZ.

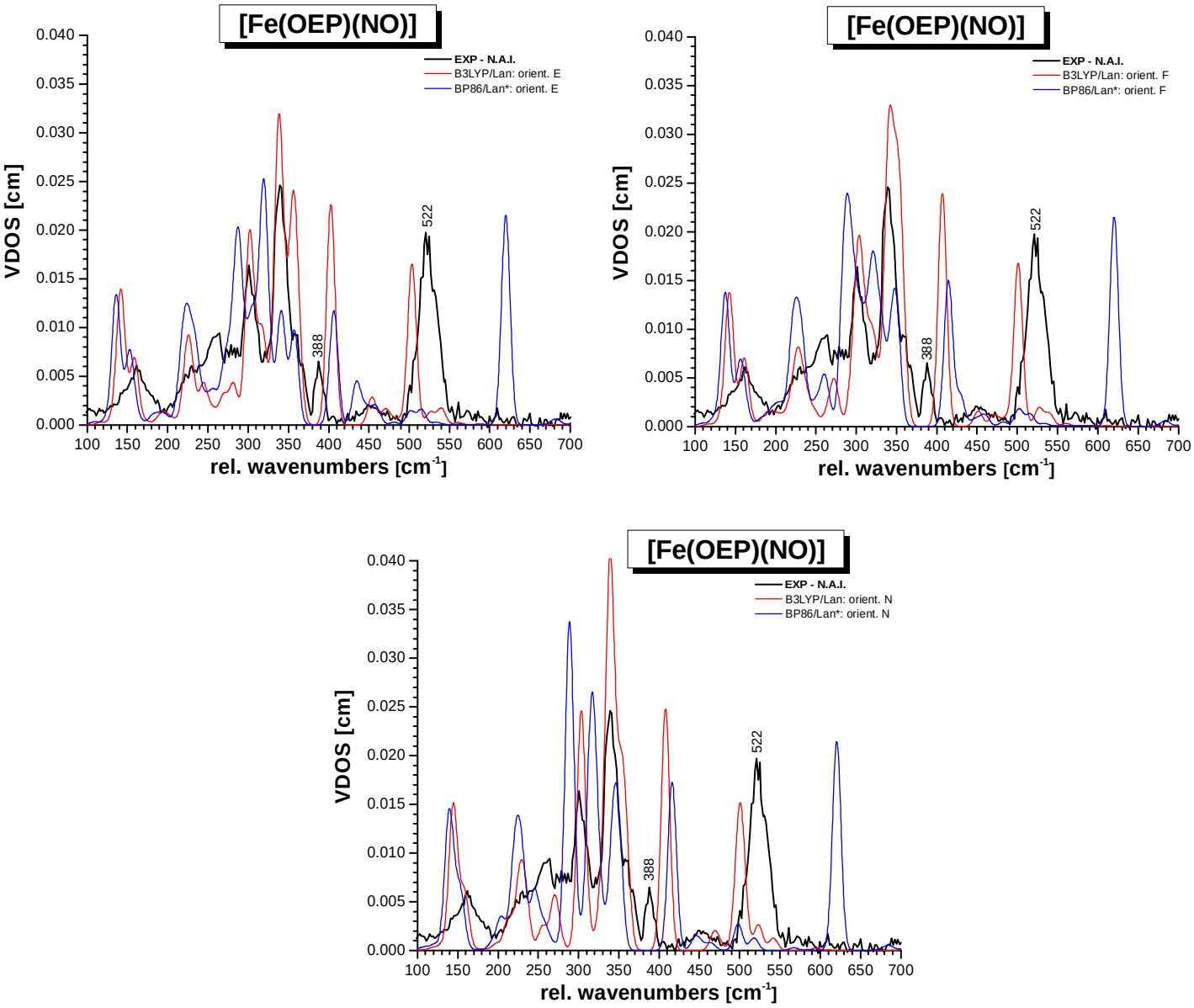

Figure S5. Calculated NRVS spectra of [Fe(OEP)(NO)] (**1**) for the selected conformers **1-E** (crystal structure form **I**), **1-F** (best fit of NRVS data with B3LYP/LanL2DZ), and **1-N** (crystal structure of form **II**) using B3LYP/LanL2DZ and BP86/LanL2DZ* in comparison.

Table S1. Results of the B3LYP/LanL2DZ and BP86/LanL2DZ* geometry optimization and frequency calculations for conformers A – H and K – N of [Fe(OEP)(NO)] (**1**).

Conformer	Geometric Parameter [a]				Vibrational Frequency [cm^{-1}]		
	r(Fe-NO)	r(N-O)	Fe-N-O	r(Fe-N_{Pyr})	ν(N-O)	ν(Fe-NO)	δ(Fe-N-O)
B3LYP/LanL2DZ: conformation **I**							
A	1.742	1.215	143	2.020	1615	504	405
B	1.742	1.215	143	2.020	1615	503/509	406
C	1.742	1.215	143	2.020	1614	502/507	404
D	1.742	1.215	143	2.020	1616	502	403
E	1.742	1.215	143	2.020	1615	503	403
F	1.742	1.215	143	2.020	1617	501	407
G	1.742	1.215	143	2.020	1615	503/508	406
H	1.742	1.215	143	2.020	1617	504/508	408
B3LYP/LanL2DZ: conformation **II**							
K	1.742	1.215	143	2.020	1614	504	404
L	1.742	1.215	143	2.020	1614	504	406
M	1.742	1.215	143	2.020	1614	504	404
N	1.742	1.215	143	2.020	1616	499/504	408
BP86/LanL2DZ*							
F	1.687	1.190	143	2.022	1712	620	414
E	1.687	1.190	144	2.023	1713	620	406
N	1.687	1.190	144	2.022	1712	620	416

[a] Distances r in [Å] and angles in [degrees]; r(Fe-N_{Pyr}) is the average Fe-N(porphyrin) distance.

Table S2. Results of the QCC-NCA fits of conformers A – H and K – N of [Fe(OEP)(NO)] (**1**) based on the B3LYP/LanL2DZ and BP86/LanL2DZ* calculations. Listed are the force constants that differ in the QCC-NCA results for the different conformers. Other force constants are listed in Table 1.

Conformer	QCC-NCA Force Constant [a]			Int. ratio NRVS [b]	Vibrational Frequency [cm^{-1}] [c]		
	Fe-NO	N-O	Fe-N-O		ν(N-O)	ν(Fe-NO) [d]	δ(Fe-N-O)
QCC-NCA: B3LYP/LanL2DZ (conformation **I**)							
A	2.829	12.166	0.341	1.48	1671 (-72)	522 (~ -13)	388 (-5)
B	2.831	12.166	0.339	1.31 *	1671 (-72)	522/(528) (~ -13)	388 (-5)
C	2.830	12.168	0.340	1.52	1671 (-72)	522 (~ -13)	388 (-5)
D	2.831	12.171	0.348	1.69	1671 (-72)	522 (~ -13)	388 (-5)
E	2.831	12.169	0.354	1.65	1671 (-72)	522 (~ -13)	388 (-5)
F	2.841	12.169	0.324	1.71	1671 (-72)	522 (~ -13)	388 (-5)
G	2.836	12.167	0.336	1.56	1671 (-72)	522 (~ -13)	388 (-5)
H	2.841	12.165	0.324	1.39 *	1671 (-72)	522/(528) (~ -13)	388 (-5)
QCC-NCA: B3LYP/LanL2DZ (conformation **II**)							
K	2.818	12.167	0.341	1.60	1671 (-73)	522/(523) (-12)	388 (-5)
L	2.812	12.158	0.335	1.28 *	1671 (-73)	521/(523) (-12)	388 (-5)
M	2.817	12.161	0.342	1.59	1671 (-73)	522/(523) (-12)	388 (-5)
N	2.831	12.168	0.325	1.64	1671 (-73)	522/(524) (-12)	388 (-5)
QCC-NCA: BP86/LanL2DZ*							
F	2.938	12.148	0.346	1.73	1671 (-73)	522 (-14)	388 (-7)
E	2.934	12.154	0.386	1.89	1671 (-73)	522 (-14)	388 (-7)
N	2.939	12.152	0.350	1.66	1671 (-73)	522 (-14)	388 (-7)

[a] Stretching force constants are given in [mdyn/Å] and bending force constants in [mdyn·Å].

[b] Predicted integral NRVS VDOS intensity ratio of $e_{Fe}^2[\nu(Fe\text{-}NO)]/e_{Fe}^2[\delta(Fe\text{-}N\text{-}O)]$; * = the Fe-N-O bend is particularly intense in these cases, which reduces the NRVS intensity ratio.

[c] Calculated for ^{57}Fe. The predicted $^{15}N^{18}O$ isotope shift is listed in brackets.

[d] For the QCC-NCA//B3LYP/LanL2DZ simulations: in the $^{15}N^{18}O$ labeled complex, ν(Fe-NO) becomes mixed with a porphyrin mode at ~507 cm^{-1}. Because of this artificial mixing that seems to be absent in the experimental data, the true isotope shift of this feature can only be estimated.

Table S3. Cartesian coordinates of the fully optimized structure of **1** in conformation A (**1-A**) using B3LYP/LanL2DZ.

Fe	0.00361300	0.01585300	0.07968000
N	0.67234500	-1.87720900	-0.07153900
N	1.92383500	0.66344300	0.08044000
N	-0.60134000	1.92351100	-0.24020200
N	-1.84518700	-0.62157200	-0.40221100
C	-0.09658200	-3.03572000	-0.18503200
C	0.74480000	-4.22558900	-0.10389700
C	0.24935400	-5.65041900	-0.16158600
C	2.04148500	-3.78214000	0.06574100
C	3.29998500	-4.60987800	0.16670000
C	1.98572900	-2.32367300	0.08769200
C	3.09940500	-1.50350100	0.23302400
H	4.06235000	-1.98639400	0.35767900
C	3.07406500	-0.11278700	0.21317500
C	4.26157500	0.73075900	0.32111500
C	5.67883800	0.22632700	0.43933300
C	3.82198200	2.03885000	0.25632400
C	4.64631800	3.30252800	0.28724400
C	2.36899000	1.98382100	0.11145000
C	1.55320500	3.10652500	0.01585500
H	2.03272000	4.07805500	0.06341000
C	0.17312800	3.07898800	-0.15689800
C	-0.65785300	4.27260300	-0.29841100
C	-0.15538700	5.69414600	-0.23386400
C	-1.95529600	3.83139000	-0.47207100
C	-3.20784000	4.65628900	-0.63969200
C	-1.90692600	2.37186400	-0.43330900
C	-3.01846700	1.54918800	-0.58503700
H	-3.97906200	2.02878200	-0.73728000
C	-2.99001400	0.15878300	-0.57477600
C	-4.16718300	-0.68456100	-0.76149700
C	-5.57643700	-0.17986500	-0.95253100
C	-3.73013800	-1.99367000	-0.69778600
C	-4.54833200	-3.25751300	-0.80036900
C	-2.28850500	-1.94216700	-0.47390500
C	-1.47503600	-3.06496100	-0.36642800
H	-1.94974700	-4.03659400	-0.44530800
N	-0.27630000	-0.09657300	1.79568900
O	-0.74680100	-0.81457300	2.65606100
H	1.06557700	-6.30934900	-0.48497100
H	-0.53833100	-5.74733600	-0.92187900
C	-0.29645200	-6.16093100	1.20025100
H	0.48448600	-6.12459000	1.96997500
H	-0.64774500	-7.19788500	1.11503000
H	-1.13248700	-5.54208300	1.54840900
H	3.04798200	-5.61517700	0.52851000
H	3.97789900	-4.17918800	0.91675800
C	4.05647700	-4.73992800	-1.18377600
H	3.42061900	-5.21561100	-1.94086900
H	4.96343200	-5.34761200	-1.06530700
H	4.35058100	-3.75576000	-1.56901100
H	6.30204300	0.99592700	0.91398400
H	5.71476700	-0.64702000	1.10541900

C	6.31455600	-0.15465400	-0.92587500
H	5.73396500	-0.93852200	-1.42776900
H	7.34034900	-0.52177800	-0.78864600
H	6.34815800	0.71368500	-1.59560400
H	4.13729100	4.07181300	0.88475600
H	5.59939600	3.10373200	0.79513600
C	4.94670600	3.87810100	-1.12425300
H	5.50925000	3.15475400	-1.72751700
H	5.54080300	4.79869700	-1.05058900
H	4.01980900	4.10984700	-1.66323000
H	0.80475100	5.78021300	-0.76160400
H	-0.85441000	6.35429700	-0.76438700
C	0.01927200	6.21897100	1.21801600
H	-0.93771400	6.20531700	1.75419000
H	0.39684400	7.25013600	1.21623400
H	0.72417700	5.59562000	1.78177100
H	-2.94363300	5.64606100	-1.03512000
H	-3.86714000	4.19519700	-1.38834200
C	-4.00136900	4.84517800	0.68246700
H	-4.30437100	3.87868700	1.10374300
H	-4.90566100	5.44423300	0.51152400
H	-3.38806900	5.35692600	1.43450400
H	-6.17125200	-0.94414100	-1.47023100
H	-5.57702200	0.70198700	-1.60830200
C	-6.28604000	0.18278500	0.38100600
H	-6.35271800	-0.69379500	1.03723600
H	-7.30403200	0.54902900	0.19294600
H	-5.73577900	0.96146800	0.92351700
H	-4.00350300	-4.01456700	-1.38168900
H	-5.47185400	-3.05156600	-1.35756400
C	-4.92521100	-3.85844000	0.58201800
H	-4.02895800	-4.09401800	1.16885200
H	-5.50874800	-4.78050700	0.45927600
H	-5.52480200	-3.14796700	1.16444700

Table S4. Cartesian coordinates of the fully optimized structure of **1** in conformation B (**1-B**) using B3LYP/LanL2DZ.

