Supporting Information for:

NMR, IR/Raman, and Structural Properties in HNO and RNO (R = alkyl and aryl) Metalloporphyrins with Implication for the HNO-myoglobin Complex

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We first investigated HNO to see for this small molecule how well we can improve over the previous predictions of the geometric structures and vibrational frequencies,[37] which will build a basis for subsequent calculations for synthetic HNO metal complexes. Compared to the experimental results,[80, 81] although the NO and NH bond lengths from using the hybrid DFT method B3LYP with a 6-311G(2d,2p) basis in the previous work are acceptable,[37] the predicted NO and HNO vibrational frequencies are of too large errors: 90 and 73 cm^{-1}, respectively. We evaluated the B3LYP calculations with some other basis sets and found that using the larger basis set in particular the diffuse functions can improve the frequency results, see Table S1. However, this improvement is insignificant, in contrast to the use of the pure DFT

method BLYP, which can have errors close to 10 cm^{-1} even with the 6-311G(2d,2p) basis,[37] Table 1. We then used another hybrid method mPW1PW91 which contains more HF exchange component compared to B3LYP to examine the effect of HF exchange on such kind of calculations. As shown in Table S1, results are even worse, e.g. the errors in ν_{NO} predictions are 143-170 cm^{-1}. These results suggest that the methods with less or no HF exchange may perform better in the investigation of HNO vibrations.

Indeed, with pure DFT methods, some better predictions of ν_{NO} and ν_{HNO} were achieved with errors of 2-8 cm^{-1} (see Table S1), even using the 6-311G(2d,2p) basis. Among all 74 different methods used in this work (see Table S1 for details), a new pure DFT method mPWVWN with a 6-311++G(2d,2p) basis produces the best predictions with only 1 and 0 cm^{-1} errors for ν_{NO} and ν_{HNO}, and 0.006 Å deviations for both NO and NH bond lengths.

Based on above calculations, the mPWVWN method was then used in geometry optimizations and frequency calculations of all HNO, RNO, and NO heme model complexes investigated here (**2**-7, **9**-**13**), with the 6-311++G(2d,2p) basis for HNO and the first coordination shell atoms, while the rest atoms were treated with a 6-31G(d) basis for computational efficiency. For calculations of the proton NMR chemical shifts, δ_H, in the HNO moieties of the HNO metal complexes, we used the method that previously yielded excellent predictions of ^{1}H NMR shifts in various metal-containing systems,[82] i.e., the B3LYP functional with a 6-311++G(2d,2p) basis for HNO and the first coordination shell atoms and a 6-31G(d) basis for the rest atoms.

We first investigated the only HNO heme model complex reported to date, Ru(TTP)(HNO)(1-MeIm) (**2**). As shown in Table S2, the use of different metal bases (SDD, CEP-121G, DGDZVP) can result in 15 cm^{-1} and 1.06 ppm differences in the predicted ν_{NO} and δ_H values, respectively. By using the all electron basis DGDZVP for Ru, the deviations from experimental ν_{NO} and δ_H data[33] are only 2 cm^{-1} and 0.46 ppm. To further examine this method, we then performed calculations of Ru(HNO)('py^{bu}S$_4$') (**3**), which compared to other known HNO metal complexes characterized by IR and NMR techniques[24-29, 31, 32] is closest to a heme model environment by having a relatively rigid ligand set in the equatorial plane and a nitrogen-coordinated ligand in the axial position. As shown in Table 2, the predicted values of 1370 cm^{-1} and 19.98 ppm are in good agreement with experimental results of 1358 cm^{-1} and 19.56 ppm.[30] The gas phase ν_{NO} prediction error (12 cm^{-1}) here is much smaller compared to the error of 155 cm^{-1} in the previous work.[30] Therefore, the all electron basis DGDZVP was chosen for Ru.

Based on above calculations, we used an all electron basis – Wachters' basis for iron in the geometry optimizations and frequencies calculations for HNO and RNO iron porphyrin complexes. The use of Wachters' basis for iron previously enabled excellent predictions of several spectroscopic properties in heme proteins and models.[42, 44-46, 52] As seen from Figure 1, the basic difference between the two RNO heme model molecules **4** and **5** is the orientation of the 1-MeIm ligand, while the ^{i}PrNO ligand orientations are essentially the same. These experimental structural features[35] were retained in the optimized structures. Moreover, the optimized key geometric parameters (NO bond length, R_{NO}; metal-NO bond length, R_{MN}; metal-NO bond angle, ∠M-N-O) are also in good accord with experimental observations, see Table 2. For example, the average error in NO bond length is 0.01 Å and that for Fe-N-O angle is 0.5°. Consequently, the errors in the predicted ν_{NO} values are only -5 and 6 cm^{-1} for **4** and **5**, respectively. Additional

calculations of these HNO, RNO, and NO heme models using the next two favorable methods (BVWN5/6-311G(2d,2p) and mPWVWN5/6-311G(2d,2p), which produced errors of 2 and 3 cm^{-1} for ν_{NO} predictions for HNO respectively) were also carried out. As shown in Table S3, their mean absolute errors of ν_{NO} predictions are 12.8 cm^{-1}, which is ca. 70% larger than that from using the mPWVWN method described above, 7.6 cm^{-1}. These results further support the use of the new pure DFT method mPWVWN in predictions of NO vibrations in HNO, RNO, and NO heme systems.

We then moved to the predictions of ^{15}N NMR chemical shifts in RNO heme model complexes, which also have experimental results to compare.[34] As the experimental data are referenced to NH_3, we first evaluated the calculations for NH_3 (**8**) itself. Using the experimental ^{15}N NMR absolute chemical shielding of 264.54 ppm,[86] the predicted ^{15}N chemical shifts from using a good variety of DFT methods are listed in Table S4. Results clearly indicate that both the exchange and correlation functionals can influence the predictions. Among the fourteen DFT methods examined here, the OP86/6-311++G(2d,2p) calculation generated the best result, with an error of 0.74 ppm. This method was then used to investigate the ^{15}N NMR properties in several RNO iron porphyrins **9-12**. Again, the first coordination shell atoms plus the NO and the atom directly bonded with NO were treated with the 6-311++G(2d,2p) basis and the rest atoms were calculated with a 6-31G(d) basis except for iron. This is designated as 6-311++G(2d,2p)|metal's basis|6-31G(d) in this work. Calculations using the OP86 method as well as a couple of other DFT methods were performed together with the examination of several types of metal basis functions on complex **9**. As seen from Table S4, the OP86 method again gives the best prediction, with an error of 11 ppm using the LanL2DZ basis: 605 ppm (expt) vs. 616 ppm (calc). Such a computational error is close to that seen in solution ^{15}N NMR for investigating protein systems due to a number of experimental effects.[87] An error of 11 ppm for **9** is much improved over the previously reported error of 23 ppm.[34] An overall comparison of the calculated ^{15}N NMR shifts with experiment for **8-12** shows an $R^2 = 0.996$ and SD of 19 ppm for RNO iron porphyrin complexes, or 3.1% of the studied experimental shift range. In addition, the predicted ^{15}N NMR chemical shift tensor elements (Table S5) are also in excellent agreement with experimental data, with an $R^2 = 0.991$ and 3.5% error over the entire experimental range of 1281 ppm.

