Supporting Information

Insight Into the Preferential *N*-binding versus *O*-binding of Nitrosoarenes to Ferrous and Ferric Heme Centers

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Protocol for Liquid Chromatography and Mass Spectrometry. Sample introduction was performed using a Waters (Milford, MA) Acquity Ultra High-Pressure Liquid Chromatography (UPLC) M-Class system. Optimum LCMS Grade Methanol (Fisher Scientific, Pittsburg, PA) was used as mobile phase carrier at 20 µL/min for injection of 2 µL sample. The UPLC eluent was introduced into a Waters G2-Si Ion Mobility Q-TOF Mass Spectrometer equipped with an electrospray ionization source operated in positive ion mode. Nitrogen gas was used as a nebulizing and drying gas with a drying gas temperature of 325ºC at 10 L/min flow rate. Capillary voltage was set at 3.2kV. Data was collected and analyzed with Mass Lynx Software (V4.1, 2015).

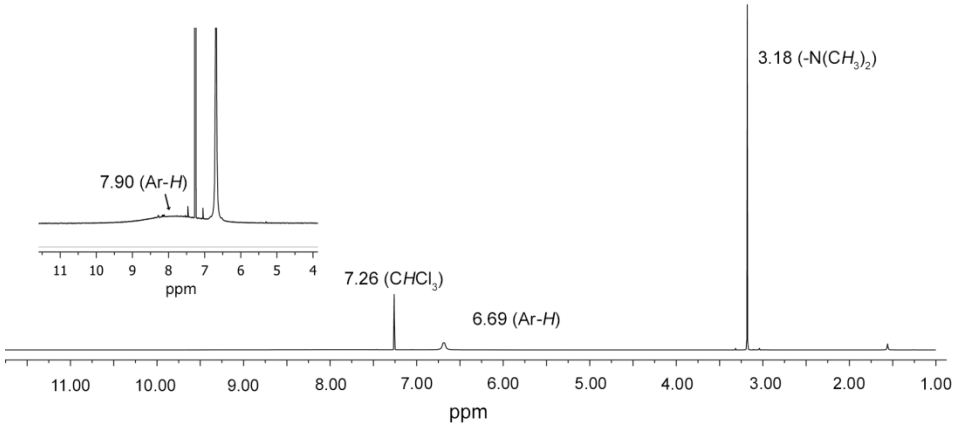


Figure S1. ^{1}H NMR spectrum of NODMA in $CDCl_3$ at 25 °C. Inset is the zoomed-in aromatic region showing a broad peak assigned to *ortho*-Ar-*H* to the NO group. The spectrum is the same as that reported for the ^{15}N-labeled analog [1-3]

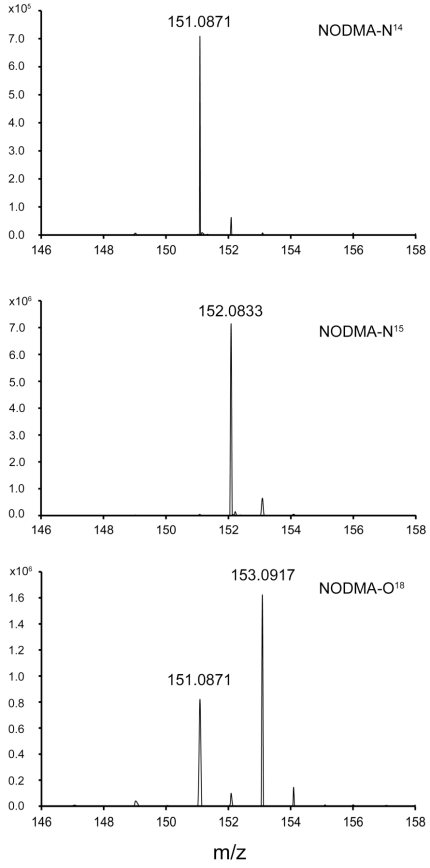


Figure S2. Truncated mass spectra for (*top*) unlabeled (^{14}N-nitroso) NODMA; (*middle*) ^{15}N-nitroso NODMA; and (*bottom*) $^{18/16}$O-nitroso NODMA in a 2:1 ratio, showing their respective molecular ion peaks (positive ion mode).