Fe	-0.01338200	0.00471700	0.08153200
N	-0.99146400	1.77453900	-0.04382900
N	-1.80427500	-0.94468500	0.07885900
N	0.89050000	-1.76255800	-0.25767000
N	1.69895000	0.94915200	-0.39993400
C	-0.42533100	3.04400300	-0.14899500
C	-1.44973200	4.07989400	-0.04554900
C	-1.19382200	5.56738300	-0.07956900
C	-2.65432600	3.42659500	0.12330300
C	-4.03239600	4.03208400	0.23785900
C	-2.35728500	1.99602200	0.12362200
C	-3.31911300	1.00026200	0.25965900
H	-4.34885800	1.31449100	0.39034000
C	-3.06479500	-0.36685600	0.22099800
C	-4.09914400	-1.39442600	0.31810300
C	-5.57956600	-1.12900900	0.44130000
C	-3.45333100	-2.61291900	0.23729600
C	-4.05919900	-3.99503700	0.24868000
C	-2.02942400	-2.32009500	0.09456800
C	-1.03896800	-3.29141600	-0.01079800
H	-1.34949600	-4.32975800	0.02539600
C	0.31701900	-3.03307500	-0.17957800
C	1.33467300	-4.06972000	-0.32721400
C	1.07590900	-5.55536000	-0.27024600
C	2.54094200	-3.41841100	-0.49804000
C	3.91277600	-4.02341000	-0.66859900
C	2.25328000	-1.98768600	-0.45198300
C	3.21393700	-0.99338500	-0.60134800
H	4.23999500	-1.30798800	-0.75620500
C	2.95581900	0.37315500	-0.58427200
C	3.97461400	1.40129900	-0.77433400
C	5.44702000	1.13715600	-0.97195400
C	3.32551600	2.61880000	-0.70368400
C	3.92058300	4.00113900	-0.81527000
C	1.91438800	2.32712000	-0.46733200
C	0.92833800	3.29989000	-0.34303200
H	1.23615500	4.33699700	-0.41879900
N	0.33934700	-0.01704700	1.78730500
O	1.22665900	-0.22629700	2.59114200
H	-2.11296300	6.09184900	-0.37130900
H	-0.44935000	5.80705400	-0.85183100
C	-0.70757800	6.13143300	1.28393100
H	-1.45945300	5.96117900	2.06456000
H	-0.52081100	7.21140700	1.21535800
H	0.21976500	5.64157200	1.60512300
H	-3.95100300	5.05865500	0.61812200
H	-4.62872000	3.48083800	0.97825900
C	-4.80056200	4.05925600	-1.11215800
H	-4.25737600	4.65594300	-1.85561800
H	-5.79985500	4.49614700	-0.98365600
H	-4.91751600	3.04785700	-1.52050800
H	-6.07016800	-2.00028300	0.89523800
H	-5.75690700	-0.28849700	1.12681700

C	-6.26637000	-0.82423100	-0.91824400
H	-5.82458800	0.05944200	-1.39513000
H	-7.33982700	-0.63914800	-0.77940800
H	-6.15047400	-1.66766300	-1.61021500
H	-3.43794800	-4.67538100	0.84802500
H	-5.03835800	-3.96121600	0.74453100
C	-4.24158600	-4.59847200	-1.17118100
H	-4.90795200	-3.97206300	-1.77714800
H	-4.67564700	-5.60552000	-1.11348200
H	-3.28169700	-4.66756200	-1.69750400
H	0.15219400	-5.79936800	-0.81369500
H	1.88411500	-6.08713800	-0.78959400
C	0.96846700	-6.10724600	1.17808900
H	1.89854800	-5.93039100	1.73237200
H	0.77521600	-7.18818800	1.16852900
H	0.15610700	-5.61794800	1.72935400
H	3.81737900	-5.03981600	-1.07330300
H	4.48847000	-3.45286100	-1.41077700
C	4.72271700	-4.08982100	0.65553500
H	4.85775000	-3.09070900	1.08759500
H	5.71494000	-4.52749900	0.48303500
H	4.20106600	-4.70432300	1.39963900
H	5.91034400	1.99813700	-1.47167200
H	5.59091600	0.28012000	-1.64478000
C	6.20336000	0.86710700	0.35800700
H	6.13895900	1.73571000	1.02504100
H	7.26433000	0.65800800	0.16726400
H	5.77333900	0.00943000	0.88950600
H	3.25445200	4.65331900	-1.39727100
H	4.86217900	3.94885300	-1.37787000
C	4.20107000	4.66543900	0.56066200
H	3.27947600	4.76826500	1.14685900
H	4.63704800	5.66457000	0.42827700
H	4.90210200	4.06063700	1.14908800

Table S5. Cartesian coordinates of the fully optimized structure of **1** in conformation C (**1-C**) using B3LYP/LanL2DZ.

Fe	0.00804800	0.01778900	0.08086400
N	-0.90494300	1.82191100	-0.04525300
N	-1.80061400	-0.86767400	0.05220900
N	0.86486800	-1.77261700	-0.26186400
N	1.76614700	0.91517900	-0.37808200
C	-0.29462100	3.07157000	-0.13771200
C	-1.28547900	4.14109800	-0.04161100
C	-0.97960500	5.61929700	-0.06636800
C	-2.51374300	3.52868500	0.10891100
C	-3.87231100	4.17897300	0.21022700
C	-2.26450300	2.08963900	0.10685900
C	-3.25856400	1.12408200	0.22797500
H	-4.27958800	1.46879100	0.34902500
C	-3.04542800	-0.24966900	0.18769300
C	-4.11024900	-1.24494900	0.27242100
C	-5.58278500	-0.93520700	0.38769700
C	-3.50191800	-2.48288200	0.19378100
C	-4.15100400	-3.84512600	0.19750100
C	-2.06896000	-2.23652900	0.06338600
C	-1.11099800	-3.23961900	-0.03787600
H	-1.45540300	-4.26717300	-0.00589700
C	0.25380000	-3.02458900	-0.19570400
C	1.23980100	-4.09131000	-0.34178800
C	0.93518400	-5.56844900	-0.29449300
C	2.46654000	-3.47618200	-0.50108500
C	3.81962100	-4.12309800	-0.66905600
C	2.22290900	-2.03748300	-0.44758100
C	3.21645100	-1.07404200	-0.58332600
H	4.23241000	-1.42173700	-0.73418400
C	3.00407500	0.30057400	-0.55906100
C	4.05831100	1.29596000	-0.73603600
C	5.52227400	0.98633700	-0.93197900
C	3.44811700	2.53298900	-0.66097900
C	4.08723200	3.89645300	-0.75929400
C	2.02566000	2.28341600	-0.43708600
C	1.06858400	3.28555800	-0.31496500
H	1.40838400	4.31326400	-0.38185500
N	0.17747300	-0.10724600	1.81002100
O	0.04676700	-0.87261000	2.74505100
H	-1.87748300	6.17565300	-0.36529200
H	-0.21949900	5.83700500	-0.82983900
C	-0.48889600	6.16122000	1.30448100
H	-1.25287000	6.01035700	2.07730500
H	-0.26851800	7.23528100	1.24316400
H	0.41998200	5.64154600	1.63151900
H	-3.76168200	5.20095100	0.59547400
H	-4.49493100	3.64494300	0.94166200
C	-4.62426700	4.23628100	-1.14792800
H	-4.05158200	4.81371000	-1.88440400
H	-5.60814600	4.70946100	-1.02930300
H	-4.77414500	3.23050600	-1.55950800
H	-6.10121400	-1.79227500	0.83769400
H	-5.73849100	-0.09120600	1.07412800

C	-6.25411900	-0.60784700	-0.97421200
H	-5.78640400	0.26473600	-1.44685400
H	-7.32267500	-0.39357600	-0.83955800
H	-6.15875400	-1.45211000	-1.66831600
H	-3.55299700	-4.54713300	0.79526200
H	-5.12986500	-3.78268200	0.69110300
C	-4.34879500	-4.43606300	-1.22554100
H	-4.99248400	-3.78569500	-1.83073300
H	-4.81593100	-5.42848800	-1.17333500
H	-3.39019800	-4.53460400	-1.74956000
H	0.00701000	-5.78107100	-0.84345100
H	1.72936900	-6.12210500	-0.81264600
C	0.80383700	-6.12370200	1.15070500
H	1.73570700	-5.97617800	1.71046600
H	0.57956400	-7.19856000	1.13482900
H	0.00342100	-5.61342200	1.70025800
H	3.69399700	-5.12990600	-1.08925600
H	4.41987500	-3.56157900	-1.39855000
C	4.61677100	-4.23569400	0.65963700
H	4.78643700	-3.24749300	1.10474300
H	5.59330100	-4.70785800	0.48847400
H	4.06745100	-4.83940900	1.39258600
H	6.01406300	1.83766700	-1.42103200
H	5.64024600	0.13310000	-1.61472100
C	6.26823300	0.67639300	0.39497600
H	6.22148400	1.53417100	1.07738300
H	7.32491300	0.44734800	0.20316500
H	5.81894400	-0.18158000	0.91013500
H	3.44108500	4.57630800	-1.33192100
H	5.02542700	3.82060400	-1.32494700
C	4.39174100	4.53537000	0.62355600
H	3.47614000	4.65188900	1.21650100
H	4.85088900	5.52547800	0.50219600
H	5.08150200	3.90583400	1.19925100

Table S6. Cartesian coordinates of the fully optimized structure of **1** in conformation D (**1-D**) using B3LYP/LanL2DZ.

Fe	-0.01913900	0.00492700	0.07917800
N	0.87668600	-1.79185800	-0.07152900
N	1.79108200	0.88624200	0.04818700
N	-0.87370900	1.81441500	-0.23942800
N	-1.78907300	-0.87160800	-0.37782700
C	0.25710000	-3.03915200	-0.17114900
C	1.24236000	-4.11321600	-0.08700700
C	0.92831200	-5.58947700	-0.12346400
C	2.47444000	-3.50910600	0.06694100
C	3.82896900	-4.16872400	0.16097800
C	2.23573800	-2.06915000	0.07732700
C	3.23707800	-1.11238800	0.20347100
H	4.25544600	-1.46570200	0.32107500
C	3.03286000	0.26297900	0.17411300
C	4.10268000	1.25224600	0.26285100
C	5.57387400	0.93413100	0.37093500
C	3.49987400	2.49351300	0.19441600
C	4.15605000	3.85245700	0.20506100
C	2.06501300	2.25521300	0.06895300
C	1.11283600	3.26510600	-0.01916800
H	1.46533800	4.28991000	0.01627100
C	-0.25503900	3.06141100	-0.16937300
C	-1.23492900	4.13673600	-0.30072800
C	-0.92080100	5.61173800	-0.24620300
C	-2.46609400	3.52984800	-0.45613900
C	-3.81672700	4.18509300	-0.61067300
C	-2.22872400	2.08843000	-0.41550300
C	-3.22801600	1.13054500	-0.55254400
H	-4.24334000	1.48424200	-0.69371700
C	-3.02293600	-0.24533200	-0.54436900
C	-4.08545300	-1.23163800	-0.72803300
C	-5.54830100	-0.90966200	-0.91186900
C	-3.48418000	-2.47404200	-0.67280800
C	-4.13259500	-3.83195400	-0.78642400
C	-2.05953100	-2.23695100	-0.45284800
C	-1.10705500	-3.24531300	-0.34681100
H	-1.45144900	-4.27075200	-0.42328600
N	-0.09522900	-0.04937600	1.81870200
O	0.55828900	-0.30927100	2.80984000
H	1.82400500	-6.14826300	-0.42426800
H	0.16916900	-5.79729800	-0.89068500
C	0.43147200	-6.13914000	1.24206200
H	1.19294800	-5.99493200	2.01856600
H	0.20898200	-7.21227200	1.17282300
H	-0.47739600	-5.61972600	1.56946600
H	3.71240100	-5.19261800	0.53921000
H	4.45602900	-3.64388600	0.89510100
C	4.57774800	-4.22104900	-1.19914100
H	3.99875800	-4.78715600	-1.93947700
H	5.55761300	-4.70384400	-1.08640700
H	4.73575300	-3.21314000	-1.60236700
H	6.09853300	1.78551000	0.82447700
H	5.72722000	0.08499900	1.05146900

C	6.23835600	0.61197900	-0.99559900
H	5.75925700	-0.25041600	-1.47546900
H	7.30457000	0.38377500	-0.86545400
H	6.15145700	1.46399500	-1.68130900
H	3.56590900	4.55283800	0.81258100
H	5.13779900	3.78068100	0.69156900
C	4.34767800	4.45418600	-1.21429200
H	4.98406100	3.80549900	-1.82894200
H	4.82031300	5.44373000	-1.15699100
H	3.38625800	4.56195800	-1.73126500
H	0.00242900	5.82286500	-0.80407500
H	-1.71748700	6.17361600	-0.75153500
C	-0.77023200	6.15705200	1.20087100
H	-1.69833300	6.01551600	1.76848000
H	-0.53531900	7.22970200	1.18949500
H	0.03063100	5.63592000	1.73968400
H	-3.68900600	5.19370000	-1.02599000
H	-4.42529800	3.63090500	-1.33885600
C	-4.60377300	4.29392700	0.72439700
H	-4.77332700	3.30400400	1.16573200
H	-5.58001000	4.77009500	0.56286300
H	-4.04707100	4.89240100	1.45614100
H	-6.04875300	-1.75201900	-1.40759400
H	-5.66457000	-0.04787200	-1.58402600
C	-6.28404200	-0.61028500	0.42321900
H	-6.23624200	-1.47539600	1.09623100
H	-7.34100700	-0.37488900	0.24093600
H	-5.82755200	0.24031100	0.94419100
H	-3.49419300	-4.50732700	-1.37296500
H	-5.07376800	-3.74220700	-1.34502000
C	-4.43245200	-4.48931500	0.58876000
H	-3.51435000	-4.61743600	1.17544500
H	-4.89556400	-5.47607400	0.45569700
H	-5.11720100	-3.86578600	1.17686100

Table S7. Cartesian coordinates of the fully optimized structure of **1** in conformation E (**1-E**) using B3LYP/LanL2DZ.