Based on these calculations for HNO and RNO heme model complexes as well as additional results in Table S6, we used the following methods for ν_{NO}, δ_H, and δ_N predictions in MbHNO models (**13-16**): mPWVWN/6-311++G(2d,2p)|Wachters|6-31G(d), B3LYP/6-311++G(2d,2p)|LanL2DZ|6-31G(d), and OP86/6-311++G(2d,2p)|LanL2DZ|6-31G(d), respectively.

Table S1. Errors in Geometry Optimizations and Frequency Calculations for HNO

Entry	DFT method	Basis	ΔR_{NO} (Å)	ΔR_{NH} (Å)	$\Delta \nu_{NO}$ (cm^{-1})	$\Delta \nu_{HNO}$ (cm^{-1})
1	B3LYP	6-311G(d)	-0.011	0.002	110	106
2		6-311G(d,p)	-0.011	0.003	107	76
3		6-311G(2d,2p)	-0.010	-0.002	91	75
4		6-311+G(d)	-0.012	0.000	108	96
5		6-311+G(d,p)	-0.011	0.001	105	65
6		6-311+G(2d,2p)	-0.010	-0.003	88	67
7		6-311++G(d)	-0.012	0.001	108	96
8		6-311++G(d,p)	-0.011	0.002	105	65
9		6-311++G(2d,2p)	-0.010	-0.003	88	65
10	mPW1PW91	6-311G(d)	-0.019	-0.002	170	128
11		6-311G(d,p)	-0.019	-0.001	168	94
12		6-311G(2d,2p)	-0.017	-0.005	146	93
13		6-311+G(d)	-0.020	-0.004	169	118
14		6-311+G(d,p)	-0.019	-0.002	166	83
15		6-311+G(2d,2p)	-0.018	-0.006	143	85
16		6-311++G(d)	-0.020	-0.003	168	117
17		6-311++G(d,p)	-0.019	-0.002	166	83
18		6-311++G(2d,2p)	-0.018	-0.006	143	84
19	BPW91	6-311G(d)	-0.001	0.021	41	49
20		6-311G(d,p)	-0.001	0.021	35	21
21		6-311G(d,2p)	0.000	0.017	36	18
22		6-311G(d,3p)	0.000	0.017	38	18
23		6-311G(d,3pd)	0.000	0.017	36	14
24		6-311G(2d)	0.000	0.020	30	25
25		6-311G(2d,p)	0.001	0.019	23	16
26		6-311G(2d,2p)	0.001	0.025	24	13
27		6-311G(2d,3p)	0.001	0.017	26	8
28		6-311G(2d,3pd)	0.001	0.016	25	8
29		6-311G(3d)	-0.001	0.018	40	30
30		6-311G(3d,p)	-0.001	0.019	34	19
31		6-311G(3d,2p)	-0.001	0.017	35	18
32		6-311G(3d,3p)	-0.001	0.018	37	17
33		6-311G(3d,3pd)	-0.001	0.018	36	15
34		6-311G(3df)	-0.004	0.019	41	24
35		6-311G(3df,p)	-0.004	0.020	38	17
36		6-311G(3df,2p)	-0.003	0.018	38	15
37		6-311G(3df,3p)	-0.004	0.019	40	14
38		6-311G(3df,3pd)	-0.004	0.018	39	13
39		6-311+G(d)	-0.002	0.018	41	44
40		6-311+G(d,p)	-0.001	0.018	34	13
41		6-311+G(2d,2p)	0.001	0.014	21	9
42		6-311++G(d)	-0.002	0.019	40	42

43		6-311++G(d,p)	-0.001	0.019	34	12
44		6-311++G(2d,2p)	0.000	0.014	21	7
45	BVWN	6-311G(2d,2p)	0.007	0.008	7	2
46	BVWN5	6-311G(2d,2p)	0.008	0.011	2	-6
47	BLYP	6-311G(2d,2p)	0.007	0.019	-6	-11
48	BPL	6-311G(2d,2p)	0.009	-0.016	126	-66
49	BP86	6-311G(2d,2p)	0.003	0.018	17	6
50	BB95	6-311G(2d,2p)	0.002	0.018	12	-1
51	BPBE	6-311G(2d,2p)	0.001	0.017	26	13
52	BTPSS	6-311G(2d,2p)	0.001	0.018	24	11
53	BVWN5	6-311+G(2d,2p)	0.008	0.008	-4	61
54		6-311++G(2d,2p)	0.008	0.008	-5	-9
55	mPWVWN	6-311G(2d,2p)	0.006	0.008	8	3
56	mPWVWN5	6-311G(2d,2p)	0.007	0.011	3	-14
57	mPWLYP	6-311G(2d,2p)	0.007	0.017	-3	-8
58	mPWPL	6-311G(2d,2p)	0.008	0.012	125	-68
59	mPWP86	6-311G(2d,2p)	0.002	0.019	18	5
60	mPWB95	6-311G(2d,2p)	0.001	0.018	13	-1
61	mPWPBE	6-311G(2d,2p)	0.000	0.017	27	12
62	mPWTPSS	6-311G(2d,2p)	0.000	0.018	25	10
63	mPWVWN	6-311+G(2d)	0.005	0.010	11	6
64		6-311+G(2d,p)	0.006	0.009	0	1
65		6-311+G(2d,2p)	0.006	0.006	2	1
66		6-311++G(2d,p)	0.006	0.009	-1	0
67		6-311++G(2d,2p)	0.006	0.006	1	0
68		6-311++G(3df,3pd)	0.002	0.008	7	6
69		cc-pvdz	0.007	0.028	7	1
70		aug-cc-pvdz	0.009	0.014	4	1
71		aug-cc-pvtz	0.003	0.008	1	1
72		aug-cc-pvqz	0.001	0.007	5	6
73	PBEPBE	6-311G(2d,2p)	0.000	0.018	28	11
74		6-311++G(2d,2p)	0.000	0.016	25	4

Table S2. Experimental and Computational Results of NO Vibrational Frequencies and ^{1}H NMR Chemical Shifts in HNO of Ru(TTP)(HNO)(1-MeIm)

