Supporting Information

Captions for Supporting Information Figures

Figure S1. Formal diagram of the porphyrinato core of [Fe(Deut)(NO)] displaying the perpendicular displacements (in units of 0.01 Å) of the core atoms from the 24-atom mean porphyrin plane. Pyrrole rings are designated I to IV based upon a standard nomenclature. Positive displacements are towards the nitrosyl coordinated face of the porphyrin. The projection of the nitrosyl ligand is shown.

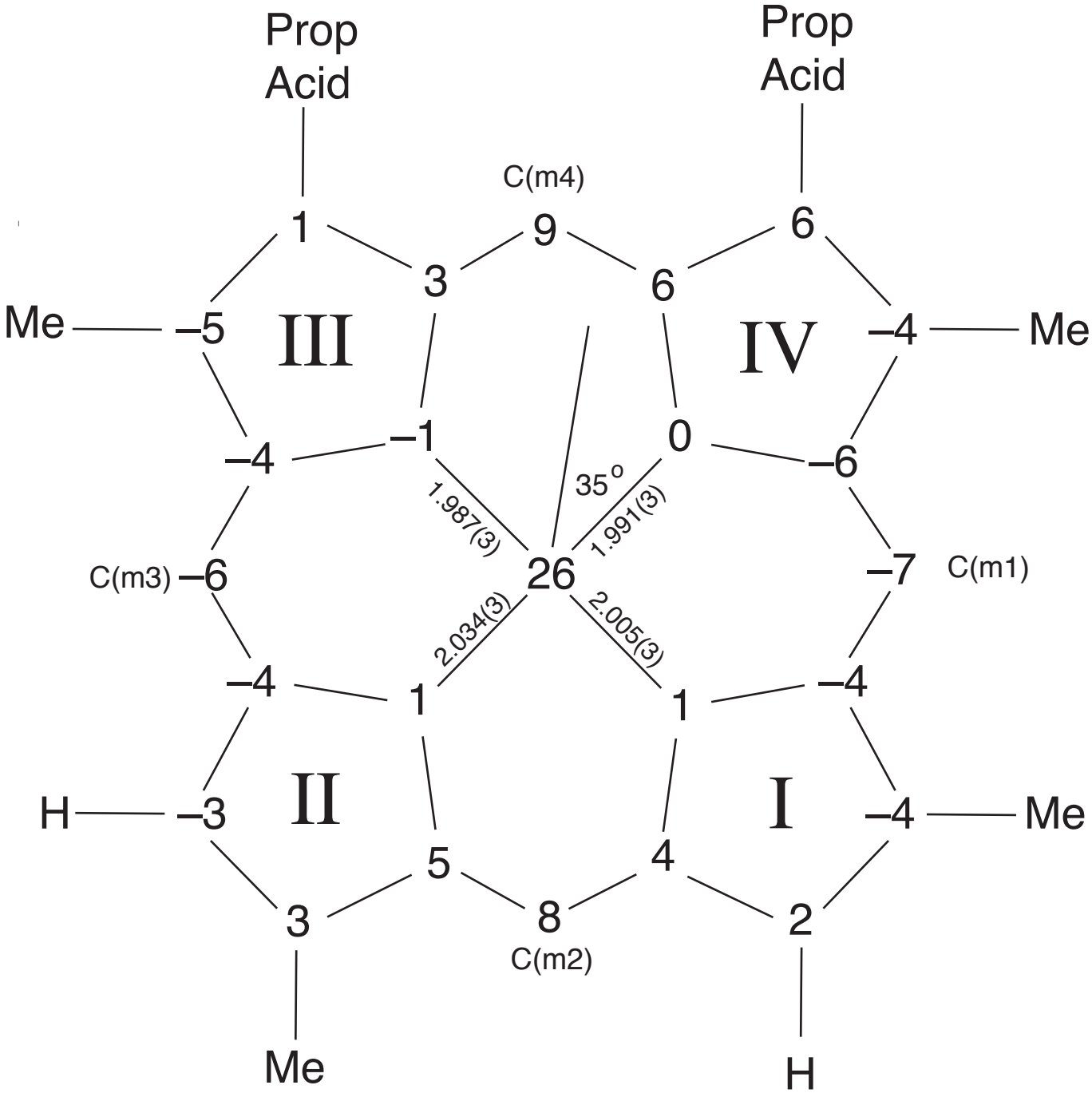
Prop
Acid
Prop
Acid
C(m4)
1
9
6
3
6
Me
–5
III
IV
–4
Me
–4
–1
0
–6
1.987(3)
35°
1.991(3)
C(m3)
–6
26
–7
C(m1)
2.034(3)
2.005(3)
–4
1
1
–4
H
–3
II
I
–4
Me
5
4
3
8
2
C(m2)
Me
H