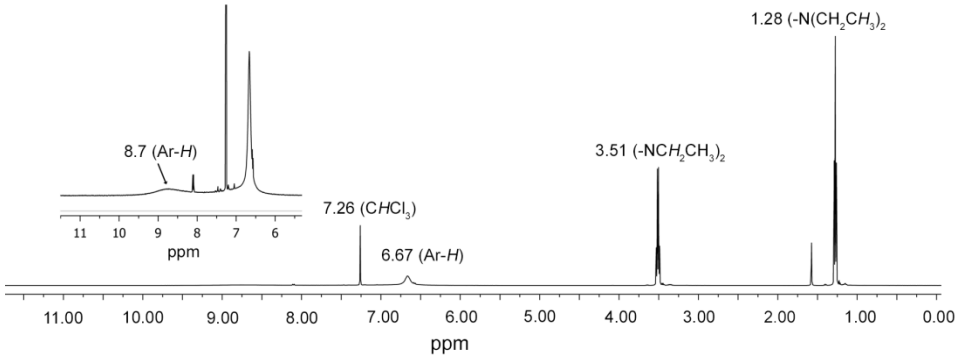


Figure S3. ^{1}H NMR spectrum of NODEA in $CDCl_3$ at 25 °C. Inset is the zoomed-in aromatic region showing a broad peak assigned to *ortho*-Ar-*H* to the NO group. The spectrum is the same as that reported for the labeled analog.[1, 3]

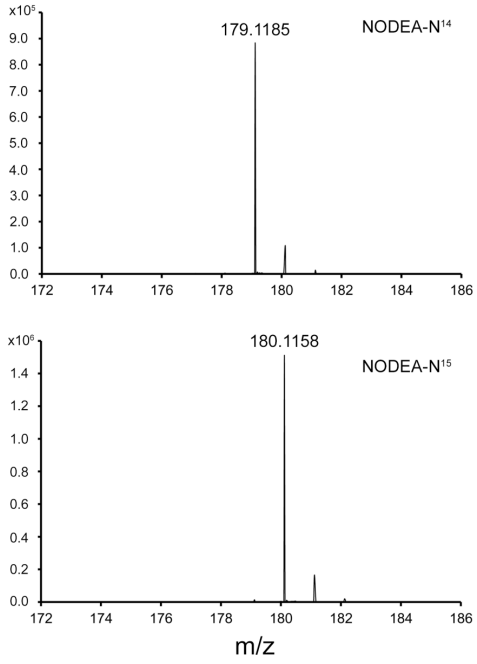
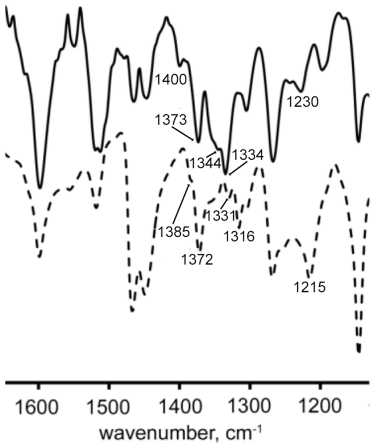


Figure S4. Truncated mass spectra for (*top*) unlabeled (^{14}N-nitroso) NODEA; and (*bottom*) ^{15}N-nitroso NODEA, showing their respective molecular ion peaks (positive ion mode).

Figure S5. See separate movie file



NO	^{15}NO (Δυ)
1400	1385 (-15)
1373	1372 (-1)
1344	1331 (-13)
1334	1316 (-18)
1230	1215 (-15)

Figure S6. Truncated FTIR spectra of crystals of the unlabeled (^{14}N-nitroso; solid line trace) and labeled (^{15}N-nitroso; broken line trace) (OEP)Fe(NODEA)($NH_2C_6H_4NEt_2$-*p*) as KBr pellets, highlighting bands that shift with ^{15}N-nitroso substitution.