Fe	-0.03306500	0.01477700	0.23187500
N	-0.73446700	-1.83910200	-0.12099200
N	-1.86209900	0.76258500	-0.21999700
N	0.72571100	1.88893100	0.10142100
N	1.84409200	-0.71466700	0.21262100
C	-0.01903600	-3.03540200	-0.06398900
C	-0.91082700	-4.17977800	-0.22349400
C	-0.47884400	-5.62578900	-0.25861200
C	-2.18548900	-3.67011900	-0.37329900
C	-3.47758700	-4.43380100	-0.53636000
C	-2.06609800	-2.21696200	-0.30546600
C	-3.13999100	-1.34089900	-0.42262800
H	-4.12378400	-1.77318700	-0.56821300
C	-3.04609600	0.04656300	-0.38803000
C	-4.18328200	0.95035000	-0.54253000
C	-5.61891100	0.52046100	-0.71998000
C	-3.67841100	2.23403400	-0.46683200
C	-4.43109800	3.53979100	-0.54202000
C	-2.23657000	2.10390100	-0.26747600
C	-1.36452200	3.18236200	-0.16002300
H	-1.79091300	4.17782600	-0.21682400
C	0.01402900	3.08279900	-0.00255800
C	0.91286200	4.23206500	0.07826400
C	0.48950300	5.67597800	-0.03665100
C	2.18736200	3.72515600	0.24225900
C	3.48725000	4.48381600	0.35134500
C	2.05750400	2.27035800	0.25674700
C	3.12718600	1.39230200	0.39888400
H	4.11390000	1.82203900	0.53154400
C	3.03057400	0.00534600	0.36474900
C	4.17320100	-0.89719400	0.47072000
C	5.61273400	-0.46549800	0.60829500
C	3.67150800	-2.18196500	0.38832800
C	4.43261000	-3.48470500	0.41398600
C	2.22550700	-2.05630800	0.23242800
C	1.35665600	-3.13571300	0.11386000
H	1.78534900	-4.13078400	0.15560000
N	-0.19392800	-0.12567900	1.96066200
O	0.01868800	-0.86973600	2.89762300
H	-1.32364200	-6.26649200	0.02569600
H	0.30382400	-5.80612500	0.49131900
C	0.04185200	-6.07376700	-1.65180500
H	-0.73763800	-5.95396800	-2.41461300
H	0.34588200	-7.12882900	-1.63340000
H	0.90537300	-5.47294500	-1.96304800
H	-3.26609000	-5.42650500	-0.95459500
H	-4.12738100	-3.92979100	-1.26536800
C	-4.25381700	-4.60862700	0.79786200
H	-3.64715900	-5.15446200	1.53111000
H	-5.18498900	-5.16791100	0.63658300
H	-4.50858000	-3.63652000	1.23769500
H	-6.18319700	1.32415900	-1.21163700
H	-5.67405200	-0.34595600	-1.39389800

C	-6.32496500	0.16400200	0.61711900
H	-5.80599300	-0.65285500	1.13377600
H	-7.36269900	-0.14734500	0.43812700
H	-6.33804400	1.02809500	1.29298600
H	-3.85264300	4.27723800	-1.11601400
H	-5.36832800	3.39097100	-1.09454300
C	-4.76575200	4.13751900	0.85251000
H	-5.39581400	3.44918600	1.42937600
H	-5.30318600	5.08954800	0.74911300
H	-3.85390900	4.31904100	1.43469800
H	-0.45256500	5.83815700	0.50550400
H	1.23583400	6.31589900	0.45262700
C	0.31359200	6.15152500	-1.50524700
H	1.25647300	6.06131300	-2.05881900
H	-0.00455100	7.20202200	-1.53866100
H	-0.43789400	5.54798000	-2.02895300
H	3.28734500	5.49849700	0.72056600
H	4.13892200	4.01083700	1.09928600
C	4.25748400	4.58776600	-0.99383500
H	4.49704700	3.59346300	-1.39077100
H	5.19716400	5.14051300	-0.86222500
H	3.65546100	5.11008600	-1.74776400
H	6.19213500	-1.27293600	1.07550000
H	5.68624100	0.39404100	1.28905700
C	6.27951100	-0.09514600	-0.74496200
H	6.27517000	-0.95279800	-1.42912100
H	7.32136600	0.21657600	-0.59260400
H	5.74482800	0.72576600	-1.23868000
H	3.87279400	-4.23772200	0.98593100
H	5.38222200	-3.34221600	0.94663700
C	4.73673500	-4.04991600	-1.00077700
H	3.81195000	-4.22635100	-1.56405900
H	5.28272200	-5.00011000	-0.93103400
H	5.34789500	-3.34526800	-1.57831800

Table S8. Cartesian coordinates of the fully optimized structure of **1** in conformation F (**1-F**) using B3LYP/LanL2DZ.

Fe	0.03948700	0.00607800	0.23165900
N	0.84485200	1.83523300	-0.09295900
N	1.83276400	-0.82544900	-0.21978200
N	-0.80962800	-1.81387700	0.07663300
N	-1.79377500	0.83857000	0.20543000
C	0.19283200	3.06576100	-0.02962100
C	1.14445100	4.16553700	-0.16438000
C	0.78692700	5.63207900	-0.18751000
C	2.39219100	3.59141700	-0.30497000
C	3.72515700	4.28623700	-0.44395500
C	2.19385800	2.14461000	-0.25926200
C	3.21990300	1.21344300	-0.38270200
H	4.22686100	1.59376300	-0.51418900
C	3.05140500	-0.16746300	-0.37517800
C	4.14077300	-1.12589000	-0.54889100
C	5.59643600	-0.76690700	-0.72142000
C	3.57125400	-2.38345800	-0.49882700
C	4.25544200	-3.72421700	-0.60562100
C	2.13887100	-2.18311500	-0.29326500
C	1.21150100	-3.21549000	-0.19631300
H	1.58322700	-4.23187300	-0.26372400
C	-0.15874800	-3.04438400	-0.03134600
C	-1.11550900	-4.14421900	0.04960200
C	-0.76943800	-5.60842800	-0.06810800
C	-2.36150100	-3.57283600	0.22224800
C	-3.69757900	-4.26462200	0.33856800
C	-2.15940800	-2.12718400	0.23758800
C	-3.18436500	-1.19732600	0.37562300
H	-4.19169900	-1.57732400	0.50385900
C	-3.01738800	0.18293400	0.34270400
C	-4.11216800	1.14366100	0.44062000
C	-5.57362700	0.78710500	0.56098900
C	-3.54281300	2.40041300	0.36725400
C	-4.23446700	3.74154400	0.38513700
C	-2.10349200	2.19986100	0.22816100
C	-1.17865500	3.23411800	0.13160100
H	-1.55648500	4.24958000	0.17643900
N	0.11588100	-0.04282800	1.97129400
O	-0.54222700	-0.28706200	2.96309000
H	1.66591800	6.22786300	0.09090300
H	0.02171100	5.84807100	0.57130900
C	0.27538200	6.11366700	-1.57310000
H	1.03688600	5.95044200	-2.34588600
H	0.03350200	7.18456300	-1.54891200
H	-0.62532200	5.56466400	-1.87427000
H	3.57335100	5.29272000	-0.85514300
H	4.35709700	3.75434900	-1.16891400
C	4.49181700	4.40698000	0.90184700
H	3.90154800	4.97038500	1.63520600
H	5.44959600	4.92501300	0.75962900
H	4.69628200	3.41828100	1.33091400
H	6.12206000	-1.59767500	-1.21071700
H	5.69613900	0.09563600	-1.39532300

C	6.31431100	-0.44493600	0.61817900
H	5.84010100	0.40276700	1.12798400
H	7.36916400	-0.19454700	0.44381400
H	6.27366900	-1.30500300	1.29803600
H	3.63020100	-4.42276600	-1.17895200
H	5.18871000	-3.61509500	-1.17402000
C	4.58439400	-4.35877800	0.77368400
H	5.26476700	-3.71555800	1.34541000
H	5.06403200	-5.33849800	0.64714000
H	3.67583300	-4.49573400	1.37301900
H	0.15386600	-5.82496000	0.48745800
H	-1.55789600	-6.20783100	0.40595200
C	-0.59802000	-6.08678100	-1.53633800
H	-1.52496000	-5.93920900	-2.10432000
H	-0.34157300	-7.15400600	-1.57002600
H	0.19577100	-5.52674300	-2.04569100
H	-3.55174100	-5.27565500	0.74185800
H	-4.33354400	-3.73752700	1.06314200
C	-4.45672000	-4.37273500	-1.01254100
H	-4.64630000	-3.38023000	-1.44003100
H	-5.42202100	-4.87833700	-0.87693300
H	-3.87091600	-4.94324300	-1.74393100
H	-6.11677700	1.62522500	1.01737700
H	-5.69919500	-0.06443200	1.24422500
C	-6.24082100	0.44541300	-0.79949600
H	-6.17446800	1.29533700	-1.49014100
H	-7.30170600	0.19813100	-0.66095300
H	-5.74914000	-0.41044700	-1.27834800
H	-3.66116900	4.45479000	0.99391800
H	-5.21236500	3.64148300	0.87432400
C	-4.44794000	4.34389100	-1.03079500
H	-3.49199600	4.48195800	-1.55092000
H	-4.94843300	5.31924600	-0.96745100
H	-5.06759700	3.67995300	-1.64626200

Table S9. Cartesian coordinates of the fully optimized structure of **1** in conformation G (**1-G**) using B3LYP/LanL2DZ.

Fe	0.01837500	0.01621300	0.23020800
N	0.57155300	1.93822700	-0.09377900
N	1.88467100	-0.57183300	-0.24742700
N	-0.59987200	-1.89393000	0.07429200
N	-1.91816700	0.61206300	0.23832100
C	-0.23426800	3.07275000	-0.01345800
C	0.56420700	4.28735000	-0.16082600
C	0.01995500	5.69545200	-0.16857800
C	1.87308100	3.88123300	-0.32886300
C	3.10161800	4.74417800	-0.48807900
C	1.86524900	2.42150900	-0.28456200
C	3.00024200	1.62933200	-0.42528400
H	3.94849100	2.13486500	-0.57125800
C	3.00957500	0.23871400	-0.41180100
C	4.21062700	-0.57310700	-0.58613500
C	5.60735500	-0.03099600	-0.76598100
C	3.80859700	-1.89332100	-0.52179700
C	4.66198800	-3.13467400	-0.61060800
C	2.36390700	-1.88009600	-0.31226500
C	1.57954300	-3.02412000	-0.21235500
H	2.08149000	-3.98277500	-0.28194000
C	0.19906700	-3.03131200	-0.04382800
C	-0.61059600	-4.24373200	0.03211100
C	-0.08124700	-5.65089800	-0.09603800
C	-1.91860000	-3.83508400	0.20786300
C	-3.15673500	-4.69101400	0.31709200
C	-1.90038000	-2.37555100	0.23634300
C	-3.03403600	-1.58577300	0.39504500
H	-3.98283200	-2.09440700	0.52558700
C	-3.04575600	-0.19475700	0.38122400
C	-4.25366900	0.61679700	0.50669000
C	-5.65552300	0.07478600	0.64075100
C	-3.84947200	1.93627900	0.44246200
C	-4.70677900	3.17732900	0.48917100
C	-2.39752400	1.92018500	0.27908000
C	-1.61254500	3.06396500	0.17510000
H	-2.11558300	4.02291000	0.23414700
N	0.30173800	-0.08875500	1.94589700
O	0.79681700	-0.79037800	2.80586800
H	0.81285700	6.39579400	0.12456600
H	-0.77136000	5.80016600	0.58677300
C	-0.54083200	6.12627400	-1.55161100
H	0.24255000	6.08457400	-2.31869300
H	-0.92906400	7.15277700	-1.51213900
H	-1.35418200	5.46365300	-1.87241400
H	2.81204900	5.72430000	-0.88889900
H	3.78244300	4.30234200	-1.22907600
C	3.87249700	4.95667100	0.84372600
H	3.23387100	5.44915800	1.58761200
H	4.76088700	5.58226700	0.68459400
H	4.19787600	3.99931400	1.26899600
H	6.22601900	-0.77826900	-1.28053400
H	5.58930500	0.85186300	-1.42006500

C	6.29716600	0.34729200	0.57361100
H	5.72180000	1.10913900	1.11393800
H	7.30617900	0.74159700	0.39406100
H	6.38273200	-0.52904500	1.22794900
H	4.14991300	-3.90469500	-1.20462800
H	5.59098400	-2.90244100	-1.14807200
C	5.02635700	-3.72877200	0.77817200
H	5.59482300	-3.00392100	1.37395300
H	5.63679500	-4.63458500	0.66551900
H	4.12500800	-3.98928200	1.34621600
H	0.87643900	-5.74417600	0.43467600
H	-0.77149100	-6.34735700	0.39818800
C	0.11264300	-6.10420600	-1.56935800
H	-0.84116400	-6.08525000	-2.11110400
H	0.51127500	-7.12646600	-1.61273300
H	0.80818100	-5.44112300	-2.09834500
H	-2.87738800	-5.69233600	0.67063400
H	-3.83546100	-4.27841400	1.07663700
C	-3.92868600	-4.83542000	-1.02329100
H	-4.24580200	-3.85709300	-1.40512700
H	-4.82296100	-5.45888700	-0.89151900
H	-3.29584300	-5.30136300	-1.78879700
H	-6.29238300	0.82571200	1.12701600
H	-5.65978200	-0.80222800	1.30291400
C	-6.29879200	-0.31627700	-0.71811100
H	-6.36430800	0.55431200	-1.38252500
H	-7.31251200	-0.71145200	-0.56954900
H	-5.70398800	-1.08169900	-1.23171100
H	-4.21297600	3.95601200	1.08718700
H	-5.64938900	2.94973900	1.00451100
C	-5.03599300	3.75359300	-0.91559700
H	-4.12061700	4.01478300	-1.46087800
H	-5.65462400	4.65683600	-0.83035900
H	-5.58345100	3.01876200	-1.51887200

Table S10. Cartesian coordinates of the fully optimized structure of **1** in conformation H (**1-H**) using B3LYP/LanL2DZ.