	Metal Basis	ν_{NO} (cm^{-1})	δ_H (ppm)
Expt		1380	13.64
Calc	SDD	1367	12.07
	CEP-121G	1376	12.88
	DGDZVP	1382	13.13

Table S3. Geometric and Vibrational Results from Other Calculations [a]

	System	R_{NO} (Å)	R_{MN} (Å)	∠M-N-O (°)	ν_{NO} (cm^{-1})	$\lvert\Delta\nu_{NO}\rvert$ (cm^{-1})
BVWN5/6-311G(2d,2p)	**2** Ru(TTP)(HNO)(1-MeIm)	1.245	1.945	132.1	1397	17
	3 Ru(HNO)('$py^{bu}S_4$')	1.247	1.961	130.8	1387	29
	4 Fe(TPP)(^{i}PrNO)(1-MeIm)	1.243	1.862	122.8	1435	2
	6 Fe(TPP)(NO)(1-MeIm)	1.186	1.736	143.8	1644	14
	7 $[Fe(OETPP)(NO)(1\text{-}MeIm)]^{+}$	1.152	1.656	180.0	1869	2
Average						12.8
mPWVWN5/6-311G(2d,2p)	**2** Ru(TTP)(HNO)(1-MeIm)	1.245	1.944	132.0	1399	19
	3 Ru(HNO)('$py^{bu}S_4$')	1.247	1.959	130.6	1388	30
	4 Fe(TPP)(^{i}PrNO)(1-MeIm)	1.243	1.860	122.9	1434	1
	6 Fe(TPP)(NO)(1-MeIm)	1.186	1.737	142.8	1643	13
	7 $[Fe(OETPP)(NO)(1\text{-}MeIm)]^{+}$	1.152	1.656	180.0	1872	1
Average						12.8

[a] $\lvert\Delta\nu_{NO}\rvert$ is the absolute error.

Table S4. Errors in the Predicted ^{15}N NMR Isotropic Chemical Shifts

Compound	Entry	Method	$\Delta\delta_N$ (ppm)
8 NH_3	1	BVWN/6-311++G(2d,2p)	11.04
	2	BVWN5/6-311++G(2d,2p)	10.55
	3	BLYP/6-311++G(2d,2p)	6.03
	4	BPW91/6-311++G(2d,2p)	4.77
	5	BP86/6-311++G(2d,2p)	3.67
	6	mPWVWN/6-311++G(2d,2p)	10.15
	7	mPWVWN5/6-311++G(2d,2p)	9.67
	8	mPWLYP/6-311++G(2d,2p)	5.11
	9	mPWPW91/6-311++G(2d,2p)	3.93
	10	mPWP86/6-311++G(2d,2p)	2.84
	11	G96P86/6-311++G(2d,2p)	4.81
	12	PW91P86/6-311++G(2d,2p)	2.05
	13	PBEP86/6-311++G(2d,2p)	1.91
	14	OP86/6-311++G(2d,2p)	0.74
9 Fe(TPP)(PhNO)(1-MeIm)	15	B3LYP/6-311++G(2d,2p)|Wachters|6-31G(d)	242
	16	BPW91/6-311++G(2d,2p)|Wachters|6-31G(d)	41
	17	OP86/6-311++G(2d,2p)|Wachters|6-31G(d)	9
	18	OP86/6-311++G(2d,2p)|LanL2DZ|6-31G(d)	11
	19	OP86/6-311++G(2d,2p)|CEP-121G|6-31G(d)	10
	20	OP86/6-311++G(2d,2p)|SDD|6-31G(d)	16

[a] The NMR calculations for NH_3 were done on the geometry optimized by using B3LYP/6-311G(d), in which the optimized R_{NH} of 1.015 Å and ∠H-N-H of 106.7° are in good agreement with experimental results of 1.015 Å and ∠H-N-H of 107.3° (Bloemink, H. I.; Legon, A. C.; Thorn, J. C. *J. Chem. Soc. Faraday Trans.* **1995,** 91, 781-787.). The predicted NMR shift of **9** is referenced to the calculated shielding of NH_3.

Table S5. ^{15}N NMR Chemical Shifts and Tensor Elements in RNO Iron Porphyrins [a]

Compound	Method	δ_N (ppm)	δ_{11} (ppm)	δ_{22} (ppm)	δ_{33} (ppm)
9 Fe(TPP)(PhNO)(1-MeIm)	Expt	605	1178	464	173
	Calc	616	1177	484	186
10 Fe(TPP)(PhNO)(py)	Expt	607	1265	469	87
	Calc	632	1215	488	193
11 Fe(TPP)(NODMA)(py)	Expt	607	1281	456	82
	Calc	590	1126	470	175
12 Fe(OEP)(PhNO)(1-MeIm) [b]	Expt	593	1247	448	84
	Calc-average	616	1178	482	188
	Calc-site 1	606	1155	475	188
	Calc-site 2	625	1200	488	189

[a] NMR calculations were performed using the OP86/6-311++G(2d,2p)|LanL2DZ|6-31G(d) method and results are referenced to the calculated shielding of NH_3. [b] The full OEP ligand was used in the calculations.

Table S6. Experimental Results of MbHNO and Computational Results of Fe(Por)(HNO)(5-MeIm)

	Metal Basis for Geometry optimization and Frequency Calculation	Metal Basis for NMR Chemical Shift Calculation	R_{MN} (Å)	R_{NO} (Å)	∠M-N-O (°)	ν_{NO} (cm^{-1})	δ_H (ppm)
Expt			1.820	1.241	131.0	1385	14.80
Calc	LanL2DZ	LanL2DZ	1.790	1.243	133.1	1411	15.05
	SDD	SDD	1.802	1.244	132.7	1404	15.83
	CEP-121G	CEP-121G	1.808	1.245	132.5	1400	15.45
	DGDZVP	DGDZVP	1.798	1.243	132.7	1409	17.02
	Wachters'	Wachters'	1.804	1.245	132.4	1400	17.17
		CEP-121G					15.95
		LanL2DZ					15.42