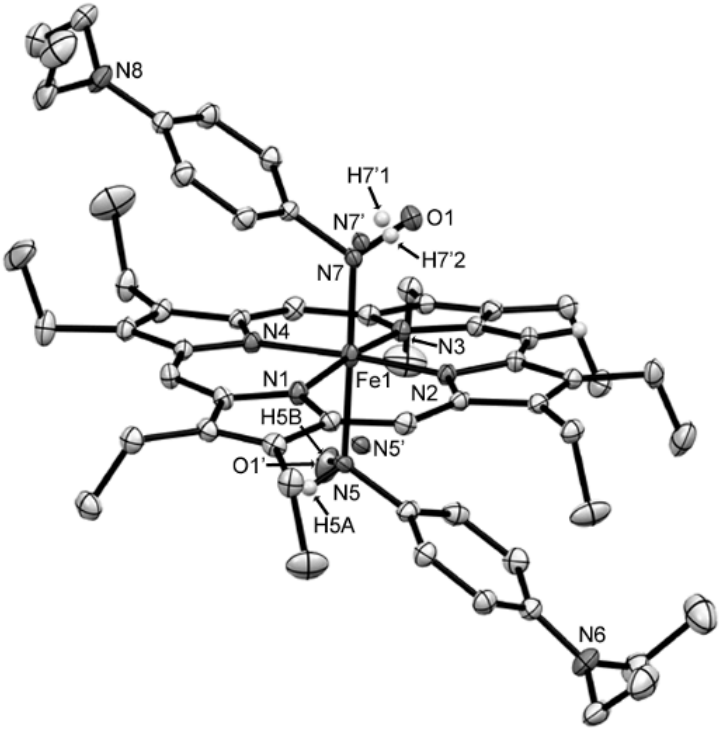
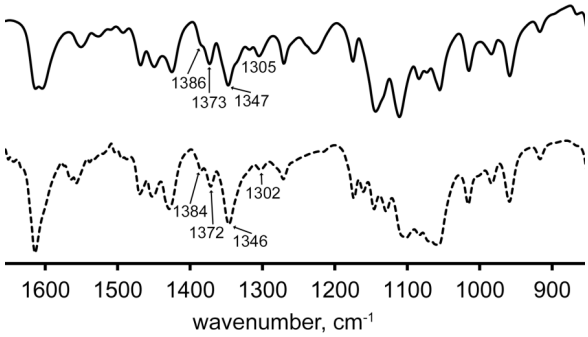
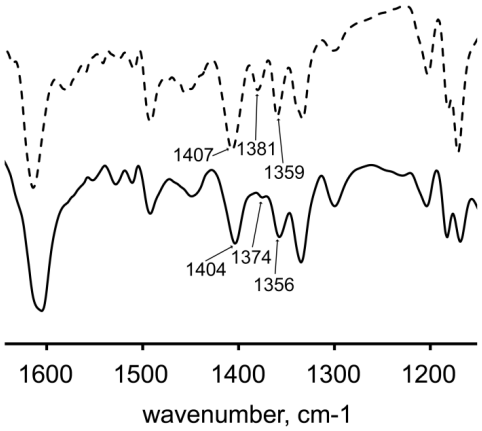


Figure S7. Molecular structure of (OEP)Fe(NODEA)($NH_2C_6H_4NEt_2$-*p*) showing the disordered fragments, with thermal ellipsoids drawn at 35% probability. Hydrogen atoms except for those of the NH_2 moieties have been omitted for clarity.



NO	^{15}NO (Δυ)
1386	1384 (-2)
1373	1372 (-1)
1347	1346 (-1)
1305	1302 (-2)

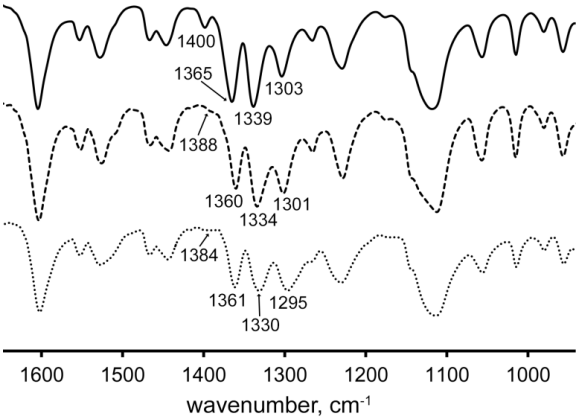
Figure S8. Truncated FTIR spectra (KBr pellets) of crystals of the unlabeled (^{14}N-nitroso; solid line trace) and labeled (^{15}N-nitroso; broken line trace) [(OEP)Fe(NODEA)]SbF_6 adducts obtained from the reactions of (OEP)Fe($FSbF_5$) with unlabeled and ^{15}N-nitroso labeled NODEA, respectively, highlighting bands that shift with ^{15}N-nitroso substitution.



ferric
[(TTP)Fe(NODMA)]$^+$

NO	^{15}NO (Δυ)
1407	1404 (-3)
1381	1374 (-7)
1359	1356 (-3)

Figure S9. Truncated FTIR spectra (KBr pellets) of crystals of the unlabeled (^{14}N-nitroso; solid line trace) and labeled (^{15}N-nitroso; broken line trace) [(TTP)Fe(NODMA)]SbF_6 adducts obtained from the reactions of (TTP)Fe($FSbF_5$) with unlabeled and ^{15}N-nitroso labeled NODMA, respectively, highlighting bands that shift with ^{15}N-nitroso substitution.