Fe	-0.01127100	0.00635700	0.23680200
N	-0.82374400	-1.80248400	-0.11242400
N	-1.77128000	0.86420100	-0.23645100
N	0.87650800	1.82267200	0.10620000
N	1.82551400	-0.85135300	0.24192000
C	-0.18437000	-3.04237600	-0.04903200
C	-1.14679200	-4.12793700	-0.21263200
C	-0.80685800	-5.59847400	-0.24674400
C	-2.38597700	-3.53884800	-0.36775500
C	-3.72390800	-4.21766100	-0.53434000
C	-2.17415300	-2.09618400	-0.30292000
C	-3.18734900	-1.15189000	-0.42974100
H	-4.19754400	-1.51813500	-0.57478500
C	-2.99997200	0.22601100	-0.40579500
C	-4.07152900	1.20212300	-0.57950800
C	-5.53100700	0.86531100	-0.76275600
C	-3.48351500	2.45056000	-0.51338800
C	-4.14839500	3.80171500	-0.61052600
C	-2.05608000	2.22954100	-0.29926500
C	-1.11738700	3.24994700	-0.19232900
H	-1.47722100	4.27044000	-0.26228500
C	0.24955000	3.06168300	-0.01498500
C	1.22216900	4.14785600	0.07275700
C	0.90023100	5.61644500	-0.05740400
C	2.45637200	3.55637400	0.26013800
C	3.80307500	4.22609900	0.38381300
C	2.22878700	2.11304100	0.27979000
C	3.23706300	1.16774500	0.43803200
H	4.24785500	1.53385700	0.57996000
C	3.05263400	-0.21076200	0.40318300
C	4.13559500	-1.18497700	0.51991800
C	5.59837300	-0.84596100	0.67153100
C	3.55334500	-2.43449600	0.43016800
C	4.22761300	-3.78424000	0.45803400
C	2.11927000	-2.21370400	0.26180700
C	1.18061700	-3.23303400	0.13727400
H	1.54093800	-4.25500500	0.17953600
N	-0.36361100	-0.03543800	1.94193200
O	-1.24302500	-0.27934200	2.74398900
H	-1.69574700	-6.18571900	0.01807600
H	-0.05138000	-5.83157300	0.51662600
C	-0.28928300	-6.07251700	-1.63260500
H	-1.04702900	-5.90469500	-2.40813500
H	-0.04807200	-7.14365400	-1.61335500
H	0.61299900	-5.52210800	-1.92630600
H	-3.57679600	-5.21937300	-0.95871500
H	-4.34115200	-3.66864100	-1.25912200
C	-4.50804300	-4.35030000	0.80022500
H	-3.93715900	-4.93938600	1.52872800
H	-5.47384200	-4.84675800	0.63685600
H	-4.69794100	-3.36666800	1.24698100
H	-6.04191300	1.70533000	-1.25170900
H	-5.63898600	0.00686200	-1.44057400

C	-6.25979500	0.54858200	0.57217900
H	-5.79009000	-0.29773600	1.08814400
H	-7.31363900	0.29929000	0.39036700
H	-6.22304600	1.41060800	1.24978700
H	-3.52145300	4.49063200	-1.19379600
H	-5.09155100	3.70606200	-1.16468000
C	-4.44791500	4.44125000	0.77318700
H	-5.12162500	3.80337000	1.35854400
H	-4.92372000	5.42359700	0.65283000
H	-3.52818100	4.57408600	1.35611300
H	-0.02734400	5.84982600	0.48421800
H	1.69080000	6.20708600	0.42412600
C	0.75552200	6.08860600	-1.53044600
H	1.68843400	5.92624500	-2.08452500
H	0.51286200	7.15872200	-1.57379500
H	-0.03799000	5.53538100	-2.04768600
H	3.66919500	5.24975400	0.75831300
H	4.41644300	3.70618300	1.13292300
C	4.58737200	4.28609100	-0.95591700
H	4.76035100	3.28018400	-1.35809200
H	5.56188300	4.77226400	-0.81511700
H	4.02700100	4.85322200	-1.70952200
H	6.12231300	-1.69164000	1.13650300
H	5.72010900	0.00247200	1.35941300
C	6.29727200	-0.50821800	-0.67403000
H	6.24502300	-1.35921900	-1.36452600
H	7.35521200	-0.26254300	-0.51197000
H	5.81781000	0.34755400	-1.16522300
H	3.62477600	-4.49616200	1.03912700
H	5.18911800	-3.70169300	0.98201600
C	4.48257700	-4.37548800	-0.95569200
H	3.54347400	-4.49659700	-1.50969400
H	4.96872800	-5.35760200	-0.88515100
H	5.13098300	-3.71331500	-1.54275600

Table S11. Cartesian coordinates of the fully optimized structure of **1** in conformation K (**1-K**) using B3LYP/LanL2DZ.

Fe	-0.01529700	0.01823300	0.15737200
N	1.38179200	-1.43050600	0.09657900
N	1.46299000	1.40303800	0.12390100
N	-1.35113100	1.48489100	-0.25795000
N	-1.42488000	-1.35030100	-0.28681500
C	1.16427500	-2.80719700	0.04179400
C	2.42092200	-3.53665800	0.18080800
C	2.56295600	-5.03825000	0.13085100
C	3.41416100	-2.58806700	0.33041100
C	4.89911500	-2.80942900	0.48268100
C	2.75831400	-1.28456200	0.27970000
C	3.42790600	-0.07039100	0.38760500
H	4.50131000	-0.10270400	0.53823800
C	2.82844600	1.18175400	0.29722900
C	3.55636700	2.44647100	0.36279000
C	5.05196900	2.58246400	0.51040000
C	2.61552700	3.44908900	0.22908600
C	2.83957800	4.94120400	0.19577700
C	1.31990900	2.78890900	0.08633200
C	0.11439700	3.46567100	-0.06774000
H	0.14666700	4.54948700	-0.07194900
C	-1.12639000	2.85996300	-0.23687300
C	-2.37378000	3.59343800	-0.43979400
C	-2.50613300	5.09678400	-0.45173100
C	-3.36846400	2.64636600	-0.58798900
C	-4.84561100	2.86912400	-0.80114900
C	-2.72115600	1.34187400	-0.47177900
C	-3.38920000	0.12599200	-0.57605000
H	-4.45935600	0.15544300	-0.74866800
C	-2.78700200	-1.12500000	-0.49426600
C	-3.50498800	-2.38921300	-0.63119900
C	-4.99231800	-2.52542700	-0.84656500
C	-2.56599000	-3.39385300	-0.49830600
C	-2.78377300	-4.88681500	-0.53114800
C	-1.27957800	-2.73734300	-0.28577100
C	-0.07558800	-3.41447000	-0.12497200
H	-0.10416000	-4.49810600	-0.14243500
N	-0.25685000	-0.12627700	1.87642400
O	-0.40307300	-0.93742300	2.76950200
H	1.73819300	-5.51397500	0.67972500
H	3.48435400	-5.33507200	0.64929000
C	2.60093200	-5.60809400	-1.31397100
H	1.68613400	-5.35544300	-1.86410300
H	2.70104300	-6.70152000	-1.29772100
H	3.44928800	-5.19478400	-1.87339600
H	5.07703100	-3.80553100	0.90933300
H	5.31649400	-2.09152500	1.20234100
C	5.68118900	-2.69549700	-0.85466700
H	5.32816800	-3.44211100	-1.57688200
H	6.75520800	-2.85667500	-0.69226000
H	5.54773700	-1.70561700	-1.30850500
H	5.28840400	3.56301300	0.94469800
H	5.43067100	1.83543100	1.22190600

C	5.82075900	2.43562600	-0.83148100
H	5.63024000	1.45828400	-1.29197700
H	6.90282100	2.53552800	-0.67314700
H	5.50647800	3.20620700	-1.54636000
H	2.04645500	5.45541000	0.75666100
H	3.77990200	5.18008400	0.71017900
C	2.89851600	5.52617200	-1.24230200
H	3.71900100	5.07420300	-1.81328000
H	3.05854200	6.61220700	-1.21347600
H	1.96739000	5.33101400	-1.78843200
H	-1.66165300	5.54677800	-0.99238400
H	-3.40960200	5.38009600	-1.00806200
C	-2.58248700	5.71977900	0.96953400
H	-3.45067400	5.33339100	1.51756400
H	-2.67265500	6.81262000	0.91049400
H	-1.68692100	5.48028300	1.55595300
H	-5.00381800	3.84988600	-1.26930900
H	-5.24145400	2.12693100	-1.50829900
C	-5.67330100	2.80582200	0.51196600
H	-5.55723300	1.83339500	1.00636800
H	-6.74079900	2.96216400	0.30734800
H	-5.34285500	3.57806700	1.21767700
H	-5.20421900	-3.48506200	-1.33676500
H	-5.34716700	-1.74688100	-1.53605700
C	-5.81443900	-2.44719200	0.46917400
H	-5.52405800	-3.25041500	1.15759500
H	-6.88874900	-2.54336900	0.26312800
H	-5.64766300	-1.49303800	0.98426700
H	-1.97135200	-5.37560800	-1.08718900
H	-3.70731200	-5.10966900	-1.08185100
C	-2.88137000	-5.52550500	0.88193600
H	-1.96962200	-5.34253700	1.46350700
H	-3.03069300	-6.61092600	0.80805900
H	-3.72268900	-5.10119200	1.44357100

Table S12. Cartesian coordinates of the fully optimized structure of **1** in conformation L (**1-L**) using B3LYP/LanL2DZ.

Fe	0.00040400	0.00004700	0.15707500
N	-1.44606100	1.41868900	0.12322800
N	-1.44437000	-1.42019800	0.12306100
N	1.36404400	-1.41529600	-0.28208300
N	1.36237000	1.41702500	-0.28210400
C	-1.26950700	2.80022100	0.07044700
C	-2.54556600	3.49434100	0.22181000
C	-2.73148600	4.99139600	0.17747500
C	-3.50905700	2.51661000	0.37710900
C	-4.99851600	2.69294600	0.54277300
C	-2.81413500	1.23261300	0.31451000
C	-3.44638000	-0.00193500	0.42196300
H	-4.51857700	-0.00258400	0.58438500
C	-2.81267900	-1.23571600	0.31434700
C	-3.50610000	-2.52053000	0.37683200
C	-4.99535600	-2.69864200	0.54243000
C	-2.54146900	-3.49712900	0.22152100
C	-2.72562700	-4.99439900	0.17710200
C	-1.26621000	-2.80153200	0.07024000
C	-0.04351500	-3.44209100	-0.10241100
H	-0.04385100	-4.52620800	-0.11792900
C	1.17762000	-2.79870400	-0.27190300
C	2.44403400	-3.49285000	-0.48604900
C	2.61896500	-4.99169400	-0.51310200
C	3.41156300	-2.51657900	-0.62576200
C	4.89387500	-2.69623400	-0.84275400
C	2.73029100	-1.23177400	-0.49531700
C	3.36535300	0.00204300	-0.58915700
H	4.43568500	0.00267500	-0.76243600
C	2.72883100	1.23511000	-0.49534200
C	3.40859000	2.52072000	-0.62578700
C	4.89069300	2.70211800	-0.84276000
C	2.43990900	3.49584700	-0.48608700
C	2.61307300	4.99489600	-0.51315800
C	1.17431000	2.80021300	-0.27189400
C	-0.04755600	3.44218300	-0.10229300
H	-0.04914100	4.52630000	-0.11779500
N	0.37880700	-0.00000200	1.85745900
O	1.30487500	-0.00182200	2.64456200
H	-1.91800200	5.48964600	0.72348000
H	-3.65851800	5.25955200	0.70155300
C	-2.79337100	5.56490300	-1.26509200
H	-1.87451700	5.34067900	-1.82079300
H	-2.92480200	6.65495800	-1.24441700
H	-3.63233600	5.12931000	-1.82176400
H	-5.20268300	3.68061500	0.97736500
H	-5.38834500	1.95819300	1.26091200
C	-5.78782300	2.56412200	-0.78898900
H	-5.46244300	3.32494900	-1.50931100
H	-6.86474900	2.69293000	-0.61713500
H	-5.62916000	1.58127600	-1.24991500
H	-5.19835000	-3.68657600	0.97697200
H	-5.38609600	-1.96439100	1.26058700

C	-5.78476900	-2.57071000	-0.78935300
H	-5.62722500	-1.58767600	-1.25026400
H	-6.86155100	-2.70075800	-0.61753100
H	-5.45849600	-3.33115500	-1.50967600
H	-1.91151800	-5.49171900	0.72302300
H	-3.65230500	-5.26369500	0.70122400
C	-2.78692300	-5.56787700	-1.26550100
H	-3.62642600	-5.13321700	-1.82209100
H	-2.91708200	-6.65808600	-1.24490100
H	-1.86836200	-5.34253800	-1.82123600
H	1.78898100	-5.45982500	-1.06086000
H	3.53156600	-5.24313700	-1.06973900
C	2.70950200	-5.62697200	0.90191100
H	3.56489600	-5.22184700	1.45638200
H	2.83071900	-6.71613600	0.83176600
H	1.80614600	-5.41904900	1.48837800
H	5.07822000	-3.66511300	-1.32585300
H	5.26904900	-1.93294700	-1.53855100
C	5.71952900	-2.63030700	0.47153000
H	5.57616800	-1.66959300	0.98122100
H	6.79086900	-2.75385500	0.26463000
H	5.41069600	-3.42220300	1.16506500
H	5.07392100	3.67131100	-1.32565200
H	5.26673100	1.93940600	-1.53872300
C	5.71643500	2.63685100	0.47150300
H	5.40675700	3.42828900	1.16518700
H	6.78763900	2.76159300	0.26461400
H	5.57411600	1.67589000	0.98101700
H	1.78238200	5.46206600	-1.06065800
H	3.52521100	5.24743100	-1.07006400
C	2.70328600	5.63024100	0.90184500
H	1.80033700	5.42126500	1.48856600
H	2.82323200	6.71954600	0.83169700
H	3.55930700	5.22608300	1.45605400

Table S13. Cartesian coordinates of the fully optimized structure of **1** in conformation M (**1-M**) using B3LYP/LanL2DZ.