Table S7. Optimized Structure of **1**

H	0.8121496358	0.	-0.553497328
N	-0.1274626995	0.	-0.0439784187
O	0.0813575068	0.	1.154688137

Table S8. Optimized Structure of **2**

N	1.4891285934	1.7809633747	-0.0857602570
N	-0.5520189598	1.0193775257	1.9457319337
N	-1.7822973691	-0.8632228815	0.0000935936
N	0.2487624019	-0.0822091856	-2.0348847970
C	2.3267957252	1.9989222056	-1.1607822139
C	1.9194518436	2.5634543797	0.9664770424
C	1.2695261482	0.4107913478	-2.8217515036
C	-0.4538281197	-1.0165764027	-2.7674455857
C	-2.1861660770	-1.6793879215	-1.0379779436
C	-2.6375413665	-1.0591829944	1.0660267194
C	-1.5895322928	0.5455071729	2.7231492776
C	0.1769797551	1.9219200501	2.6942332223
C	-2.5442538561	-0.4066250514	2.3116855005
H	-3.2973629395	-0.6764043008	3.0493434345
C	1.3139430443	2.6216080143	2.2387674136
H	1.7807713624	3.2916436242	2.9582545195
C	2.2149260090	1.3725074825	-2.4162890474
H	2.9599219625	1.6523166262	-3.1582617235
C	-1.5674273931	-1.7469217168	-2.3029358911
H	-2.0065972620	-2.4467761294	-3.0112211027
C	-3.6359541766	-2.0508811867	0.6838297606
C	-3.3583025278	-2.4315126792	-0.6065736193
C	0.1474745700	-1.1130558160	-4.0918561159
C	1.2044746511	-0.2364545085	-4.1253878997
C	3.3380756930	2.9739512672	-0.7719548057
C	3.0888777892	3.3199090061	0.5334528212
C	-0.4333037333	2.0284741556	4.0133166951
C	-1.5174496546	1.1839105238	4.0313592564
H	-0.1961295741	-1.7709598078	-4.8823652331
H	1.8840381952	-0.0444023982	-4.9479880416
H	4.1317059583	3.3349445874	-1.4163751679
H	3.6423845699	4.0157214878	1.1543136576
H	-0.0722551202	2.6634627320	4.8148592738
H	-2.2063305348	1.0031517015	4.8489499429
H	-4.4378252953	-2.4024089752	1.3233845791
H	-3.8913227856	-3.1531519141	-1.2156869315
N	1.0231723961	-1.0125349919	0.6042315526
H	0.6069464453	-1.6267903160	1.3332441486
O	2.1814485829	-1.3595129429	0.2970255914
N	-1.4962915110	2.1149169422	-0.7633996498
C	-2.4991689944	2.0365240281	-1.7181638217
C	-1.4743669667	3.3773079950	-0.3461777114
H	-0.8070921692	3.7806840285	0.4009565135
C	-3.0859186395	3.2743876614	-1.8716527083
N	-2.4254050494	4.1284198407	-0.9899014932

H	-2.7231557623	1.1079141182	-2.2211167501
Ru	-0.1110725136	0.4259965555	-0.0330203955
C	-2.6917885225	5.5584974665	-0.7899304843
H	-2.5365268873	6.1102969901	-1.7237300560
H	-3.7211135799	5.7112870770	-0.4469000791
H	-2.0045679270	5.9431739438	-0.0325222696
H	-3.8875381355	3.6220282089	-2.5069731509

Table S9. Optimized Structure of **3**

Ru	1.3122268633	-0.8459342268	0.4536191033
S	-0.2448304614	-1.0600151641	-1.4428305745
S	-0.3256244203	0.6530266864	1.3915007219
S	2.6092057432	-2.7839900181	-0.1906339191
S	2.7227059686	-0.8488806144	2.5097113498
N	0.0798828985	-2.3808113698	1.4743806615
N	2.4094426118	0.5138153774	-0.4198179359
H	3.3986304178	0.2727940558	-0.6279965209
O	2.1332321998	1.6801495236	-0.7736737975
C	-1.6547343807	-0.0803504435	-0.9798360604
C	-2.7785071319	0.0132977240	-1.8677234372
C	-3.8659014419	0.8237393707	-1.5122245771
C	-3.9154206292	1.5773572497	-0.3170824657
C	-2.8133098626	1.4895348424	0.5443841085
C	-1.7182326141	0.6604351553	0.2258461324
C	-0.9060166391	-0.5233694553	2.7490762101
C	3.7447777493	-2.2925866489	2.3418311738
C	4.6776637943	-2.6279979491	3.3821823129
C	5.5128823805	-3.7420498147	3.2225104035
C	5.5033520330	-4.5630500741	2.0707796538
C	4.5965692936	-4.2328812442	1.0551587468
C	3.7228710772	-3.1343601322	1.2004813875
C	1.2141992657	-4.0309982828	0.0492067500
C	-0.8438636169	-1.9964073068	2.3909108905
C	-1.6684990065	-2.9426070563	3.0223773584
C	-1.4958353068	-4.3023325754	2.7310236803
C	-0.5227020403	-4.6838362851	1.7974889865
C	0.2398221933	-3.6905007666	1.1612187582
C	-2.7958875129	-0.7417561695	-3.1869173441
C	-5.1172178680	2.4519106851	0.0097819139
C	4.7726134987	-1.7857012061	4.6438042139
C	6.4543970611	-5.7440297320	1.9409876858
H	7.5030617647	-5.4154441628	1.9088412444
H	6.3616823936	-6.4328081310	2.7922061899
H	6.2599392051	-6.3165175520	1.0266102502
H	5.0581239567	-0.7504048814	4.4122424245
H	3.8067132319	-1.7315644934	5.1643841446
H	5.5145795903	-2.2004920404	5.3354278266
H	6.2119557964	-3.9777955671	4.0249104265
H	4.5626569301	-4.8253156049	0.1418612165
H	0.6981830300	-4.0073239454	-0.9186643351
H	1.6588673720	-5.0211746927	0.1858120140
H	-0.3685863922	-5.7300181270	1.5479529092
H	-2.1105876201	-5.0525168074	3.2224157454
H	-2.4155991069	-2.6169206911	3.7409063462

H	-0.2071774559	-0.3089826371	3.5670673931
H	-1.9109569807	-0.2244112679	3.0616361121
H	-4.7081841524	0.8832203165	-2.2014673385
H	-1.9635502188	-0.4330032131	-3.8338733583
H	-2.6852653694	-1.8239063134	-3.0323463735
H	-3.7336370737	-0.5652640332	-3.7258792655
H	-2.7945285034	2.0694754704	1.4659664390
H	-5.3282410263	3.1642035628	-0.7996234883
H	-6.0276507860	1.8519607157	0.1528232059
H	-4.9540907022	3.0299899611	0.9267647003