Table S1A. Summary of Nitrosyl Geometry in Five-coordinate Heme Protein Derivatives.

Complex	PDB Code	Resolution[a]	Fe–N_{NO}[a]	∠FeNO[b]	N–O[a]	ϕ[b,c]	ϕ^* [b,d]	ref
(T243N-P450nor)NO	1F25	1.4	1.9[e]	131[e]	1.45[e]	41	−49	18
(cytc')NO **(1)**[f]	1E85	1.35	2.0	124	1.16[e]	24	−114	19
(NP1)NO **(I)**[g]	4NP1	2.3	NA	125	NA	44	134	20
(NP1)NO **(II)**[h]	4NP1	2.3	NA	135	NA	45	135	20
(eNOS)NO(+4HB)[i,j]	1FOP	2.30	1.80	160	1.15	44	136	21
(eNOS)NO(−4HB)[i,k]	1FOO	2.00	1.80	160	1.14	34	146	21
(α-Hb)NO	− − −	2.8	1.74	145	1.1	25	245	22
(NP4)NO **(I)**[l]	1ERX	1.4	2.0	110	NA	1	269	23
(T243A-P450nor)NO	1F24	1.4	2.1[e]	120[e]	1.42[e]	14	−284	18
(T243V-P450nor)NO	1F26	1.4	2.0[e]	119[e]	1.36[e]	16	−286	18
(cytc')NO **(2)**[m]	1E85	1.35	2.0	132	1.17[e]	38	−322	19
(α-T-Hb_A)NO	− − −	2.2	1.74	150	1.13	NA	NA	24

Table S1B. Summary of Nitrosyl Geometry in Six-coordinate Protein Derivatives.

Complex	PDB Code	Resolution[a]	Fe–N_{NO}[a]	∠FeNO[b]	N–O[a]	Fe–L[a]	ϕ[b,c]	ϕ^* [b,d]	ref
(cd_1-NIR(*tp*))NO	1AOM	1.8	2.0	131	1.35[e]	1.99[e]	30	120	25
(SiRHP)NO	6GEP	1.80	1.76	125	1.17[e]	2.65[n]	40	−140	26
(hh-Mb)NO	1NPF	1.90	2.03	147	1.14	2.11	∼10	∼−190	27
(sw-L29F-Mb)NO	IJDO	1.7	1.86[e]	130	1.14[e]	NA	11	−191	28
(sw-Mb)NO	1HJT	1.7	1.89	112	1.15	2.18	25	−205	29
(α-SNO-nitrosylHbA)NO	1BUW	1.8	1.75	131	1.13	2.28	44	−224	30
(β-SNO-nitrosylHbA)NO	1BUW	1.8	1.74	123	1.11	2.28	34	−236	30
(β-Hb)NO[o]	—	2.8	1.74	145	1.1	NA	15	255	22
(fungal-NOR)NO	1CL6	1.7	1.63	161	1.16	2.31[n]	28	−298	31
(S286T-fungal-NOR)NO	1CMJ	1.7	1.65	162	1.13	2.33[n]	29	−299	31
(S286V-fungal-NOR)NO	1CMN	1.7	1.62	162	1.13	2.37[n]	45	−315	31
(SHP)NO	1DW2	2.2	1.8	112	1.36[e]	2.16[e]	45	315	32
(cd_1-NIR(*pa*))NO	1NNO	2.65	1.8	135	1.15	1.99[e]	26	334	33
(lupin-Lb^{II})NO	1GDL	1.8	1.72	147	1.355[e]	2.20	2	358	34
(β-T-Hb_A)NO	—	2.2	1.74	155	1.12	2.30	NA	NA	24
(CCP)NO **(1)**[p]	2CYP	1.85	1.82	135	NA	2.04	NA	NA	35
(CCP)NO **(2)**[q]	2CYP	1.85	1.82	125	NA	2.04	NA	NA	35
(hh-Mb)NO	MS-XAFS[r]	NA	1.76	150	1.12	2.05	NA	NA	36
(soybean-Lb^{II})NO	MS-XAFS[r]	NA	1.77	147	1.12	1.98	NA	NA	37