NO	^{15}NO (Δυ)	N^{18}O (Δυ)
1400	1388 (-12)	1384 (-16)
1365	1360 (-5)	1361 (-4)
1339	1334 (-5)	1330 (-9)
1303	1301 (-2)	1295 (-8)

Figure S10. Truncated FTIR spectra (KBr pellets) of crystals of the unlabeled (^{14}N-nitroso; solid line trace) and labeled (^{15}N-nitroso = broken line trace, and ^{18}O-nitroso = dotted line trace) product prepared from the in situ reduction of (OEP)FeCl by Zn/Hg followed by reaction with excess NODMA, highlighting bands that shift with ^{15}N- and ^{18}O-nitroso substitution.

Table S1. Crystal Data and Structural Refinement

Compound	(OEP)Fe(NODEA)($NH_2C_6H_4NEt_2$-*p*)[a]	[(OEP)Fe(NODEA)]SbF_6•(CH_2Cl_2)[b]	[(TTP)Fe(NODMA)]SbF_6[b]
CCDC	2011046	2011047	2011048
Empirical Formula	$C_{56}H_{74}FeN_8O$	$C_{47}H_{60}FeN_6OCl_2F_6Sb$	$C_{56}H_{46}FeN_6O_1F_6Sb$
Formula weight	931.08	1087.51	1110.59 (1181.485)[c]
Crystal system	Monoclinic	Triclinic	Monoclinic
Space group	$P2_1/n$	$P\bar{1}$	$P2_1/c$
a (Å), α(°)	14.1052(13), 90	13.2553(8), 79.6981(10)	21.4336(11), 90
b (Å), β(°)	14.6434(15), 105.549(3)	13.6557(8), 77.0265(10)	15.7973(8), 97.599(2)
c (Å), γ(°)	24.980(2), 90	15.0672(9), 64.4348(9)	16.4555(8), 90
V, *Z/Z'*	4970.7(8) $Å^3$, 4	2387.1(2) $Å^3$, 2	5522.8(5) $Å^3$, 4
D(calcd), g/cm^3	1.244	1.513	1.336 (1.421)[c]
Abs coeff, mm^{-1}	0.352	1.048	0.814 (0.91)[c]
F(000)	2000	1114	2252
Crystal size (mm)	0.040 x 0.156 x 0.173	0.080 x 0.240 x 0.420	0.024 x 0.132 x 0.233
θ range for data collection	2.191–27.366°	1.393-29.784°	2.310–25.383°
Reflections collected	72590	55564	80385
Independent reflns	11216 [R_{int} = 0.0828]	13621 [R_{int} = 0.0400]	10138 [R_{int} = 0.0842]
Data / restraints / parameters	11216 / 51 / 611	13621 / 624 / 654	10138 / 1157 / 708
Goodness-of-fit on F^2	1.027	1.005	1.053
Final R indices [$I>2\sigma(I)$]	R1 = 0.0468	R1 = 0.0417	R1 = 0.0636
R indices (all data)	wR2 = 0.1064	wR2 = 0.1056	wR2 = 0.1637
Largest diff. peak and hole, e.$Å^{-3}$	0.419 and –0.732	1.495 and –0.573	0.573 d –0.965

[a] Using a D8 Quest κ-geometry diffractometer with a Bruker Photon II cmos area detector and an Incoatec Iμs microfocus Mo Kα source.
[b] Using a diffractometer with a Bruker APEX ccd area detector and graphite-monochromated Mo Kα radiation.
[c] Data in brackets represent corresponding values when the squeezed solvent is included.

Cartesian coordinates of DFT-optimized iron porphyrins with favorable spin states