Table S10. Optimized Structure of **4**

Fe	-0.1604608492	0.0502358273	-0.2001491297
O	-1.3101101454	0.4753642524	-2.6499631562
N	1.3951456117	0.4590706769	-1.4519130543
N	-0.6964544664	2.0154577405	-0.2057522179
N	-1.6205210043	-0.3390917981	1.1861026452
N	0.4694434719	-1.8980483708	-0.0635006901
N	1.1747064132	0.4933883868	1.4866998744
N	2.9808174391	0.5188646395	2.7962087008
N	-1.2667089479	-0.2695346781	-1.6548099765
C	2.2790548584	-0.4519284248	-2.0006189138
C	3.1855217467	0.2272965183	-2.9137475114
H	3.9739251817	-0.2589434624	-3.4774920701
C	2.8369414574	1.5520016611	-2.9077245733
H	3.2824805817	2.3679908568	-3.4654231264
C	1.7102754319	1.6882619187	-1.9977947848
C	1.0345221677	2.8852066280	-1.7367834642
C	-0.0931166784	3.0308939566	-0.9217639430
C	-0.8197712337	4.2757597447	-0.7245128358
H	-0.5512985679	5.2252220259	-1.1736368944
C	-1.8727106052	3.9942295175	0.1045626640
H	-2.6392598309	4.6674208108	0.4716958828
C	-1.7899932967	2.5774515276	0.4261566786
C	-2.6706980645	1.8959639591	1.2760192388
C	-2.5767146050	0.5484873540	1.6482517847
C	-3.4392548302	-0.1129870369	2.6137946819
H	-4.2707848160	0.3591202894	3.1250413552
C	-2.9834280457	-1.3995708376	2.7405202871
H	-3.3689425027	-2.1907901080	3.3736481157
C	-1.8465614490	-1.5352517404	1.8438674851
C	-1.1106444578	-2.7123210928	1.6546836326
C	-0.0449633609	-2.8833612450	0.7610535889
C	0.6683323611	-4.1315764074	0.5443454861
H	0.4602738041	-5.0604914723	1.0634253680
C	1.6149905091	-3.8881007549	-0.4175077352
H	2.3367459973	-4.5782895856	-0.8401261872
C	1.4927628142	-2.4873511958	-0.7866449676
C	2.3180630341	-1.8206013402	-1.7025653415
C	0.9069989748	1.2735983699	2.6018284472
H	-0.0503002765	1.7536627732	2.7346357226
C	2.0127305769	1.3013349753	3.4241053770
H	2.2005046728	1.7889975147	4.3697506536
C	4.3378959059	0.2442047921	3.2833714667
H	4.3005439572	-0.2525628374	4.2594221096
H	4.9085860156	1.1753569810	3.3744991058
H	4.8428136456	-0.4127337860	2.5709001338

C	2.4218267612	0.0562906475	1.6312409950
H	2.9499295133	-0.5807613108	0.9379643688
C	-2.2264903523	-1.4771004538	-1.7636838289
H	-2.0854528330	-2.0409318731	-0.8462621094
C	-1.8246494098	-2.3414363465	-2.9738450954
H	-0.7897850068	-2.6883201014	-2.8852647765
H	-1.9306167216	-1.7784207850	-3.9073013251
H	-2.4787323968	-3.2221579151	-3.0176733162
C	-3.6783111990	-0.9677420999	-1.8447645950
H	-3.9306456146	-0.3537555250	-0.9739004941
H	-4.3593341502	-1.8286144707	-1.8659249433
H	-3.8330224008	-0.3749631087	-2.7527288970
H	3.0760616190	-2.4149054462	-2.2079759455
H	1.3966852896	3.7770843991	-2.2427870210
H	-3.4835920041	2.4731856076	1.7107544455
H	-1.4074494533	-3.5792894227	2.2405679841

Table S11. Optimized Structure of **5**

Fe	-0.4564702536	6.7002838742	5.1060710812
O	1.8729028571	8.1048702090	5.4173503430
N	-0.1660507138	4.7622656519	5.7280664590
N	0.6259284432	6.3299173191	3.4209887916
N	-1.6898218430	7.0011485134	6.7198959564
N	1.0607595976	7.3359870385	5.9619370485
C	-0.6796607100	4.1575647900	6.8643089760
C	-0.2005128178	2.7884852927	6.9546102711
C	0.5993362424	2.5733241250	5.8605572067
C	0.6128122721	3.8078310601	5.0948689996
C	1.2882918658	3.9937608634	3.8818744858
H	1.8621667688	3.1504661456	3.5043064288
C	1.2883299139	5.1589548145	3.1059889379
C	2.0020936209	5.3169811813	1.8473668381
C	1.7698595410	6.5955767801	1.4167504445
C	0.9123744527	7.2255399798	2.4093690880
C	-2.3633822246	8.1696098714	7.0283868765
C	-3.1350177523	7.9892000597	8.2475430302
C	-2.9255221169	6.7011343522	8.6658902513
C	-2.0221316702	6.0876112359	7.7049452576
C	-1.5480062489	4.7708322487	7.7785389934
H	-1.8822590341	4.1713191398	8.6223563111
C	1.4549563608	6.9740505101	7.4116373907
H	0.6720496973	6.3111776521	7.7674463505
C	2.8040070658	6.2296231854	7.4005595629
H	2.7542469336	5.3322802653	6.7748069360
H	3.0513276492	5.9204513046	8.4245507999
H	3.6039667685	6.8773296932	7.0260997049
C	1.4810733118	8.2538535330	8.2692557003
H	0.5094288961	8.7588493846	8.2550905805
H	2.2467855848	8.9494343458	7.9095819123
H	1.7112509946	7.9833526225	9.3081477668
N	-0.8656525661	8.5785587511	4.4319574474
C	0.4594362873	8.5478078147	2.3487039839
H	0.7796950987	9.1420583071	1.4960742022
C	-0.3535004832	9.1792809798	3.2964065710
C	-0.8042921952	10.5598037452	3.2212046536
C	-1.5866010213	10.7832336417	4.3236235366
C	-1.6177466861	9.5408766874	5.0795798240
C	-2.3167449028	9.3506223602	6.2777155229
N	-2.2442683904	5.9876336368	4.0026237494
N	-3.9170029981	4.6874103675	3.3012093547
C	-2.9464170384	6.6569815199	3.0106846255
H	-2.6583173518	7.6467131291	2.6931697175
C	-3.9841411107	5.8686100316	2.5633481379

C	-2.8481932705	4.8126037779	4.1520273442
H	-2.5574849104	4.0410912487	4.8480261153
C	-4.8004277840	3.5220336309	3.1740788384
H	-4.5376089972	2.7934538567	3.9450214372
H	-4.6845955368	3.0556496459	2.1888653891
H	-5.8453923369	3.8213722025	3.3104811693
H	-2.8820613648	10.1985516278	6.6576072640
H	-3.7524188167	8.7531829675	8.7066826422
H	-3.3359186954	6.2000052437	9.5354110415
H	-0.4510988537	2.0968677047	7.7512685011
H	1.1323689605	1.6698539993	5.5858443230
H	2.6002317503	4.5454801667	1.3755243547
H	2.1367846192	7.0820361744	0.5200637389
H	-2.0957380353	11.6954923288	4.6137657035
H	-0.5463918745	11.2512975845	2.4270482934
H	-4.7447149489	6.0284698250	1.8127337370