Fe	0.01535900	0.01819200	0.15738700
N	-1.46153800	1.40434500	0.12382700
N	-1.38308000	-1.42921600	0.09659300
N	1.42368200	-1.35167200	-0.28684600
N	1.35267600	1.48363300	-0.25785400
C	-1.31711600	2.79009600	0.08629800
C	-2.61210500	3.45150800	0.22899600
C	-2.83470200	4.94384200	0.19569400
C	-3.55392200	2.44980000	0.36261900
C	-5.04939500	2.58728300	0.51015500
C	-2.82723000	1.18438000	0.29710700
C	-3.42791300	-0.06717500	0.38747800
H	-4.50135500	-0.09844300	0.53805400
C	-2.75947200	-1.28198800	0.27963700
C	-3.41654800	-2.58486900	0.33030300
C	-4.90171500	-2.80482600	0.48250400
C	-2.42418800	-3.53439400	0.18076800
C	-2.56763300	-5.03585500	0.13085900
C	-1.16685700	-2.80611300	0.04179300
C	0.07243000	-3.41455300	-0.12499500
H	0.09997400	-4.49821400	-0.14246200
C	1.27706200	-2.73856800	-0.28580400
C	2.56286100	-3.39629800	-0.49832300
C	2.77919900	-4.88947000	-0.53123900
C	3.50281800	-2.39254800	-0.63113600
C	4.99003100	-2.53017500	-0.84640100
C	2.78602000	-1.12764700	-0.49422800
C	3.38942400	0.12277100	-0.57594200
H	4.45961400	0.15118900	-0.74852600
C	2.72256100	1.33930300	-0.47165600
C	3.37112600	2.64318000	-0.58785000
C	4.84847900	2.86453700	-0.80102100
C	2.37734000	3.59120100	-0.43967900
C	2.51110100	5.09442400	-0.45164300
C	1.12925600	2.85890000	-0.23679400
C	-0.11097900	3.46575000	-0.06769900
H	-0.14225600	4.54959200	-0.07189500
N	0.25644000	-0.12659400	1.87647400
O	0.39785600	-0.93798700	2.77009900
H	-2.04111000	5.45726900	0.75662800
H	-3.77482300	5.18363300	0.71004500
C	-2.89299200	5.52888600	-1.24238000
H	-1.96202700	5.33284000	-1.78846500
H	-3.05197400	6.61507400	-1.21355000
H	-3.71388000	5.07771400	-1.81341000
H	-5.28483300	3.56790900	0.94482100
H	-5.42893600	1.84037100	1.22133800
C	-5.81823700	2.44178400	-0.83184100
H	-5.50309300	3.21231800	-1.54639100
H	-6.90020400	2.54276700	-0.67354400
H	-5.62872500	1.46442300	-1.29271500
H	-5.08059400	-3.80072400	0.90923200
H	-5.31846000	-2.08646800	1.20207700

C	-5.68360100	-2.69028000	-0.85490300
H	-5.54901600	-1.70063900	-1.30892700
H	-6.75780700	-2.85022200	-0.69251600
H	-5.33138400	-3.43743100	-1.57695500
H	-1.74337900	-5.51233700	0.67984300
H	-3.48936800	-5.33177100	0.64921700
C	-2.60600100	-5.60575000	-1.31393200
H	-3.45387500	-5.19163700	-1.87349400
H	-2.70720500	-6.69907500	-1.29761600
H	-1.69088300	-5.35405800	-1.86397200
H	1.96620300	-5.37746900	-1.08713300
H	3.70241500	-5.11320000	-1.08213500
C	2.87648000	-5.52829400	0.88180500
H	3.71893300	-5.10552600	1.44290500
H	3.02375700	-6.61399200	0.80787500
H	1.96542700	-5.34362700	1.46392700
H	5.20106700	-3.49005000	-1.33650200
H	5.34564700	-1.75201800	-1.53594100
C	5.81214100	-2.45257000	0.46938200
H	5.64664700	-1.49798100	0.98408200
H	6.88633600	-2.55032200	0.26347400
H	5.52057500	-3.25511500	1.15809300
H	5.00759300	3.84506500	-1.26936900
H	5.24365300	2.12184700	-1.50802100
C	5.67609100	2.80074000	0.51211700
H	5.34651700	3.57359600	1.21756700
H	6.74376600	2.95581000	0.30745200
H	5.55892800	1.82861000	1.00684700
H	1.66710000	5.54518600	-0.99241000
H	3.41490100	5.37687400	-1.00787400
C	2.58785700	5.71740700	0.96960700
H	1.69193000	5.47889200	1.55587500
H	2.67918900	6.81014900	0.91052400
H	3.45553300	5.33013200	1.51781900

Table S14. Cartesian coordinates of the fully optimized structure of **1** in conformation N (**1-N**) using B3LYP/LanL2DZ.

Fe	0.03243600	-0.00002700	0.15531900
N	-1.39768300	1.41576000	0.09570500
N	-1.39821700	-1.41519600	0.09567800
N	1.41660100	-1.42024900	-0.26290400
N	1.41713800	1.41987100	-0.26285600
C	-1.21489100	2.79916600	0.05143800
C	-2.49195900	3.49410900	0.18256900
C	-2.67430500	4.99168000	0.13921600
C	-3.46106500	2.51882600	0.31824300
C	-4.95270600	2.69895500	0.45793300
C	-2.77042700	1.23370000	0.26513100
C	-3.40677200	0.00064600	0.35969700
H	-4.48126800	0.00084400	0.50515000
C	-2.77089800	-1.23264600	0.26504200
C	-3.46200800	-2.51751000	0.31800400
C	-4.95373200	-2.69709000	0.45752100
C	-2.49325900	-3.49315100	0.18232700
C	-2.67614300	-4.99065200	0.13883100
C	-1.21592400	-2.79866700	0.05132100
C	0.00747200	-3.44209200	-0.10093500
H	0.00375700	-4.52623800	-0.11367400
C	1.23254700	-2.80164100	-0.25597500
C	2.50143500	-3.49700800	-0.45552800
C	2.67691500	-4.99580100	-0.48001500
C	3.46890200	-2.51972800	-0.58683900
C	4.95331500	-2.69811300	-0.79090200
C	2.78325500	-1.23486200	-0.46394300
C	3.41917900	-0.00054300	-0.55123200
H	4.49102100	-0.00074400	-0.71600800
C	2.78371500	1.23401200	-0.46392000
C	3.46981900	2.51863200	-0.58684800
C	4.95428800	2.69650500	-0.79095500
C	2.50269200	3.49625200	-0.45553400
C	2.67868100	4.99498600	-0.48007900
C	1.23357200	2.80131400	-0.25595100
C	0.00872000	3.44217700	-0.10083900
H	0.00536600	4.52632700	-0.11353600
N	0.12689000	-0.00024600	1.89475900
O	-0.55270700	-0.00232200	2.90212500
H	-1.86924400	5.48708900	0.69994100
H	-3.60930300	5.25980700	0.64882400
C	-2.71202900	5.56897500	-1.30262400
H	-1.78442300	5.34558600	-1.84391500
H	-2.84303600	6.65905300	-1.28116700
H	-3.54212100	5.13552000	-1.87405300
H	-5.16202900	3.68792600	0.88691000
H	-5.35633800	1.96663500	1.17084700
C	-5.71898500	2.56911500	-0.88713400
H	-5.37919500	3.32734900	-1.60357700
H	-6.79836200	2.70118700	-0.73428600
H	-5.55507500	1.58472300	-1.34287800
H	-5.16348100	-3.68605900	0.88629800
H	-5.35714900	-1.96474600	1.17053500

C	-5.71983100	-2.56669400	-0.88759000
H	-5.55548600	-1.58227800	-1.34312700
H	-6.79927400	-2.69836600	-0.73486800
H	-5.38027800	-3.32491900	-1.60415500
H	-1.87134100	-5.48639700	0.69962600
H	-3.61131200	-5.25848300	0.64827900
C	-2.71388300	-5.56779600	-1.30307800
H	-3.54372900	-5.13395400	-1.87456800
H	-2.84532000	-6.65782300	-1.28175500
H	-1.78611100	-5.34470800	-1.84420900
H	1.85235600	-5.46427900	-1.03567400
H	3.59500100	-5.24764900	-1.02745000
C	2.75332800	-5.63064200	0.93600500
H	3.60321600	-5.22528600	1.49881000
H	2.87537100	-6.71983600	0.86757300
H	1.84409700	-5.42275500	1.51339000
H	5.14250500	-3.66748700	-1.27118200
H	5.33363900	-1.93548700	-1.48462600
C	5.76873000	-2.63015400	0.52961600
H	5.62277300	-1.66789000	1.03584900
H	6.84159000	-2.75513500	0.33156700
H	5.45375800	-3.42034300	1.22240800
H	5.14378500	3.66576800	-1.27133700
H	5.33436500	1.93368200	-1.48459900
C	5.76968800	2.62841200	0.52957100
H	5.45494100	3.41874100	1.22230300
H	6.84258500	2.75307400	0.33152000
H	5.62345200	1.66622500	1.03586800
H	1.85431100	5.46371100	-1.03581200
H	3.59688200	5.24649600	-1.02747400
C	2.75521400	5.62986900	0.93591500
H	1.84589200	5.42226400	1.51326000
H	2.87756900	6.71902600	0.86744700
H	3.60495600	5.22429700	1.49878500

Table S15. Cartesian coordinates of the fully optimized structure of **1** in conformation E (**1-E**) using BP86/LanL2DZ*.

Fe	-0.03119700	0.00446500	0.26291300
N	-0.71913000	-1.83972200	-0.12225500
N	-1.86905500	0.74735400	-0.21792000
N	0.71368100	1.89522400	0.09844800
N	1.84772700	-0.69672300	0.20339800
C	-0.00367400	-3.02861900	-0.05818100
C	-0.87805600	-4.18465100	-0.21659800
C	-0.43254300	-5.62784900	-0.25299300
C	-2.15980000	-3.68255800	-0.37301000
C	-3.44778700	-4.45480200	-0.54126100
C	-2.04192100	-2.23086900	-0.30480400
C	-3.12793400	-1.36130500	-0.42303500
H	-4.11802100	-1.80732100	-0.57119000
C	-3.04468200	0.03285400	-0.38659200
C	-4.19424300	0.91972700	-0.54046100
C	-5.62606700	0.47646300	-0.72607300
C	-3.69636700	2.21046600	-0.45996400
C	-4.45395600	3.51473200	-0.53697200
C	-2.25538100	2.07812600	-0.26003200
C	-1.38796400	3.16768800	-0.14924200
H	-1.82760900	4.17028100	-0.20201100
C	-0.00195500	3.07904600	0.00240700
C	0.87704900	4.24295500	0.08104600
C	0.43508100	5.68286300	-0.02979900
C	2.16076500	3.74633400	0.24091500
C	3.45670500	4.51402900	0.35012900
C	2.03307800	2.29200500	0.25099800
C	3.11473000	1.41860900	0.39119200
H	4.10896000	1.85978000	0.52545800
C	3.02692900	0.02571700	0.35452100
C	4.18134000	-0.85929200	0.46020100
C	5.61830800	-0.41300100	0.59095300
C	3.68743500	-2.15243400	0.38490500
C	4.45578200	-3.45221200	0.41313000
C	2.24232400	-2.02815100	0.23303500
C	1.37780800	-3.11924400	0.12408200
H	1.81827200	-4.12150800	0.17305900
N	-0.16348900	-0.16955700	1.93548200
O	0.05681500	-0.90741300	2.84290300
H	-1.27917000	-6.27790500	0.04080700
H	0.35839900	-5.80137500	0.50348100
C	0.08617900	-6.07379600	-1.64574100
H	-0.70289600	-5.96302300	-2.41279700
H	0.40454200	-7.13397000	-1.62714400
H	0.94828600	-5.45945000	-1.96557600
H	-3.22340900	-5.45104700	-0.96894100
H	-4.10176300	-3.94910000	-1.27919600
C	-4.22613900	-4.64077900	0.78825600
H	-3.61396200	-5.18950200	1.52804700
H	-5.16104800	-5.20981300	0.62160100
H	-4.49018600	-3.66476800	1.23603800
H	-6.19530100	1.28294700	-1.22870900
H	-5.66809200	-0.39548900	-1.40893200

C	-6.33943900	0.11470200	0.60364500
H	-5.81349100	-0.70335800	1.13016200
H	-7.38153500	-0.20862200	0.41621100
H	-6.36589200	0.98482700	1.28576300
H	-3.87351200	4.25638900	-1.12133700
H	-5.39666200	3.35696900	-1.09658300
C	-4.79181400	4.11608800	0.85331700
H	-5.42694600	3.42403900	1.43704800
H	-5.33446700	5.07513300	0.74642500
H	-3.87460500	4.30128800	1.44270600
H	-0.51294500	5.83253900	0.52434700
H	1.18230600	6.33286100	0.46626400
C	0.24818400	6.16230600	-1.49393700
H	1.19700900	6.08591500	-2.05689900
H	-0.08645000	7.21719700	-1.52343600
H	-0.50239500	5.54611400	-2.02284200
H	3.24456700	5.53272300	0.72973100
H	4.11521000	4.03968300	1.10495500
C	4.22585300	4.63069600	-0.99252600
H	4.47320600	3.63256200	-1.39955600
H	5.17007700	5.19273300	-0.85780300
H	3.61678100	5.15711500	-1.75083900
H	6.20714800	-1.22061300	1.06840200
H	5.68486300	0.45577000	1.27579300
C	6.28073600	-0.04471600	-0.76287200
H	6.28363300	-0.91192100	-1.44925600
H	7.32850800	0.27970200	-0.61291000
H	5.73443300	0.77482100	-1.26573300
H	3.89802000	-4.20899300	1.00004900
H	5.41290000	-3.29728600	0.94850100
C	4.75855900	-4.02492000	-0.99695100
H	3.82621300	-4.20882000	-1.56263800
H	5.31231700	-4.98069300	-0.92334500
H	5.37043900	-3.31688500	-1.58632000

Table S16. Cartesian coordinates of the fully optimized structure of **1** in conformation F (**1-F**) using BP86/LanL2DZ*.