(i) Fe^{II}-N (bis NODMA) *S*=0

Fe	3.41371700	3.43764000	5.27106300
O	4.67688700	5.61569800	3.98042700
N	1.64173100	4.10455300	5.97380000
N	2.75701200	3.64969800	3.37451900
N	4.30801300	5.25261300	5.07353200
N	6.49356100	8.12552800	9.35725700
C	1.24786800	4.16128100	7.27716200
C	-0.12805600	4.59229900	7.36308300
H	-0.67758500	4.72706200	8.28622400
C	-0.55909300	4.77027300	6.08998500
H	-1.53724300	5.08184300	5.74599700
C	0.55384800	4.44388100	5.22860200
C	0.49152400	4.43123000	3.84214100
C	1.52224500	4.06518400	2.98783100
C	1.43702200	4.11340700	1.54532300
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C	3.47137300	3.46067200	2.23215800
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C	4.85194000	6.00460900	6.15007700
C	4.08783600	6.24836500	7.28873200
H	3.06474000	5.89833000	7.33077900
C	4.61891800	6.97130900	8.33826300
H	3.99280700	7.15972800	9.20121400
C	5.95291400	7.43877300	8.29808700
C	6.71270100	7.17386900	7.13336000
H	7.74509700	7.49340700	7.06468700
C	6.16088200	6.48587600	6.07110300
H	6.75083600	6.26938800	5.18669600
C	5.75464700	8.22645500	10.59922900
C	7.88194500	8.53458100	9.32005600
N	5.19571000	2.78784200	4.56866900
N	4.06956000	3.21578700	7.16867100
C	5.59583200	2.75222600	3.26618600
C	6.97830100	2.34414000	3.18143900
H	7.53400700	2.22912200	2.25931000
C	7.40575000	2.15400600	4.45444500
H	8.38652600	1.85099100	4.79865600
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C	6.33847500	2.44237500	6.70154000
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C	5.38345100	2.73335200	8.99752100
H	6.25906500	2.42778400	9.55619900
C	4.16940100	3.10968400	9.46674500
H	3.83552900	3.18241000	10.49415900
C	3.35565900	3.40594600	8.31107700
C	2.04001100	3.84107500	8.37217300
O	2.09080400	1.29702700	6.54258700
N	2.52254600	1.62283600	5.46029600
N	0.69553000	-1.51931500	1.19729400
C	2.06688900	0.81245700	4.38569400
C	2.89527900	0.56798900	3.29280600
H	3.89933800	0.97025900	3.28422900
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H	3.12939700	-0.40869400	1.42444300
C	1.14712200	-0.76175400	2.24888500
C	0.31895800	-0.49342400	3.36585400
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C	0.78183500	0.26385200	4.42261100
H	0.14008700	0.47885000	5.27037200
C	1.50570700	-1.64722900	0.00332100
H	2.45056500	-2.16455700	0.21253400
H	0.96267300	-2.23438000	-0.73849100
H	1.73883000	-0.66873800	-0.43873500
C	-0.66524500	-2.01413800	1.19312300
H	-1.40348100	-1.19936200	1.18920300
H	-0.82413300	-2.62085100	0.30054500
H	-0.85865600	-2.64994600	2.06553000
H	-0.44670100	4.73436700	3.38607200
H	5.24805300	2.97064100	1.18689700
H	7.27634800	2.13916000	7.15827800
H	4.82720900	8.79813500	10.46900400
H	5.49646200	7.23763600	11.00306400
H	6.36419900	8.74753300	11.33877800
H	8.07786700	9.19196600	8.46456600
H	8.11567400	9.09487500	10.22646300
H	8.56756300	7.67683200	9.26059700
H	1.59064900	3.93741300	9.35646400

(ii) Fe^{II}-O (bis NODMA) *S* = 0

Fe	3.94447600	5.24617900	4.93258200
O	5.54356200	5.20137600	6.10572100
N	3.00283300	6.52092700	6.18079700
N	3.20624600	3.68192600	5.97079600
N	4.88618800	3.97144500	3.68441300

N	4.68271000	6.81044500	3.89438600
N	5.98203700	6.24458300	6.57497600
N	10.43016500	5.93824600	9.91144000
C	3.02941600	7.88005800	6.13210700
C	2.24108700	8.43656700	7.20786700
H	2.10033200	9.49482200	7.38991400
C	1.74126400	7.38566700	7.90325600
H	1.10335300	7.39658100	8.77826600
C	2.22709700	6.19212800	7.24909100
C	1.93709800	4.90022500	7.66482500
C	2.39526700	3.73730200	7.06185400
C	2.06855600	2.40362300	7.51279200
H	1.43836600	2.17397100	8.36297500
C	2.69794000	1.54746800	6.67096800
H	2.69520400	0.46455500	6.68316400
C	3.40646200	2.36189100	5.71022700
C	4.17627600	1.85480100	4.67336000
C	4.85974800	2.61231500	3.73321700
C	5.64798700	2.05580000	2.65739400
H	5.78884900	0.99754400	2.47543000
C	6.14754100	3.10669300	1.96180300
H	6.78531400	3.09577500	1.08669100
C	5.66170800	4.30023600	2.61596000
C	5.95158900	5.59213900	2.20014900
C	5.49356300	6.75506000	2.80323600
C	5.82041000	8.08873600	2.35238800
H	6.45052000	8.31838200	1.50214300
C	5.19131700	8.94490000	3.19442000
H	5.19423100	10.02781400	3.18234400
C	4.48274000	8.13048600	4.15512700
C	3.71303500	8.63757700	5.19207200
C	7.09812000	6.08691800	7.39579500
C	7.61651200	7.26334600	7.94863500
H	7.12974700	8.20350500	7.70683800
C	8.71698200	7.22542400	8.78000600
H	9.09538700	8.15183400	9.19305800
C	9.34052500	5.99156200	9.08755600
C	8.80178200	4.80581800	8.51593400
H	9.25318900	3.84465800	8.72841100
C	7.70450800	4.85356100	7.68877300
H	7.29384000	3.94800100	7.25460100
C	10.96373300	7.15614800	10.48911600
H	11.82153400	6.91106100	11.11609600
H	10.22012800	7.66438000	11.11639200
H	11.30015200	7.85685500	9.71413600
C	11.05592300	4.66593000	10.21631000