Table S12. Optimized Structure of **6**

O	2.0527854630	7.9419205540	5.8237961840
N	-0.0883653910	4.6765750390	5.6803367630
N	0.7503821270	6.3089408400	3.4449934940
N	-1.6049643360	6.9099309360	6.7321061020
N	1.1055312640	7.2429624980	5.9910930070
C	-0.5575301020	4.0757787240	6.8334561630
C	-0.0893314640	2.7005515820	6.8972427210
C	0.6657476810	2.4838250850	5.7736055110
C	0.6675297050	3.7270734520	5.0207540820
C	1.3416146730	3.9344330000	3.8115397040
H	1.8970724020	3.0931011950	3.4041928680
C	1.3813282330	5.1305590790	3.0869938450
C	2.1097812100	5.3215245620	1.8442450140
C	1.9229699380	6.6253266290	1.4673912700
C	1.0724426710	7.2382779130	2.4733410220
C	-2.2868429200	8.0644695040	7.0588756780
C	-3.0172377170	7.8731234190	8.3019447840
C	-2.7577698730	6.5949768490	8.7215116050
C	-1.8722269870	5.9980121080	7.7332315620
C	-1.3797289630	4.6882301960	7.7878377310
H	-1.6706709060	4.0872764780	8.6463223560
N	-0.7562466520	8.5329770690	4.4897816630
C	0.6323440330	8.5663409070	2.4481533420
H	0.9750865640	9.1856125730	1.6228475470
C	-0.2216635700	9.1645535910	3.3817282300
C	-0.7030618430	10.5335891800	3.3158190680
C	-1.5280592300	10.7187328300	4.3946162350
C	-1.5510536400	9.4670229190	5.1316518450
C	-2.2670481360	9.2494268230	6.3141006220
N	-2.3234390400	5.9335936710	3.8822059270
N	-4.1270141330	4.7505944070	3.2955450640
C	-2.9422138960	6.5581827880	2.8113470110
H	-2.5442054400	7.4699983580	2.3897331410
C	-4.0598429530	5.8436028590	2.4318511340
C	-3.0526299460	4.8577854410	4.1473846480
H	-2.8546456190	4.1414655620	4.9320192380
C	-5.1457099240	3.6941729450	3.2955200290
H	-4.9219719610	2.9880810220	4.0992404580
H	-5.1431511150	3.1565102360	2.3404029520
H	-6.1409344410	4.1205664120	3.4653708450
H	-2.8503603400	10.0834736900	6.6968450250
H	-3.6355733070	8.6255390250	8.7781797840
H	-3.1226555190	6.0909121760	9.6093687590
H	-0.3150439270	2.0072340430	7.6996789780
H	1.1822342650	1.5787925890	5.4743826050

H	2.6853516390	4.5519273750	1.3427011910
H	2.3119553620	7.1361456770	0.5939662510
H	-2.0718070000	11.6120490200	4.6800754580
H	-0.4393318600	11.2440997300	2.5407443700
H	-4.7955066130	5.9986485630	1.6554100790
Fe	-0.3069184640	6.6576988710	5.1461170380

Table S13. Optimized Structure of **7**

O	1.8005928600	7.4759893277	6.5107487500
N	-0.1378992819	4.6499057082	5.6027237272
N	0.6642543337	6.3079982051	3.3540680299
N	-1.6840877457	6.8451230528	6.6688705646
N	0.8838679514	7.1196489146	5.9134692311
C	-0.5187519829	4.0630259734	6.7994360072
C	-0.0174140239	2.7027682430	6.8449866374
C	0.6647769900	2.4832345102	5.6761833237
C	0.6062318021	3.7116488313	4.9071511595
C	1.2426622248	3.9232723738	3.6806558453
H	1.7905222875	3.0858458982	3.2583722534
C	1.2935761973	5.1324062333	2.9812416672
C	2.0575708775	5.3625381245	1.7696816395
C	1.9082399457	6.6846720097	1.4408221410
C	1.0356555907	7.2776521666	2.4363278640
C	-2.4042493732	7.9855893700	6.9828078033
C	-3.0747392940	7.7919037233	8.2543100351
C	-2.7257074207	6.5476565330	8.7122609420
C	-1.8514232686	5.9549630956	7.7182740845
C	-1.3022450253	4.6700679591	7.7868051210
H	-1.5189535530	4.0854303456	8.6762579564
N	-0.8809187291	8.5021427414	4.4198531745
C	0.6029726150	8.6077203653	2.4421462066
H	0.9808860284	9.2555014500	1.6564827472
C	-0.2963603529	9.1687148157	3.3547685969
C	-0.7996144681	10.5282849267	3.3072735040
C	-1.6813966099	10.6699296392	4.3469436000
C	-1.7159979209	9.4048493162	5.0560989793
C	-2.4449172846	9.1582823723	6.2230155032
N	-2.1015956214	5.9571710149	3.9784777806
N	-3.9760733027	4.8949670489	3.4443578886
C	-2.4620954523	6.3294244010	2.6894168667
H	-1.8763102470	7.0240240568	2.1102921278
C	-3.6235312993	5.6772164186	2.3465172978
C	-3.0307542462	5.0946084722	4.4050127142
H	-3.0506736386	4.6121549175	5.3689438493
C	-5.1557113467	4.0135307370	3.5467635962
H	-5.1560000569	3.5360939991	4.5287043671
H	-5.1131324908	3.2434978888	2.7706789123
H	-6.0708142491	4.6019521923	3.4310102550
H	-3.0590391574	9.9701842372	6.6016941550
H	-3.7148805714	8.5261723414	8.7280990392
H	-3.0284193718	6.0614172878	9.6317538955
H	-0.1789455725	2.0161659031	7.6671967818
H	1.1758895944	1.5833024282	5.3563188258

H	2.6364280474	4.6042881183	1.2565006783
H	2.3359862249	7.2207302298	0.6023153319
H	-2.2538803118	11.5457736531	4.6271026272
H	-0.5123078420	11.2633823983	2.5653097221
H	-4.2169026239	5.6972553789	1.4444178001
Fe	-0.4349698342	6.6061206510	5.0586783920