Fe	0.03860600	0.00156600	0.26891100
N	0.88636600	1.81982200	-0.09211100
N	1.82442700	-0.86108500	-0.20603600
N	-0.83661400	-1.79201900	0.06985700
N	-1.76637300	0.87372500	0.20702500
C	0.26473500	3.05857400	-0.06244500
C	1.22877000	4.14512300	-0.20800200
C	0.89327800	5.61663300	-0.27707400
C	2.47182700	3.54408900	-0.31539800
C	3.82142200	4.20969600	-0.45115700
C	2.23559800	2.10481100	-0.24022800
C	3.25122000	1.14962100	-0.33094600
H	4.27859700	1.51424500	-0.44405100
C	3.05479600	-0.23368700	-0.32944400
C	4.13450900	-1.20340700	-0.49709700
C	5.60007600	-0.86834200	-0.64132500
C	3.53638500	-2.45323600	-0.47839200
C	4.18913800	-3.80974400	-0.60003400
C	2.10771100	-2.21474500	-0.29429600
C	1.15223400	-3.23212100	-0.23058100
H	1.50468100	-4.26618800	-0.31688500
C	-0.21959300	-3.03133900	-0.06663700
C	-1.19170300	-4.11693500	-0.00456500
C	-0.87672900	-5.58449900	-0.17209500
C	-2.42631800	-3.52144400	0.20192400
C	-3.77904700	-4.18293000	0.31724100
C	-2.18301200	-2.08417900	0.24579300
C	-3.18941400	-1.13203600	0.42093800
H	-4.21183900	-1.49657600	0.57131600
C	-2.99546600	0.25030200	0.37979400
C	-4.07621600	1.22371900	0.48592700
C	-5.54094700	0.89161200	0.64514400
C	-3.48451100	2.47254800	0.37686400
C	-4.15028000	3.82812500	0.38350400
C	-2.05436900	2.23473200	0.21730400
C	-1.10984500	3.25544200	0.09339400
H	-1.47388100	4.28893900	0.11959800
N	0.06574800	-0.06522300	1.95456500
O	-0.59081400	-0.32600900	2.91235000
H	1.78518700	6.20933200	0.00415600
H	0.11596200	5.86589100	0.47269200
C	0.41007600	6.06777200	-1.68103300
H	1.19111700	5.88505000	-2.44249700
H	0.16627000	7.14768000	-1.68691400
H	-0.49173000	5.50745700	-1.99023600
H	3.69061200	5.21560100	-0.89477300
H	4.45514300	3.64481600	-1.16356900
C	4.57257700	4.34933200	0.89955000
H	3.98438600	4.95396800	1.61480800
H	5.55441500	4.84035300	0.75599800
H	4.74490800	3.36102000	1.36479400
H	6.11959600	-1.71194800	-1.13645800
H	5.72591400	0.00343100	-1.31421500

C	6.30177300	-0.57225100	0.71047400
H	5.82373600	0.27839700	1.23078700
H	7.36991800	-0.32654000	0.55466700
H	6.24352700	-1.44766000	1.38378300
H	3.56512800	-4.47484000	-1.22986000
H	5.15399700	-3.70405600	-1.13355800
C	4.44616700	-4.49876800	0.76642800
H	5.11956600	-3.88706900	1.39521900
H	4.91446200	-5.49188300	0.62463100
H	3.50368000	-4.63798500	1.32807100
H	0.05253300	-5.83860300	0.37614600
H	-1.68060400	-6.18441800	0.29738500
C	-0.72703400	-6.01980400	-1.65398600
H	-1.66289100	-5.83714400	-2.21428900
H	-0.48734000	-7.09825000	-1.72532000
H	0.07745400	-5.45263900	-2.15785100
H	-3.64729900	-5.22202700	0.67751200
H	-4.38690300	-3.66923700	1.08851800
C	-4.57017800	-4.21229100	-1.01728000
H	-4.73569600	-3.19002500	-1.40527500
H	-5.55715800	-4.69452200	-0.87994300
H	-4.01586000	-4.77554800	-1.79087500
H	-6.05946000	1.75181800	1.11206400
H	-5.66164400	0.04527900	1.35041100
C	-6.25005500	0.54542600	-0.69069600
H	-6.20044600	1.39602200	-1.39579000
H	-7.31621500	0.30211800	-0.51854900
H	-5.77337400	-0.32243000	-1.18327200
H	-3.54412700	4.54564600	0.97173200
H	-5.12360600	3.75288200	0.90670800
C	-4.38928500	4.40769600	-1.03569900
H	-3.43756700	4.51907900	-1.58775200
H	-4.87435900	5.40119500	-0.97906600
H	-5.04065900	3.73922500	-1.62881100

Table S17. Cartesian coordinates of the fully optimized structure of **1** in conformation N (**1-N**) using BP86/LanL2DZ*.

Fe	0.02942300	-0.00000100	0.18880200
N	-1.39031200	1.41227100	0.08919600
N	-1.39051000	-1.41203500	0.08921000
N	1.42179000	-1.42126400	-0.25872100
N	1.42201300	1.42108200	-0.25869300
C	-1.21558000	2.79067600	0.02254200
C	-2.48632900	3.49354400	0.15595400
C	-2.66896300	4.99114700	0.08259700
C	-3.45390700	2.51658500	0.33167600
C	-4.94450800	2.69393000	0.49611100
C	-2.75403500	1.23774400	0.28746300
C	-3.39020400	0.00026600	0.40659600
H	-4.47251900	0.00034400	0.57811600
C	-2.75421000	-1.23730300	0.28748700
C	-3.45427000	-2.51603800	0.33170500
C	-4.94489600	-2.69316000	0.49615800
C	-2.48684000	-3.49314400	0.15597500
C	-2.66970600	-4.99071900	0.08262600
C	-1.21599000	-2.79046900	0.02254400
C	0.00963900	-3.43799100	-0.14278800
H	0.00205200	-4.53326000	-0.17408500
C	1.24289500	-2.79527600	-0.27617900
C	2.50767200	-3.49900300	-0.46647600
C	2.67652000	-4.99913300	-0.51768500
C	3.48168500	-2.51805800	-0.56333900
C	4.97018000	-2.69180400	-0.74998400
C	2.78571900	-1.24017700	-0.43161100
C	3.42647600	-0.00023700	-0.49952300
H	4.51290400	-0.00032100	-0.64440200
C	2.78591200	1.23980200	-0.43157900
C	3.48206900	2.51758200	-0.56327200
C	4.97059000	2.69111300	-0.74990400
C	2.50819800	3.49866800	-0.46639400
C	2.67726800	4.99877500	-0.51757300
C	1.24331600	2.79512000	-0.27612700
C	0.01015100	3.43801400	-0.14275500
H	0.00272900	4.53328400	-0.17404100
N	0.07254700	-0.00006900	1.87531800
O	-0.61052800	-0.00051200	2.84997100
H	-1.85868900	5.49997900	0.64228000
H	-3.61152600	5.26727700	0.59452100
C	-2.70714800	5.54324700	-1.36721300
H	-1.77257200	5.30914500	-1.91003200
H	-2.83975500	6.64234100	-1.36565300
H	-3.54270600	5.09649700	-1.93751500
H	-5.14571300	3.69323000	0.92949900
H	-5.33419300	1.96084000	1.23004300
C	-5.73656400	2.55610900	-0.83091300
H	-5.41163700	3.31769500	-1.56401000
H	-6.82215900	2.68600300	-0.65712100
H	-5.57691500	1.56303400	-1.29071000
H	-5.14624400	-3.69241600	0.92958000
H	-5.33446400	-1.95999000	1.23007200

C	-5.73694300	-2.55526200	-0.83086300
H	-5.57716000	-1.56222100	-1.29068600
H	-6.82255500	-2.68500100	-0.65705900
H	-5.41212700	-3.31691200	-1.56394200
H	-1.85951100	-5.49967500	0.64231200
H	-3.61231200	-5.26669800	0.59454900
C	-2.70797600	-5.54282200	-1.36718100
H	-3.54346000	-5.09594300	-1.93748900
H	-2.84075700	-6.64189400	-1.36561300
H	-1.77336100	-5.30887500	-1.90999900
H	1.85306900	-5.45372700	-1.10409900
H	3.60916300	-5.24275900	-1.06340200
C	2.72857000	-5.66469700	0.88322300
H	3.57795300	-5.27343900	1.47339500
H	2.84710300	-6.76179300	0.79359600
H	1.80521300	-5.46273600	1.45727100
H	5.16426000	-3.66164600	-1.24888900
H	5.35904400	-1.91391400	-1.43681200
C	5.77011800	-2.64286600	0.57867600
H	5.61534300	-1.68158200	1.10306900
H	6.85440800	-2.76382200	0.39072900
H	5.44689700	-3.44960800	1.26264800
H	5.16481500	3.66091300	-1.24883300
H	5.35935300	1.91314900	-1.43670500
C	5.77050700	2.64210000	0.57876600
H	5.44738100	3.44889700	1.26271900
H	6.85481500	2.76291400	0.39082900
H	5.61560600	1.68084600	1.10317800
H	1.85392700	5.45349500	-1.10404500
H	3.60998700	5.24226900	-1.06321600
C	2.72931000	5.66432000	0.88334500
H	1.80588000	5.46249100	1.45732200
H	2.84801200	6.76139800	0.79373500
H	3.57859000	5.27293100	1.47357900

Table S18. Polarization functions applied for the LanL2DZ* basis set. See refs:
(a) Praneeth, V. K. K.; Neese, F.; Lehnert, N. *Inorg. Chem.* **2005**, *44*, 2570-2572.
(b) Praneeth, V. K. K.; Näther, C.; Peters, G.; Lehnert, N. *Inorg. Chem.* **2006**, *45*, 2795-2811.

```
Fe 0
F    1 1.00
 0.1050000000D+01  0.1000000000D+01
****
O 0
D    1 1.00
 0.1292000000D+01  0.1000000000D+01
****
C 0
D    1 1.00
 0.6260000000D+00  0.1000000000D+01
****
N 0
D    1 1.00
 0.9130000000D+00  0.1000000000D+01
****
```