H	11.43344300	4.17387500	9.31097400
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H	11.90131900	4.83335900	10.88438000
H	6.59159900	5.70244100	1.32900700
H	4.24675200	0.77368700	4.58824800
H	1.29694600	4.78993500	8.53586400
H	3.64271700	9.71869200	5.27730300
O	2.34543700	5.29094100	3.75954000
N	1.90704100	4.24776500	3.29013800
C	0.79090000	4.40548500	2.46939800
C	0.27252100	3.22909700	1.91647300
C	0.18440600	5.63884000	2.17664900
H	0.75935300	2.28893600	2.15812500
C	-0.82804300	3.26705500	1.08522200
C	-0.91294000	5.68662300	1.34958600
H	0.59498900	6.54435600	2.61099400
H	-1.20644300	2.34066500	0.67213200
C	-1.45160400	4.50093300	0.77776300
H	-1.36454600	6.64776000	1.13744200
N	-2.54120400	4.55432200	-0.04619500
C	-3.07645400	3.33617300	-0.62178100
C	-3.16770200	5.82650800	-0.35004400
H	-3.93460400	3.58127000	-1.24828300
H	-3.41269900	2.63666500	0.15437200
H	-2.33390700	2.82657100	-1.24918400
H	-2.47081400	6.51112300	-0.85002100
H	-3.54673600	6.31721700	0.55542700
H	-4.01202700	5.65927200	-1.01952000

(iii) Fe^{III}-O (mono NODMA) *S* = 3/2

Fe	3.90795600	5.33070000	4.94146300
O	5.57465900	5.08919500	6.15002500
N	2.83853900	6.40499300	6.22665400
N	2.99395900	3.68569900	5.58733700
N	4.65382200	4.28992200	3.41907900
N	4.49644200	7.00964400	4.05597800
N	5.95263900	6.14027300	6.72436800
N	10.33336300	6.00541500	10.05673000
C	2.85909600	7.76859500	6.38742400
C	2.07184600	8.15427800	7.52017200
H	1.92308500	9.17530200	7.84529400
C	1.57468800	7.01288400	8.05867100
H	0.93077500	6.89636500	8.92009000
C	2.05542600	5.93163900	7.25146000
C	1.75113600	4.60774200	7.48485900

C	2.18638000	3.56708400	6.69274500
C	1.83643000	2.19635300	6.91649100
H	1.20266200	1.84825900	7.72107500
C	2.43730300	1.47402400	5.93816300
H	2.40281700	0.40620300	5.76852700
C	3.15725400	2.40375800	5.12045600
C	3.90756700	2.03783600	4.02376700
C	4.60180100	2.92932500	3.23450200
C	5.38027900	2.54504400	2.09542000
H	5.48833900	1.52888900	1.74051400
C	5.91712500	3.68195400	1.58629200
H	6.55946200	3.79850300	0.72372000
C	5.46225200	4.75998400	2.41226400
C	5.79369100	6.08075600	2.19866800
C	5.32812000	7.12496900	2.96846000
C	5.64954200	8.49925000	2.72384000
H	6.28044500	8.84760800	1.91710500
C	5.00867100	9.22591800	3.67316000
H	5.00115200	10.29874100	3.81207500
C	4.30032000	8.29443400	4.49916700
C	3.53881200	8.66168900	5.58759800
C	7.03219700	6.02458100	7.52286900
C	7.45185600	7.21675000	8.16635300
H	6.88786200	8.12477800	7.97671200
C	8.53449000	7.22146200	9.00002600
H	8.83187400	8.14585800	9.47678600
C	9.26665800	6.01688300	9.23912200
C	8.83351300	4.81476800	8.58252100
H	9.36811800	3.88797200	8.74491800
C	7.75279800	4.81900700	7.75256400
H	7.42858400	3.90960000	7.25890000
C	10.76787800	7.22942900	10.72319700
H	11.63794700	7.01068900	11.34006800
H	9.97966600	7.62431300	11.37278500
H	11.05037600	7.99559600	9.99352800
C	11.07872400	4.77258700	10.29551200
H	11.50101500	4.38061800	9.36442200
H	10.44127100	4.00846700	10.75244100
H	11.90071900	4.98039000	10.97857400
H	3.46544900	9.71730100	5.82552300
H	1.11587000	4.37238600	8.33168700
H	3.95087300	0.98586100	3.76381000
H	6.44485400	6.31405500	1.36342200