Table S14. Optimized Structure of **13**

N	1.4417542132	1.7741064661	-0.1276822705
N	-0.5351876267	1.0706361231	1.8702294864
N	-1.7569517897	-0.7678479275	0.0084402930
N	0.2295393635	-0.0683834278	-1.9816368047
C	2.2776268451	2.0016461040	-1.2040898077
C	1.9184181139	2.5526835335	0.9109906919
C	1.2342460182	0.4036061382	-2.8043710243
C	-0.4421959722	-1.0407766871	-2.6998755784
C	-2.1654819095	-1.6326367127	-0.9916638588
C	-2.6414988183	-0.9349873382	1.0581894297
C	-1.5809408605	0.6465849309	2.6705699703
C	0.2177240346	1.9446313824	2.6367391718
C	-2.5668665148	-0.2726553351	2.2897822225
H	-3.3295068690	-0.5126571879	3.0269222934
C	1.3597421453	2.6243763564	2.1937862082
H	1.8518117675	3.2794562624	2.9091476215
C	2.1731736191	1.3786970967	-2.4521349915
H	2.9095312119	1.6512079186	-3.2044235286
C	-1.5471076799	-1.7695073864	-2.2407720857
H	-1.9741364809	-2.4994400067	-2.9246530071
C	-3.6439806652	-1.9276695621	0.7052308363
C	-3.3465231286	-2.3620725704	-0.5601154260
C	0.1528234265	-1.1776103954	-4.0199482956
C	1.1864536432	-0.2811587558	-4.0861021835
C	3.3035404519	2.9651156068	-0.8388815308
C	3.0840200770	3.3028497136	0.4702794099
C	-0.3753427010	2.0773744057	3.9568767271
C	-1.4895840252	1.2784505555	3.9765850564
H	-0.1845246641	-1.8734892212	-4.7798574554
H	1.8657675339	-0.0962980137	-4.9104226112
H	4.0849682642	3.3164882234	-1.5030418155
H	3.6497571680	3.9866598219	1.0930861521
H	0.0190603589	2.7005149388	4.7517444140
H	-2.1872965586	1.1172961708	4.7906360047
H	-4.4552518529	-2.2428471498	1.3516875209
H	-3.8674291736	-3.1026163158	-1.1565692367
N	0.9219479895	-0.8636733373	0.5820413881
H	0.5177504022	-1.4015414160	1.3755826398
O	2.0487020383	-1.2792753051	0.2521019054
N	-1.4281047800	2.0675911443	-0.7757255047
C	-2.2716104903	2.0389012253	-1.8794373549
C	-1.5594429595	3.2730078924	-0.2366084624
H	-1.0437036026	3.6333965334	0.6403012610
C	-2.9278040086	3.2464555275	-2.0173602784
N	-2.4564130018	4.0236255890	-0.9542821500

H	-2.3517592430	1.1579764899	-2.4979637516
C	-3.9293766063	3.7441104609	-3.0213654092
H	-4.8793137753	4.0330785874	-2.5493242994
H	-3.5571570885	4.6152406708	-3.5794468944
H	-4.1474485580	2.9547264098	-3.7476357136
H	-2.7265881787	4.9768657577	-0.7462964745
Fe	-0.1176344530	0.4685315446	-0.0508699392

Table S15. Optimized Structure of **14**

N	-1.1596343889	1.6263154123	0.3824048760
N	1.5046790053	1.4961147457	-0.7398580099
N	1.1917365177	-1.3413100571	-1.1430515585
N	-1.4736505017	-1.2010280638	-0.0221698384
C	-2.4099566428	1.4867440911	0.9563207997
C	-0.8606449179	2.9767270521	0.4180667888
C	-2.6748757024	-0.9641029632	0.6192895788
C	-1.4693574284	-2.5417185922	-0.3639631089
C	0.8267951673	-2.6623676551	-1.3381136571
C	2.4968799324	-1.2249289170	-1.5854138211
C	2.7685410153	1.2292267850	-1.2356536829
C	1.4390510445	2.8664481417	-0.5489087153
C	3.2366585347	-0.0360694667	-1.6113791823
H	4.2538781256	-0.0944149005	-1.9912418689
C	0.3358988629	3.5540320472	-0.0274751902
H	0.4260703509	4.6339610355	0.0641740222
C	-3.1026831035	0.2797895760	1.0937679806
H	-4.0834805646	0.3210326746	1.5599185607
C	-0.4133490112	-3.2142012510	-0.9930087971
H	-0.5577193146	-4.2715111570	-1.2028403263
C	2.9732435506	-2.5136148523	-2.0602349707
C	1.9380342549	-3.4000791205	-1.9145986620
C	-2.7098675620	-3.1645276151	0.0697972415
C	-3.4499586833	-2.1913469074	0.6880134023
C	-2.9118551865	2.7859698916	1.3703643230
C	-1.9575639617	3.7081953474	1.0306218304
C	2.7006249913	3.4778324792	-0.9311639212
C	3.5251553813	2.4652992562	-1.3484054769
H	-2.9611633129	-4.2086520918	-0.0790917667
H	-4.4330217256	-2.2745861638	1.1364271518
H	-3.8726735309	2.9534998884	1.8430974488
H	-1.9790504746	4.7826965589	1.1732937358
H	2.9129513894	4.5397831768	-0.8797413978
H	4.5452994279	2.5338992743	-1.7088837006
H	3.9653006933	-2.6969570360	-2.4570564716
H	1.9154291214	-4.4545711718	-2.1654356919
N	-0.6119968709	0.4642030172	-2.0927127717
H	0.1327960560	0.5353688726	-2.8123376868
O	-1.7502004545	0.6191731645	-2.5918076728
N	0.7982165890	-0.2236202581	1.5605321255
C	0.9930908131	-1.4549483044	2.1746665362
C	1.2006725758	0.6954367675	2.4294632694
H	1.1877932513	1.7634345197	2.2738244205
C	1.5227602224	-1.2847599759	3.4386490884
N	1.6480313265	0.1007414604	3.5815435700

H	0.7404112657	-2.3762268412	1.6722625631
C	1.9158169790	-2.2632898052	4.5094040928
H	2.9828239349	-2.1908204244	4.7641043894
H	1.3421707438	-2.1149342700	5.4354234204
H	1.7269076570	-3.2843595374	4.1631710342
H	2.0069192268	0.5866446429	4.3939478312
Fe	-0.0186808954	0.1544058439	-0.4273635924
H	-3.7546870323	0.3609634795	-2.1329712584
O	-4.6294435219	-0.0709926075	-2.1904379386
H	-4.3841353218	-1.0041723996	-2.3247991385