[a] Value in angstroms. [b] Value in degrees. [c] dihedral angle between Fe–N–O plane and closest Fe–N_p vector. [d] Signed torsion angle for the unit O–N–Fe–N_p of pyrrole ring IV. Positive values refer to NO coordinated on the "top" of the porphyrin and represent a clockwise rotation about the N(NO)–Fe axis between the O–N–Fe and N–Fe-N_p planes whilst negative values represent NO coordinated on the "bottom" and a counterclockwise rotation is required. Both sets of values are comparable, for example ϕ^* angles of 90 and $-90°$ representing two NOs coordinated one each face of the porphyrin and orientated directly above each other. Absolute ϕ^* values of 270, 180 and 90° result in NO orientations coincident with the Fe–N_p bonds of pyrrole rings I, II and III respectively. [e] Value not reported in original literature report. Taken from PDB coordinates. [f] Nitrosyl conformer 1. [g] 2 molecules in asymmetric unit, molecule I. [h] 2 molecules in asymmetric unit, molecule II. [i] Values reported are averaged for both subunits. [j] Cofactor tetrahydrobiopterin present. [k] Cofactor tetrahydrobiopterin absent. [l] 2 orientations of NO observed, orientation I. [m] Nitrosyl conformer 2. [n] Fe–S bond. [o] Differs from α form by orientation of NO with respect to the heme and coordination number. [p] Disordered oxygen, position 1. [q] Disordered oxygen, position 2. [r] Structure determined by multiple scattering XAFS.

Abbreviations:

CCP	Yeast cytochrome *c* peroxidase.
cd_1-NIR(*pa*)	Cytochrome cd_1 nitrite reductase from *Pseudomonas aeruginosa*.
cd_1-NIR(*tp*)	Cytochrome cd_1 nitrite reductase from *Thiosphaera pantotropha*.
cyt c′	Cytochrome c' from *Alcaligenes xylosoxidons*.
4HB	Co-factor tetrahydrobiopterin.
α-Hb	Nitrosylated horse hemoglobin, α subunit.
β-Hb	Nitrosylated horse hemoglobin, β subunit.
α-T-Hb$_A$	T-state human hemoglobin A, α subunit.
α-T-Hb$_A$	T-state human hemoglobin A, β subunit.
Lupin-Lb^{II}	Lupin ferrous leghemoglobin.
fungal-NOR	Fungal nitric oxide reductase
S286T-fungal-NOR	Threonine mutant of fungal nitric oxide reductase
S286V-fungal-NOR	Valine mutant of fungal nitric oxide reductase
hh-Mb	Horse Heart Myoglobin.
sw-Mb	Sperm Whale Myoglobin.
sw-L29F-Mb	Mutant (L29F) Sperm Whale Myoglobin.
NOS	Bovine endothelial nitric oxide synthase.
NP1	Nitrophorin 1 from *Rhodnius prolixus* saliva.
NP4	Nitrophorin 4 from *Rhodnius prolixus* saliva.
SHP	Sphaeroides Heme Protein from *Rhodobacter sphaeroides*.
SiRHP	Sulfite reductase heme protein from *Escherichia coli*..
α-SNO-nitrosylHbA	S-Nitroso form of human hemoglobin, alpha subunit.
β-SNO-nitrosylHbA	S-Nitroso form of human hemoglobin, beta subunit.
soybean-Lb^{II}	Soybean ferrous leghemoglobin A.
soybean-Lb^{III}	Soybean ferric leghemoglobin A.
T243A-P450nor	Mutant (T243A) Cytochrome P450nor (fungal nitric oxide reductase).