(iv) Fe^{III}-O (mono NODMA) *S* = 5/2

Fe	4.08298100	5.24795500	5.05335900
O	5.76348300	5.01456000	6.26854000
N	2.82883100	6.39043700	6.29685600
N	2.90403000	3.57572000	5.55635100
N	4.62930400	4.20570000	3.30641300
N	4.55717200	7.02490500	4.03597600
N	6.10566700	6.08290900	6.83130100
N	10.47838200	6.11529100	10.19121500
C	2.88362400	7.76049600	6.43980400
C	2.04286600	8.15590300	7.56117900
H	1.89165900	9.17278300	7.89891500
C	1.49489900	7.02102100	8.05452100
H	0.80435800	6.91586800	8.88089100
C	2.00382300	5.92858700	7.23923200
C	1.65010200	4.55887100	7.41159100
C	2.04898500	3.49819100	6.63623400
C	1.61042500	2.11927600	6.79881400
H	0.93131300	1.76779700	7.56440500
C	2.19762700	1.40595900	5.81012600
H	2.10023000	0.34919400	5.59919700
C	3.00111000	2.34537400	5.04389000
C	3.76474100	1.99828800	3.89230700
C	4.49067700	2.84993400	3.09700100
C	5.20402500	2.47861800	1.88345900
H	5.26081900	1.47818800	1.47512700
C	5.74171800	3.61677600	1.38655200
H	6.33169600	3.74090100	0.48807400
C	5.36226000	4.68586100	2.29699200
C	5.71108800	6.05577000	2.11544100
C	5.33120100	7.11714600	2.89930400
C	5.64674100	8.51665000	2.64986600
H	6.23564600	8.88477400	1.82009300
C	5.04698500	9.22954500	3.63165400
H	5.04453500	10.30242800	3.77234100
C	4.36783000	8.26753500	4.48614300
C	3.59168000	8.61369900	5.63025200
C	7.18780600	6.00965900	7.64142500
C	7.56867100	7.21838200	8.27246900
H	6.98032000	8.10835800	8.07112700
C	8.64773500	7.26425100	9.11233100
H	8.91500400	8.20249600	9.57995900
C	9.41317000	6.08600400	9.36815100
C	9.01780900	4.86619600	8.72435400
H	9.57707300	3.95635400	8.89942100

C	7.94032100	4.83030300	7.88842300
H	7.64454700	3.90663100	7.40349200
C	10.87267600	7.35860600	10.84443600
H	11.74791800	7.17420900	11.46546200
H	10.07148300	7.73696900	11.48838900
H	11.13293700	8.12605700	10.10748100
C	11.25731000	4.90794600	10.44610500
H	11.69254100	4.51579200	9.52080500
H	10.64166100	4.13069900	10.91132000
H	12.07209500	5.14710300	11.12778100
H	3.53184500	9.67331600	5.86212100
H	0.96634500	4.34125700	8.22702700
H	3.74096000	0.95222300	3.60087100
H	6.31771000	6.28085900	1.24298400

(v) Fe^{III}-N (mono NODMA) *S* = 3/2

Fe	3.57032000	3.46746200	5.19445500
N	2.13142200	4.50776700	6.13504200
N	2.98905600	4.26513700	3.45007700
C	1.90279100	4.54504700	7.49858000
C	0.71349900	5.33645600	7.77797000
H	0.31946200	5.52836700	8.76690700
C	0.23480300	5.74419000	6.58648500
H	-0.63775900	6.34843100	6.37804700
C	1.14016000	5.21552300	5.57905900
C	0.98353200	5.44695900	4.19397400
C	1.85211300	5.02450900	3.23107300
C	1.74653900	5.36041000	1.82073800
H	0.94751200	5.94493200	1.38482000
C	2.82874200	4.82989900	1.21735600
H	3.11323900	4.88011500	0.17481000
C	3.58808000	4.14889900	2.25272000
C	4.77827600	3.43864500	2.00346000
N	5.15295200	2.63885800	4.28022000
N	4.28247000	2.84680100	6.96509200
C	5.48426200	2.74100500	2.94680900
C	6.68191000	1.96172800	2.67198600
H	7.15588000	1.88058400	1.70283500
C	7.04855800	1.39411000	3.83920800
H	7.89089700	0.74623600	4.04088100
C	6.08812100	1.83875000	4.83185600
C	6.16296800	1.49322700	6.19373300
C	5.33730100	1.97934100	7.16916100
C	5.46339300	1.67536800	8.58616500
H	6.21094500	1.02019000	9.01267500