Table S16. Optimized Structure of **15**

N	1.2021418480	0.8767772553	-0.0026110448
N	0.7545737094	-1.9076571159	-0.6465606539
N	-1.9122173996	-1.2692690956	-1.5345015544
N	-1.4595845891	1.5114230561	-0.8925003513
C	1.2205770794	2.2286388456	0.2811467246
C	2.4660656532	0.3986129042	0.2931693214
C	-1.0828831220	2.7778478290	-0.4877712771
C	-2.7229158990	1.6372466763	-1.4399082301
C	-3.1189681699	-0.7652752237	-1.9877842898
C	-1.9804595661	-2.6417892134	-1.6890399137
C	0.3262418182	-3.1966864640	-0.9089228058
C	2.0797655734	-2.0073947297	-0.2544144829
C	-0.9491908301	-3.5409048168	-1.3821710032
H	-1.1499269751	-4.5981003793	-1.5424433257
C	2.8786037735	-0.9336567254	0.1615516570
H	3.9059948595	-1.1611224350	0.4370264373
C	0.1516189683	3.1082856066	0.0798544553
H	0.3112682530	4.1503985897	0.3463747830
C	-3.4866762300	0.5855830533	-1.9617960875
H	-4.4679155227	0.8376288004	-2.3573445118
C	-3.2683989019	-3.0140827839	-2.2539561609
C	-3.9679409911	-1.8519989565	-2.4475242839
C	-3.1585645318	3.0235539126	-1.3680415911
C	-2.1472752266	3.7276915243	-0.7715922614
C	2.5279977856	2.6117129996	0.7894615766
C	3.3009559253	1.4812136200	0.7897479945
C	2.4996105551	-3.3982660458	-0.2830760722
C	1.4119383509	-4.1361414596	-0.6776094000
H	-4.1118966588	3.3905811365	-1.7311666883
H	-2.1039486044	4.7879003364	-0.5497301410
H	2.8041503953	3.6164372258	1.0884586671
H	4.3369792323	1.3739629744	1.0908978460
H	3.4907882895	-3.7510250696	-0.0204417374
H	1.3387054427	-5.2105048451	-0.8054572002
H	-3.5771503152	-4.0300178032	-2.4730643396
H	-4.9651171716	-1.7271579949	-2.8543017004
N	0.2907338608	0.0894750705	-2.4921172086
H	0.3609160390	-0.7436309516	-3.1152944687
O	0.6845476567	1.1291758502	-3.0566776925
N	-1.0960963717	-0.5381396337	1.2187446901
C	-2.3943807145	-0.3621080068	1.6812580933
C	-0.3835828952	-0.9524701253	2.2584282793
H	0.6710277086	-1.1832072156	2.2525846933
C	-2.4759114583	-0.6737137256	3.0245868664
N	-1.1753911376	-1.0496282838	3.3752338570

H	-3.1805693527	-0.0236296153	1.0233501530
C	-3.6201128939	-0.6574148408	3.9990059003
H	-3.8189830900	-1.6532158974	4.4204778259
H	-3.4380674894	0.0283770175	4.8388575212
H	-4.5315447963	-0.3246991233	3.4921980586
H	-0.8665576607	-1.3432071433	4.2935501303
Fe	-0.3327802234	-0.1730536514	-0.8190461289
O	0.8322605613	-2.4170508322	-4.1597283456
H	1.7095412509	-2.5832670178	-3.7659652198
H	0.2357041989	-2.9736370628	-3.6208053587

Table S17. Optimized Structure of **16**

N	-1.2063264450	1.5413925794	0.6495145818
N	1.6038049069	1.4165454202	-0.0148288223
N	1.2343415889	-1.2408270934	-1.0632607172
N	-1.5746899356	-1.1095461245	-0.3945777876
C	-2.5423971591	1.3913835395	0.9707380324
C	-0.8626860509	2.8349865583	0.9988476544
C	-2.8547066226	-0.9148167915	0.0882730304
C	-1.5766332972	-2.3413247290	-1.0235658010
C	0.8483118042	-2.4537791621	-1.6063882249
C	2.6074537558	-1.1666024035	-1.2083148926
C	2.9296951585	1.1317141190	-0.2870127123
C	1.5676791128	2.7263916225	0.4355798869
C	3.4009290789	-0.0760415716	-0.8237820183
H	4.4738474232	-0.1631916201	-0.9814862603
C	0.4175350917	3.3918264633	0.8810600089
H	0.5374575413	4.4237955678	1.2028428811
C	-3.2999321947	0.2372646739	0.7440608661
H	-4.3431801420	0.2612809667	1.0475661587
C	-0.4605351007	-2.9522618014	-1.6100306528
H	-0.6168654118	-3.9247979859	-2.0710125709
C	3.1024078714	-2.3701994418	-1.8585096588
C	2.0125438021	-3.1605511683	-2.1142243074
C	-2.9007692928	-2.9380462672	-0.9355852171
C	-3.6870954796	-2.0618285916	-0.2363371847
C	-3.0544915445	2.6233878369	1.5486031838
C	-2.0185904457	3.5192258884	1.5568919325
C	2.9093228495	3.2841119373	0.4363274723
C	3.7542976706	2.2940395223	0.0015428545
H	-3.1726197160	-3.9012643356	-1.3524959402
H	-4.7349781186	-2.1552892212	0.0231242096
H	-4.0749855165	2.7701374944	1.8828947803
H	-2.0199436706	4.5461485426	1.9044629084
H	3.1598379929	4.2927088014	0.7457015426
H	4.8311210071	2.3346678338	-0.1195838197
H	4.1440004735	-2.5660530160	-2.0869857310
H	1.9854624681	-4.1337838534	-2.5910791775
N	-0.3190317591	0.8614644108	-1.8961891979
H	0.5104612820	1.0318401798	-2.5032718693
O	-1.3791582065	1.1977230280	-2.4723524963
N	0.4220108278	-0.6684516978	1.7221591430
C	0.3715544163	-2.0040145554	2.1022663989
C	0.7883139318	0.0125073357	2.8004193432
H	0.9246003582	1.0817522650	2.8582570306
C	0.7128418820	-2.1405151174	3.4336198289
N	0.9759741568	-0.8356376496	3.8623510113

H	0.0916369643	-2.7740500337	1.3994503938
C	0.8181049164	-3.3400345839	4.3330327726
H	1.8348666560	-3.4705666001	4.7304142264
H	0.1322926282	-3.2754355387	5.1898462783
H	0.5631811551	-4.2452724958	3.7729257047
H	1.2556696144	-0.5593193653	4.7952806863
Fe	-0.0135511435	0.1753885316	-0.2598355116
O	2.1162216813	1.6226846617	-3.5622154768
H	2.2763765338	2.4751550898	-3.1147743270
H	2.7249203190	1.0089950552	-3.1054945326
H	-3.4350691845	0.9860290464	-2.3543971713
O	-4.2939128839	0.6767398765	-2.7041207635
H	-4.0367383445	-0.1373504165	-3.1734453444

Table S18. The SCF Energies of All Structures Optimized by using the mPWVWN method Described in the Text

Compound	E (Hartrees)
1	-131.34503
2	-5841.03125
3	-7126.74936
4	-2779.67104
5	-2779.67036
6	-2659.99393
7	-2659.77029
13	-2660.63454
14	-2737.61552
15	-2737.61781
16	-2814.53615