T243N-P450nor	Mutant (T243N) Cytochrome P450nor (fungal nitric oxide reductase).
T243V-P450nor	Mutant (T243V) Cytochrome P450nor (fungal nitric oxide reductase).

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Table S2. Complete Crystallographic Details for [Fe(deut)(NO)]

formula	$C_{32}H_{32}FeN_5O_5$
FW, amu	622.48
a, Å	11.3518(14)
b, Å	11.6492(15)
c, Å	12.0065(15)
α, deg	78.915(2)
β, deg	77.590(2)
γ, deg	64.663(2)
V, Å^3	1392.4(3)
space group	$P\bar{1}$
Z	2
D_c, g/cm^3	1.485
F(000)	650
μ, mm^{-1}	0.594
crystal dimensions, mm	0.28 × 0.24 × 0.21
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	100(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	1.95–25.04
index range	$-13 \leq h \leq 13$
	$-13 \leq k \leq 13$
	$-14 \leq l \leq 14$
total data collected	11640
absorption correction	Empirical
relative transmission coefficients (I)	1.00 and 0.759
unique data	4918 (R_{int} = 0.0394)
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	4918/0/398
goodness-of-fit (pased on F^2)	1.050
final R indices [I > 2σ(I)]	R_1 = 0.0594, wR_2 = 0.1460
final R indices (all data)	R_1 = 0.0738, wR_2 = 0.1543

Table S3. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(deut)(NO)][a]

atom	x	y	z	U(eq)
Fe(1)	0.37474(5)	0.45148(5)	1.41143(4)	0.0218(2)
N(1)	0.2074(3)	0.6019(3)	1.3860(3)	0.0222(7)
N(2)	0.2976(3)	0.4205(3)	1.5752(3)	0.0263(7)
N(3)	0.5553(3)	0.3311(3)	1.4538(3)	0.0291(8)
N(4)	0.4650(3)	0.5118(3)	1.2666(3)	0.0219(7)
N(5)	0.3344(3)	0.3549(3)	1.3482(3)	0.0233(7)
O(5)	0.2805(3)	0.3547(3)	1.2739(2)	0.0301(6)
C(a1)	0.1803(3)	0.6790(4)	1.2844(3)	0.0239(8)
C(a2)	0.0887(4)	0.6368(4)	1.4597(3)	0.0251(8)
C(a3)	0.1687(4)	0.4781(4)	1.6236(3)	0.0288(9)
C(a4)	0.3604(4)	0.3232(4)	1.6582(3)	0.0297(9)
C(a5)	0.5827(4)	0.2465(4)	1.5521(4)	0.0308(9)
C(a6)	0.6754(4)	0.3030(4)	1.3833(4)	0.0287(9)
C(a7)	0.5977(4)	0.4584(4)	1.2205(3)	0.0251(8)
C(a8)	0.4060(4)	0.6021(3)	1.1810(3)	0.0223(8)
C(b1)	0.0407(4)	0.7636(4)	1.2936(4)	0.0307(9)
C(b2)	−0.0136(4)	0.7388(4)	1.4027(4)	0.0297(9)
C(b3)	0.1495(4)	0.4150(4)	1.7409(3)	0.0298(9)
C(b4)	0.2667(4)	0.3218(4)	1.7584(4)	0.0331(9)
C(b5)	0.7227(4)	0.1650(4)	1.5397(4)	0.0325(10)
C(b6)	0.7791(4)	0.1992(4)	1.4394(4)	0.0319(9)
C(b7)	0.6199(4)	0.5180(4)	1.1066(3)	0.0284(9)
C(b8)	0.5009(4)	0.6069(4)	1.0806(3)	0.0244(8)
C(m1)	0.0714(4)	0.5775(4)	1.5708(3)	0.0316(9)
C(m2)	0.4919(4)	0.2426(4)	1.6448(4)	0.0313(9)
C(m3)	0.6948(4)	0.3618(4)	1.2757(4)	0.0305(9)
C(m4)	0.2726(4)	0.6785(3)	1.1880(3)	0.0232(8)
C(1)	0.0211(4)	0.4557(4)	1.8195(4)	0.0368(10)
C(2)	0.7860(4)	0.0615(4)	1.6335(4)	0.0397(10)
C(3)	0.7510(4)	0.4840(5)	1.0299(4)	0.0372(10)
C(4)	0.4726(4)	0.6947(4)	0.9713(3)	0.0288(9)
C(5)	0.4867(5)	0.8189(4)	0.9727(3)	0.0352(10)
C(6)	0.4867(4)	0.8996(4)	0.8597(4)	0.0311(9)
O(1)	0.4338(3)	0.8720(3)	0.7849(2)	0.0332(7)