Table S19. Complete force field of [Fe(OEP)(NO)] used for the QCC-NCA simulation. The definition of the internal coordinates follows the usual terminology where type 1 is a bond stretch, 2 an in-plane angle bend, 3 an out-of-plane bend, 4 a torsion, and 6 a linear bend. The atomic numbering scheme corresponds to the structures provided in Tables S3 – S17.

```
[Fe(OEP)(NO)] BP86/LanL2DZ*
   0   0   0
   1   1  38                                R:Fe-N(O)
   1  38  39                                R:N-O
   1   1   2                                R:Fe-N2
   1   1   3                                R:Fe-N3
   1   1   4                                R:Fe-N4
   1   1   5                                R:Fe-N5
   1   2   6                                R:N2-C6
   1   2  11                                R:N2-C11
   1   3  14                                R:N3-C14
   1   3  19                                R:N3-C19
   1   4  22                                R:N4-C22
   1   4  27                                R:N4-C27
   1   5  30                                R:N5-C30
   1   5  35                                R:N5-C35
   1   6   7                                R:C6-C7
   1   7   9                                R:C7-C9
   1   9  11                                R:C9-C11
   1  14  15                                R:C14-C15
   1  15  17                                R:C15-C17
   1  17  19                                R:C17-C19
   1  22  23                                R:C22-C23
   1  23  25                                R:C23-C25
   1  25  27                                R:C25-C27
   1  30  31                                R:C30-C31
   1  31  33                                R:C31-C33
   1  33  35                                R:C33-C35
   1  11  12                                R:C11-M12
   1  12  14                                R:M12-C14
   1  19  20                                R:C19-M20
   1  20  22                                R:M20-C22
   1  27  28                                R:C27-M28
   1  28  30                                R:M28-C30
   1  35  36                                R:C35-M36
   1  36   6                                R:M36-C6
   1  12  13                                R:M12-H
   1  20  21                                R:M20-H
   1  28  29                                R:M28-H
   1  36  37                                R:M36-H
   1   7   8                                R:C7-C8
   1   9  10                                R:C9-C10
   1  15  16                                R:C15-C16
   1  17  18                                R:C17-C18
   1  23  24                                R:C23-C24
   1  25  26                                R:C25-C26
   1  31  32                                R:C31-C32
   1  33  34                                R:C33-C34
   2   1  38  39                            a:Fe-N-O
```

```
2  38   1   2                    a1:N(O)-Fe-N2
2  38   1   3                    a1:N(O)-Fe-N3
2  38   1   4                    a1:N(O)-Fe-N4
2  38   1   5                    a1:N(O)-Fe-N5
2   2   1   3                    a1:N2-Fe-N3
2   3   1   4                    a1:N3-Fe-N4
2   4   1   5                    a1:N4-Fe-N5
2   5   1   2                    a1:N5-Fe-N2
2   1   2   6                    a2:Fe-N2-C6
2   2   6   7                    a2:N2-C6-C7
2   6   7   9                    a2:C6-C7-C9
2   7   9  11                    a2:C7-C9-C11
2   9  11   2                    a2:C9-C11-N2
2  11   2   1                    a2:C11-N2-Fe
2   1   3  14                    a2:Fe-N3-C14
2   3  14  15                    a2:N3-C14-C15
2  14  15  17                    a2:C14-C15-C17
2  15  17  19                    a2:C15-C17-C19
2  17  19   3                    a2:C17-C19-N3
2  19   3   1                    a2:C19-N3-Fe
2   1   4  22                    a2:Fe-N4-C22
2   4  22  23                    a2:N4-C22-C23
2  22  23  25                    a2:C22-C23-C25
2  23  25  27                    a2:C23-C25-C27
2  25  27   4                    a2:C25-C27-N4
2  27   4   1                    a2:C27-N4-Fe
2   1   5  30                    a2:Fe-N5-C30
2   5  30  31                    a2:N5-C30-C31
2  30  31  33                    a2:C30-C31-C33
2  31  33  35                    a2:C31-C33-C35
2  33  35   5                    a2:C33-C35-N5
2  35   5   1                    a2:C35-N5-Fe
2  11  12  14                    a3:C11-M12-C14
2  19  20  22                    a3:C19-M20-C22
2  27  28  30                    a3:C27-M28-C30
2  35  36   6                    a3:C35-M36-C6
2   6   7   8                    a4:C6-C7-H
2   9   7   8                    a4:C9-C7-H
2   7   9  10                    a4:C7-C9-H
2  11   9  10                    a4:C11-C9-H
2  14  15  16                    a4:C14-C15-H
2  17  15  16                    a4:C17-C15-H
2  15  17  18                    a4:C15-C17-H
2  19  17  18                    a4:C19-C17-H
2  22  23  24                    a4:C22-C23-H
2  25  23  24                    a4:C25-C23-H
2  23  25  26                    a4:C23-C25-H
2  27  25  26                    a4:C27-C25-H
2  30  31  32                    a4:C30-C31-H
2  33  31  32                    a4:C33-C31-H
2  31  33  34                    a4:C31-C33-H
2  35  33  34                    a4:C35-C33-H
2  11  12  13                    a5:C11-M12-H
2  14  12  13                    a5:C14-M12-H
2  19  20  21                    a5:C19-M20-H
2  22  20  21                    a5:C22-M20-H
2  27  28  29                    a5:C27-M28-H
```

```
 2  30  28  29                    a5:C30-M28-H
 2  35  36  37                    a5:C35-M36-H
 2   6  36  37                    a5:C6-M36-H
 3   1   2   6  11                g:Pyrr
 3  36   6   7   2                g:Pyrr
 3   8   7   9   6                g:Pyrr
 3  10   9  11   7                g:Pyrr
 3  12  11   2   9                g:Pyrr
 3   1   3  14  19                g:Pyrr
 3  12  14  15   3                g:Pyrr
 3  16  15  17  14                g:Pyrr
 3  18  17  19  15                g:Pyrr
 3  20  19   3  17                g:Pyrr
 3   1   4  22  27                g:Pyrr
 3  20  22  23   4                g:Pyrr
 3  24  23  25  22                g:Pyrr
 3  26  25  27  23                g:Pyrr
 3  28  27   4  25                g:Pyrr
 3   1   5  30  35                g:Pyrr
 3  28  30  31   5                g:Pyrr
 3  32  31  33  30                g:Pyrr
 3  34  33  35  31                g:Pyrr
 3  36  35   5  33                g:Pyrr
 3  13  12  14  11                g:Meth
 3  21  20  22  19                g:Meth
 3  29  28  30  27                g:Meth
 3  37  36   6  35                g:Meth
 4   4   1  38   1                t:Fe-N(O)
 2   3   4   5
39
 4   2   2   6   2                t:N-C
 1  11
 7  36
 4   2   6   7   2                t:C-C(H)
 2  36
 8   9
 4   2   7   9   2                t:(H)C-C(H)
 6   8
10  11
 4   2   9  11   2                t:C(H)-C
 7  10
 2  12
 4   2  11   2   2                t:C-N
 9  12
 1   6
 4   2   3  14   2                t:N-C
 1  19
12  15
 4   2  14  15   2                t:C-C(H)
 3  12
16  17
 4   2  15  17   2                t:(H)C-C(H)
14  16
18  19
 4   2  17  19   2                t:C(H)-C
15  18
 3  20
```

```
 4   2  19   3   2                    t:C-N
17  20
 1  14
 4   2   4  22   2                    t:N-C
 1  27
20  23
 4   2  22  23   2                    t:C-C(H)
 4  20
24  25
 4   2  23  25   2                    t:(H)C-C(H)
22  24
26  27
 4   2  25  27   2                    t:C(H)-C
23  26
 4  28
 4   2  27   4   2                    t:C-N
25  28
 1  22
 4   2   5  30   2                    t:N-C
 1  35
28  31
 4   2  30  31   2                    t:C-C(H)
 5  28
32  33
 4   2  31  33   2                    t:(H)C-C(H)
30  32
34  35
 4   2  33  35   2                    t:C(H)-C
31  34
 5  36
 4   2  35   5   2                    t:C-N
33  36
 1  30
 4   2  11  12   2                    t:(H)C-M(H)
 2   9
13  14
 4   2  12  14   2                    t:(H)M-C(H)
11  13
 3  15
 4   2  19  20   2                    t:(H)C-M(H)
 3  17
21  22
 4   2  20  22   2                    t:(H)M-C(H)
19  21
 4  23
 4   2  27  28   2                    t:(H)C-M(H)
 4  25
29  30
 4   2  28  30   2                    t:(H)M-C(H)
27  29
 5  31
 4   2  35  36   2                    t:(H)C-M(H)
 5  33
 6  37
 4   2  36   6   2                    t:(H)M-C(H)
35  37
 2   7
```

```
1   8  40                    R:C8-H
1   8  41                    R:C8-H
1   8  42                    R:C8-C42
1  42  43                    R:C42-H
1  42  44                    R:C42-H
1  42  45                    R:C42-H
1  10  46                    R:C10-H
1  10  47                    R:C10-H
1  10  48                    R:C10-C48
1  48  49                    R:C48-H
1  48  50                    R:C48-H
1  48  51                    R:C48-H
1  16  52                    R:C16-H
1  16  53                    R:C16-H
1  16  54                    R:C16-C54
1  54  55                    R:C54-H
1  54  56                    R:C54-H
1  54  57                    R:C54-H
1  18  58                    R:C18-H
1  18  59                    R:C18-H
1  18  60                    R:C18-C60
1  60  61                    R:C60-H
1  60  62                    R:C60-H
1  60  63                    R:C60-H
1  24  64                    R:C24-H
1  24  65                    R:C24-H
1  24  66                    R:C24-C66
1  66  67                    R:C66-H
1  66  68                    R:C66-H
1  66  69                    R:C66-H
1  26  70                    R:C26-H
1  26  71                    R:C26-H
1  26  72                    R:C26-C72
1  72  73                    R:C72-H
1  72  74                    R:C72-H
1  72  75                    R:C72-H
1  32  76                    R:C32-H
1  32  77                    R:C32-H
1  32  78                    R:C32-C78
1  78  79                    R:C78-H
1  78  80                    R:C78-H
1  78  81                    R:C78-H
1  34  82                    R:C34-H
1  34  83                    R:C34-H
1  34  84                    R:C34-C84
1  84  85                    R:C84-H
1  84  86                    R:C84-H
1  84  87                    R:C84-H
2   7   8  40                A6:C7-C8-H
2   7   8  41                a6:C7-C8-H
2   7   8  42                a6:C7-C8-C42
2  40   8  42                a6:H-C8-C42*
2  41   8  42                a6:H-C8-C42*
2   8  42  43                a6:C8-C42-H
2   8  42  44                a6:C8-C42-H
2   8  42  45                a6:C8-C42-H
2  43  42  44                a6:H-C42-H
```

```
2  43  42  45                a6:H-C42-H
2  44  42  45                a6:H-C42-H
2   9  10  46                A6:C9-C10-H
2   9  10  47                a6:C9-C10-H
2   9  10  48                a6:C9-C10-C48
2  46  10  48                a6:H-C10-C48*
2  47  10  48                a6:H-C10-C48*
2  10  48  49                a6:C10-C48-H
2  10  48  50                a6:C10-C48-H
2  10  48  51                a6:C10-C48-H
2  49  48  50                a6:H-C48-H
2  49  48  51                a6:H-C48-H
2  50  48  51                a6:H-C48-H
2  15  16  52                A6:C15-C16-H
2  15  16  53                a6:C15-C16-H
2  15  16  54                a6:C15-C16-C54
2  52  16  54                a6:H-C16-C54*
2  53  16  54                a6:H-C16-C54*
2  16  54  55                a6:C16-C54-H
2  16  54  56                a6:C16-C54-H
2  16  54  57                a6:C16-C54-H
2  55  54  56                a6:H-C54-H
2  55  54  57                a6:H-C54-H
2  56  54  57                a6:H-C54-H
2  17  18  58                A6:C17-C18-H
2  17  18  59                a6:C17-C18-H
2  17  18  60                a6:C17-C18-C60
2  58  18  60                a6:H-C18-C60*
2  59  18  60                a6:H-C18-C60*
2  18  60  61                a6:C18-C60-H
2  18  60  62                a6:C18-C60-H
2  18  60  63                a6:C18-C60-H
2  61  60  62                a6:H-C60-H
2  61  60  63                a6:H-C60-H
2  62  60  63                a6:H-C60-H
2  23  24  64                A6:C23-C24-H
2  23  24  65                a6:C23-C24-H
2  23  24  66                a6:C23-C24-C66
2  64  24  66                a6:H-C24-C66*
2  65  24  66                a6:H-C24-C66*
2  24  66  67                a6:C24-C66-H
2  24  66  68                a6:C24-C66-H
2  24  66  69                a6:C24-C66-H
2  67  66  68                a6:H-C66-H
2  67  66  69                a6:H-C66-H
2  68  66  69                a6:H-C66-H
2  25  26  70                A6:C25-C26-H
2  25  26  71                a6:C25-C26-H
2  25  26  72                a6:C25-C26-C72
2  70  26  72                a6:H-C26-C72*
2  71  26  72                a6:H-C26-C72*
2  26  72  73                a6:C26-C72-H
2  26  72  74                a6:C26-C72-H
2  26  72  75                a6:C26-C72-H
2  73  72  74                a6:H-C72-H
2  73  72  75                a6:H-C72-H
2  74  72  75                a6:H-C72-H
```

```
 2  31  32  76                    A6:C31-C32-H
 2  31  32  77                    a6:C31-C32-H
 2  31  32  78                    a6:C31-C32-C78
 2  76  32  78                    a6:H-C32-C78*
 2  77  32  78                    a6:H-C32-C78*
 2  32  78  79                    a6:C32-C78-H
 2  32  78  80                    a6:C32-C78-H
 2  32  78  81                    a6:C32-C78-H
 2  79  78  80                    a6:H-C78-H
 2  79  78  81                    a6:H-C78-H
 2  80  78  81                    a6:H-C78-H
 2  33  34  82                    A6:C33-C34-H
 2  33  34  83                    a6:C33-C34-H
 2  33  34  84                    a6:C33-C34-C84
 2  82  34  84                    a6:H-C34-C84*
 2  83  34  84                    a6:H-C34-C84*
 2  34  84  85                    a6:C34-C84-H
 2  34  84  86                    a6:C34-C84-H
 2  34  84  87                    a6:C34-C84-H
 2  85  84  86                    a6:H-C84-H
 2  85  84  87                    a6:H-C84-H
 2  86  84  87                    a6:H-C84-H
 4   2   7   8   3                T:C-Et
 6   9
40  41  42
 4   3   8  42   3                t:Et-Et
 7  40  41
43  44  45
 4   2   9  10   3                t:C-Et
 7  11
46  47  48
 4   3  10  48   3                t:Et-Et
 9  46  47
49  50  51
 4   2  15  16   3                T:C-Et
14  17
52  53  54
 4   3  16  54   3                t:Et-Et
15  52  53
55  56  57
 4   2  17  18   3                t:C-Et
15  19
58  59  60
 4   3  18  60   3                t:Et-Et
17  58  59
61  62  63
 4   2  23  24   3                T:C-Et
22  25
64  65  66
 4   3  24  66   3                t:Et-Et
23  64  65
67  68  69
 4   2  25  26   3                t:C-Et
23  27
70  71  72
 4   3  26  72   3                t:Et-Et
25  70  71
```

```
73  74  75
 4   2  31  32   3                    T:C-Et
30  33
76  77  78
 4   3  32  78   3                    t:Et-Et
31  76  77
79  80  81
 4   2  33  34   3                    t:C-Et
31  35
82  83  84
 4   3  34  84   3                    t:Et-Et
33  82  83
85  86  87
```

Table S20. Cartesian coordinates of the fully optimized structure of [Fe(P)(NO)] (P = porphine^{2-}) using BP86/LanL2DZ*.

Fe	-0.02494400	0.00042600	0.07906100
N	-1.33674300	1.53898100	-0.15804700
N	-1.58485000	-1.29163600	-0.14957700
N	1.23529100	-1.52988600	-0.22741900
N	1.47990500	1.28528800	-0.22947600
C	-1.04314900	2.89392100	-0.19833600
C	-2.25563500	3.69236100	-0.20441000
H	-2.28231800	4.78626200	-0.24380700
C	-3.30728200	2.80310000	-0.16030900
H	-4.38240600	3.01071900	-0.15708000
C	-2.72260200	1.47405400	-0.13061900
C	-3.48002200	0.29940400	-0.09768300
H	-4.57270900	0.39539200	-0.07555700
C	-2.93829900	-0.98930200	-0.12291000
C	-3.74340400	-2.19779300	-0.14609100
H	-4.83819500	-2.21760300	-0.14161400
C	-2.86044700	-3.25497200	-0.18682900
H	-3.07489400	-4.32815300	-0.22189400
C	-1.52858100	-2.67690100	-0.18504600
C	-0.35367400	-3.43396200	-0.22388600
H	-0.44625900	-4.52687500	-0.24639400
C	0.93198700	-2.88776100	-0.24978400
C	2.14086100	-3.68663400	-0.31597500
H	2.16134200	-4.78057400	-0.35722500
C	3.19784600	-2.80227800	-0.32102900
H	4.27081200	-3.01499700	-0.36905000
C	2.62326600	-1.47178100	-0.26295400
C	3.38243900	-0.29861600	-0.26396100
H	4.47495200	-0.39363200	-0.28972900
C	2.83728700	0.98796300	-0.26352900
C	3.63303200	2.19875800	-0.32441800
H	4.72665700	2.22278300	-0.37119700
C	2.74498200	3.25276500	-0.32381600
H	2.95429200	4.32655500	-0.36870800
C	1.41628300	2.67550500	-0.25725000
C	0.24479900	3.43643900	-0.23673100
H	0.34291500	4.52875900	-0.26321400
N	0.18324200	-0.00575700	1.75452900
O	0.99478700	-0.01053300	2.62165200

Table S21. Cartesian coordinates of the fully optimized structure of [Fe(P)(NO)] (P = porphine^{2-}) using BP86/6-31G*.