C	4.49384200	2.37044700	9.21279000
H	4.26570300	2.41062200	10.26936000
C	3.76605200	3.08710800	8.17815900
C	2.64867700	3.90942900	8.44510800
O	1.58096500	1.48801800	6.37283000
N	2.10400100	1.59425100	5.27527400
N	0.81125800	-2.04617600	1.27319000
C	1.74777300	0.66164200	4.30797500
C	2.36218400	0.76457700	3.05004500
H	3.08525500	1.55334600	2.87967000
C	2.06203000	-0.12260200	2.04295400
H	2.55589900	-0.01643800	1.08573300
C	1.11871300	-1.16480800	2.25611000
C	0.50312900	-1.25597900	3.54053800
H	-0.22032300	-2.03568900	3.74185900
C	0.81150300	-0.36679300	4.53723300
H	0.33962200	-0.44263600	5.51070000
C	1.44624900	-1.93934800	-0.03061700
H	2.53419700	-2.05390400	0.04466200
H	1.06862600	-2.72869200	-0.67961400
H	1.22396500	-0.97586100	-0.50454300
C	-0.15415700	-3.10954500	1.51022100
H	-1.14052300	-2.70432900	1.76391300
H	-0.25832200	-3.70602900	0.60454600
H	0.17423900	-3.77443100	2.31738200
H	6.96156900	0.82209800	6.49208800
H	5.15029400	3.43455500	0.98425500
H	0.12988100	6.04060500	3.88413200
H	2.35154800	4.01673800	9.48302200

(vi) Fe^{III}-N (mono NODMA) *S* = 5/2

Fe	3.44959700	3.27847200	5.19487300
N	2.05384900	4.47729700	6.19194900
N	2.96400600	4.23280400	3.40600700
C	1.83314600	4.50736200	7.55473100
C	0.66207000	5.33202700	7.82368600
H	0.25762900	5.53658300	8.80601800
C	0.21556600	5.77577100	6.62716100
H	-0.63041200	6.41916000	6.42527600
C	1.11246100	5.22422000	5.61963500
C	1.00927100	5.47092800	4.21803300
C	1.85866800	5.04041400	3.22634900
C	1.77554200	5.41831900	1.82509700
H	1.00981300	6.05149900	1.39686000
C	2.84079600	4.85815000	1.20409600

H	3.12309200	4.93565900	0.16247600
C	3.57378300	4.12143400	2.21826300
C	4.77010600	3.38898100	1.98421800
N	5.18239200	2.57826700	4.24816600
N	4.29476100	2.83877400	7.04358500
C	5.50900000	2.69515300	2.91669500
C	6.75742900	1.98972700	2.67069000
H	7.25495300	1.91864600	1.71248100
C	7.15696300	1.47940900	3.86013600
H	8.04846400	0.90552100	4.07539900
C	6.15773100	1.87431700	4.83768900
C	6.23478500	1.58645400	6.23101900
C	5.40157000	2.03336200	7.22731700
C	5.55378500	1.76272100	8.64892900
H	6.33986000	1.16241600	9.08735100
C	4.54662000	2.41161200	9.27897900
H	4.33625400	2.44927800	10.33948000
C	3.76933200	3.07493800	8.24535500
C	2.60516100	3.86925700	8.48831000
O	1.59774500	1.41447400	6.34817400
N	2.10078100	1.52414800	5.23897800
N	0.75557400	-2.07375400	1.22876200
C	1.73790000	0.60724600	4.26803400
C	2.34773000	0.71030100	3.00556100
H	3.08156500	1.48867500	2.83103200
C	2.03247000	-0.16874100	1.99838100
H	2.52321100	-0.06487000	1.03949100
C	1.07756100	-1.20233000	2.21240200
C	0.46738800	-1.29292400	3.50088400
H	-0.26427200	-2.06472400	3.70228400
C	0.79120600	-0.41322900	4.49913800
H	0.32361200	-0.48771500	5.47463800
C	1.38393200	-1.96809000	-0.07964400
H	2.47059100	-2.09518800	-0.01061700
H	0.99348900	-2.75051500	-0.72917500
H	1.16840600	-1.00028400	-0.54714300
C	-0.22094800	-3.12846700	1.46513600
H	-1.20123500	-2.71288200	1.72453500
H	-0.33512000	-3.71931500	0.55716800
H	0.10463700	-3.79996800	2.26758000
H	7.07538900	0.97189700	6.54017600
H	5.14785500	3.40138400	0.96603200
H	0.18570600	6.10789300	3.90865800
H	2.31208200	3.97716600	9.52839500

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