Fe	0.02580900	0.00001300	0.07366400
N	1.46324000	-1.40611300	-0.14735400
N	1.45115600	1.41814800	-0.14775400
N	-1.36055100	1.39881800	-0.23007200
N	-1.34863500	-1.41070900	-0.22998300
C	1.29768100	-2.78203900	-0.21236700
C	2.57433200	-3.46091100	-0.21155600
H	2.70020200	-4.54369100	-0.26579600
C	3.53440700	-2.48699100	-0.13688900
H	4.62021500	-2.59649000	-0.11916600
C	2.83750500	-1.22012500	-0.09953800
C	3.47898500	0.01460400	-0.05538800
H	4.57296300	0.01931400	-0.01732900
C	2.82697800	1.24378900	-0.09995700
C	3.51312900	2.51650300	-0.13773000
H	4.59797300	2.63518300	-0.12011700
C	2.54485200	3.48224500	-0.21258700
H	2.66154000	4.56604000	-0.26711700
C	1.27399400	2.79261300	-0.21309500
C	0.04025600	3.43464900	-0.27157400
H	0.03390000	4.52836000	-0.31476300
C	-1.18652700	2.77887400	-0.27785100
C	-2.46062600	3.45746300	-0.33487900
H	-2.58096600	4.54069400	-0.39213800
C	-3.42672900	2.48688100	-0.30348100
H	-4.51177000	2.60046500	-0.33288100
C	-2.73853800	1.21834500	-0.23796700
C	-3.38303800	-0.01455100	-0.22138000
H	-4.47748900	-0.01920800	-0.22684900
C	-2.72809800	-1.24193600	-0.23807700
C	-3.40549400	-2.51628900	-0.30357400
H	-4.48952500	-2.63909800	-0.33313200
C	-2.43117100	-3.47862100	-0.33467600
H	-2.54227400	-4.56284700	-0.39179900
C	-1.16288800	-2.78921600	-0.27752300
C	0.06943200	-3.43452500	-0.27090200
H	0.07241100	-4.52826100	-0.31387700
N	-0.17747800	-0.00029800	1.74738100
O	-0.99162400	-0.00053500	2.61751600

Table S22. Cartesian coordinates of the fully optimized structure of [Fe(P)(NO)] (P = porphine^{2-}) using BP86/6-311G*.

Fe	0.02671300	-0.00000700	0.06803600
N	1.46129700	-1.41542900	-0.14718200
N	1.46083700	1.41590400	-0.14721900
N	-1.35946700	1.40837100	-0.22614800
N	-1.35901700	-1.40878600	-0.22623300
C	1.28591600	-2.78699200	-0.21299800
C	2.55972600	-3.46887600	-0.21119300
H	2.68605800	-4.55036600	-0.26573200
C	3.52181800	-2.50107200	-0.13572600
H	4.60539300	-2.62010200	-0.11759400
C	2.83256400	-1.23127300	-0.09829000
C	3.47624400	0.00056000	-0.05469800
H	4.56907900	0.00073900	-0.01656800
C	2.83216600	1.23218300	-0.09836600
C	3.52102000	2.50219500	-0.13589100
H	4.60455700	2.62156700	-0.11779700
C	2.55862200	3.46969200	-0.21138600
H	2.68461300	4.55121900	-0.26598800
C	1.28502600	2.78740900	-0.21309100
C	0.05401600	3.43128600	-0.27194100
H	0.05216800	4.52379100	-0.31695500
C	-1.17547300	2.78366100	-0.27743200
C	-2.44662100	3.46530200	-0.33535400
H	-2.56720400	4.54716900	-0.39455200
C	-3.41493100	2.50098400	-0.30219100
H	-4.49770900	2.62404400	-0.33163200
C	-2.73455500	1.22969100	-0.23405900
C	-3.38102900	-0.00053000	-0.21767000
H	-4.47433100	-0.00070400	-0.22339800
C	-2.73416200	-1.23054300	-0.23418700
C	-3.41412900	-2.50204900	-0.30241200
H	-4.49686600	-2.62545300	-0.33191500
C	-2.44551100	-3.46605900	-0.33555400
H	-2.56575300	-4.54796100	-0.39479000
C	-1.17458300	-2.78401900	-0.27753700
C	0.05511200	-3.43125400	-0.27193800
H	0.05361100	-4.52376000	-0.31693200
N	-0.17747400	-0.00006200	1.75105200
O	-0.98735300	-0.00022000	2.61081500

Table S23. Cartesian coordinates of the fully optimized structure of [Fe(P)(NO)] (P = porphine^{2-}) using BP86/TZVP [Praneeth, V. K. K.; Neese, F.; Lehnert, N. *Inorg. Chem.* **2005**, *44*, 2570-2572].

Fe	0.026411	0.000294	0.089784
N	1.527839	-1.350679	-0.151542
N	1.396344	1.482247	-0.156643
N	-1.425869	1.344832	-0.228134
N	-1.295755	-1.474373	-0.228719
C	1.411306	-2.726598	-0.192501
C	2.714102	-3.347471	-0.198612
H	2.888498	-4.420646	-0.240291
C	3.630278	-2.337557	-0.153917
H	4.716196	-2.406448	-0.152167
C	2.886439	-1.100745	-0.122699
C	3.469589	0.158665	-0.094830
H	4.559729	0.209277	-0.074378
C	2.772426	1.358518	-0.129018
C	3.399025	2.658467	-0.167089
H	4.473955	2.827074	-0.167316
C	2.393668	3.579522	-0.213479
H	2.468368	4.664066	-0.259043
C	1.153552	2.841580	-0.201526
C	-0.105227	3.425117	-0.241807
H	-0.157483	4.514808	-0.274638
C	-1.302561	2.724893	-0.260280
C	-2.602325	3.344888	-0.331891
H	-2.771827	4.418406	-0.382830
C	-3.523004	2.337884	-0.330065
H	-4.607490	2.410290	-0.379269
C	-2.787792	1.099563	-0.260552
C	-3.373526	-0.158055	-0.258386
H	-4.463323	-0.208309	-0.286925
C	-2.674249	-1.356335	-0.261935
C	-3.291736	-2.657450	-0.332311
H	-4.364793	-2.829986	-0.382293
C	-2.281741	-3.574786	-0.333425
H	-2.350951	-4.659423	-0.384412
C	-1.045066	-2.836960	-0.260039
C	0.211688	-3.423588	-0.236502
H	0.260060	-4.513520	-0.267566
N	-0.187524	-0.003513	1.780776
O	-0.971492	-0.007520	2.661471

Table S24. Cartesian coordinates of the fully optimized structure of [Fe(P)(NO)] (P = porphine^{2-}) using B3LYP/LanL2DZ [Praneeth, V. K. K.; Näther, C.; Peters, G.; Lehnert, N. *Inorg. Chem.* **2006**, *45*, 2795-2811].

Fe	0.022853	0.054551	0.017189
N	0.031498	0.032574	2.041022
N	2.050535	0.026275	0.042678
N	0.070533	-0.391838	-1.945225
N	-1.941365	-0.380679	0.048056
C	-1.076066	-0.018100	2.887738
C	-0.663549	0.133866	4.271680
H	-1.337353	0.122381	5.118213
C	0.702331	0.281578	4.266932
H	1.368630	0.414587	5.109108
C	1.130085	0.219063	2.880230
C	2.456630	0.317558	2.469179
H	3.213737	0.466005	3.233615
C	2.880801	0.214567	1.146897
C	4.271372	0.272222	0.731102
H	5.108391	0.406011	1.403697
C	4.287080	0.118712	-0.634232
H	5.139247	0.102034	-1.300842
C	2.905972	-0.031813	-1.057207
C	2.507770	-0.218093	-2.378379
H	3.279072	-0.241291	-3.142621
C	1.187855	-0.393275	-2.784133
C	0.784070	-0.618628	-4.159997
H	1.466246	-0.670549	-4.998261
C	-0.583683	-0.748931	-4.160939
H	-1.242748	-0.929230	-4.999907
C	-1.023632	-0.605863	-2.785320
C	-2.351606	-0.689788	-2.376559
H	-3.107444	-0.855833	-3.138379
C	-2.772398	-0.595560	-1.053016
C	-4.152554	-0.729780	-0.625544
H	-4.986410	-0.907664	-1.291697
C	-4.163799	-0.594456	0.741809
H	-5.008672	-0.639723	1.416280
C	-2.790853	-0.374718	1.157353
C	-2.395047	-0.198457	2.480102
H	-3.164944	-0.215786	3.245869
N	-0.245339	1.755700	-0.247210
O	-0.962388	2.542673	-0.826440

Table S25. Cartesian coordinates of the fully optimized structure of [Fe(P)(NO)] (P = porphine^{2-}) using B3LYP/LanL2DZ*.

Fe	-0.02934000	0.00147800	0.05991800
N	-1.26771600	1.59657600	-0.15172100
N	-1.63935900	-1.22408100	-0.14705100
N	1.17140500	-1.58610800	-0.21644300
N	1.53918900	1.22241100	-0.22281900
C	-0.91127400	2.92652500	-0.18501400
C	-2.08512300	3.77359300	-0.19425000
H	-2.06626800	4.85940800	-0.22754700
C	-3.16798700	2.93660100	-0.16319300
H	-4.22417200	3.19170600	-0.16599200
C	-2.64527200	1.58646300	-0.13593500
C	-3.44665700	0.44771200	-0.11308800
H	-4.52572100	0.58989700	-0.10065100
C	-2.96738700	-0.85993200	-0.13180000
C	-3.82047900	-2.02982400	-0.15373400
H	-4.90673000	-2.00492400	-0.15555900
C	-2.98944200	-3.11753300	-0.18092400
H	-3.25054200	-4.17182900	-0.20969200
C	-1.63715700	-2.60081600	-0.17461900
C	-0.49802200	-3.40183300	-0.20378000
H	-0.63678700	-4.48122400	-0.22044800
C	0.80681200	-2.91787400	-0.23214300
C	1.97727300	-3.76535500	-0.29841700
H	1.95340200	-4.85105500	-0.33182200
C	3.06384400	-2.93244200	-0.31651400
H	4.11766700	-3.19160100	-0.36910600
C	2.54962300	-1.58143600	-0.26304400
C	3.35230500	-0.44398100	-0.27450100
H	4.43081800	-0.58519300	-0.30981700
C	2.86975300	0.86193200	-0.26833600
C	3.71503600	2.03398800	-0.32737700
H	4.80004800	2.01243800	-0.37949400
C	2.88035000	3.11943100	-0.31374200
H	3.13739600	4.17440500	-0.35175200
C	1.53112800	2.60322700	-0.24456700
C	0.39539800	3.40740700	-0.21799400
H	0.53887000	4.48607200	-0.23940600
N	0.15397900	-0.01144800	1.76174300
O	0.98200500	-0.04038400	2.58691200

Table S26. Cartesian coordinates of the fully optimized structure of [Fe(P)(NO)] (P = porphine^{2-}) using B3LYP/TZVP.

Fe	0.02828500	0.00051600	0.08013300
N	1.66199200	-1.19352900	-0.14426000
N	1.23858000	1.61545100	-0.15390700
N	-1.55868000	1.18940700	-0.22626300
N	-1.14008000	-1.60794500	-0.21802200
C	1.68050800	-2.56372000	-0.18974600
C	3.03723400	-3.04653700	-0.19459700
H	3.32002000	-4.08707400	-0.23655200
C	3.84038500	-1.95508400	-0.14495300
H	4.91873700	-1.91526400	-0.13857600
C	2.97613900	-0.80324500	-0.11367800
C	3.42111300	0.50658300	-0.08603800
H	4.49134700	0.66808300	-0.06352600
C	2.61024800	1.62673100	-0.12251600
C	3.09901200	2.98106300	-0.16306000
H	4.14193100	3.25813500	-0.15826000
C	2.01183800	3.78931800	-0.21870100
H	1.97795100	4.86674200	-0.26757600
C	0.85564000	2.93111500	-0.20830600
C	-0.45290600	3.37761500	-0.25582500
H	-0.61498700	4.44712400	-0.29578700
C	-1.57065400	2.56408000	-0.26999000
C	-2.92427500	3.04562700	-0.34113300
H	-3.20264500	4.08669500	-0.39640000
C	-3.73198800	1.95615900	-0.32927000
H	-4.80949900	1.91937400	-0.37370400
C	-2.87614900	0.80231300	-0.25604800
C	-3.32520100	-0.50572600	-0.24997200
H	-4.39535900	-0.66585200	-0.27566100
C	-2.51272600	-1.62489500	-0.24990300
C	-2.99222200	-2.98001600	-0.31524100
H	-4.03298400	-3.26132300	-0.36051500
C	-1.90016300	-3.78398300	-0.31948800
H	-1.86048500	-4.86124400	-0.36729400
C	-0.74747800	-2.92527100	-0.25178100
C	0.55998300	-3.37431400	-0.23308900
H	0.71875400	-4.44461500	-0.26576100
N	-0.17421100	-0.00937700	1.78629100
O	-0.99142300	-0.01114000	2.61116200