Table S3. Continued

atom	x	y	z	U(eq)
C(7)	0.4401(5)	0.9398(4)	0.6708(4)	0.0431(12)
O(2)	0.5326(4)	0.9790(3)	0.8360(3)	0.0498(9)
C(8)	−0.0297(4)	0.8516(4)	1.1970(4)	0.0382(10)
C(9)	−0.0603(4)	0.9921(4)	1.1948(4)	0.0382(10)
C(10)	0.0527(5)	1.0286(4)	1.1360(4)	0.0399(11)
O(3)	0.0431(4)	1.1349(3)	1.1708(4)	0.0648(11)
C(11)	0.1455(7)	1.1774(6)	1.1141(8)	0.088(2)
O(4)	0.1413(3)	0.9719(3)	1.0653(3)	0.0505(9)
C(12)	−0.1550(4)	0.8011(4)	1.4582(4)	0.0364(10)

[a] U(eq) is defined as one third of the trace of the orthogonalized $\mathbf{U}_{ij}$ tensor. The estimated standard deviations of the least significant digits are given in parentheses.

Table S4. Bond Lengths for [Fe(deut)(NO)][a]

bond	length (Å)	bond	length (Å)
Fe(1)–N(5)	1.723(3)	C(a7)–C(m3)	1.373(6)
Fe(1)–N(4)	1.987(3)	C(a7)–C(b7)	1.433(6)
Fe(1)–N(1)	1.992(3)	C(a8)–C(m4)	1.383(5)
Fe(1)–N(2)	2.005(3)	C(a8)–C(b8)	1.443(5)
Fe(1)–N(3)	2.035(3)	C(b1)–C(b2)	1.356(6)
N(1)–C(a1)	1.375(5)	C(b1)–C(8)	1.509(6)
N(1)–C(a2)	1.385(5)	C(b2)–C(12)	1.509(5)
N(2)–C(a3)	1.369(5)	C(b3)–C(b4)	1.338(6)
N(2)–C(a4)	1.402(5)	C(b3)–C(1)	1.493(6)
N(3)–C(a6)	1.382(5)	C(b5)–C(b6)	1.312(6)
N(3)–C(a5)	1.383(5)	C(b5)–C(2)	1.524(6)
N(4)–C(a8)	1.374(5)	C(b7)–C(b8)	1.361(6)
N(4)–C(a7)	1.391(5)	C(b7)–C(3)	1.505(5)
N(5)–O(5)	1.187(4)	C(b8)–C(4)	1.502(5)
C(a1)–C(m4)	1.383(5)	C(4)–C(5)	1.526(5)
C(a1)–C(b1)	1.458(5)	C(5)–C(6)	1.495(6)
C(a2)–C(m1)	1.395(5)	C(6)–O(2)	1.206(5)
C(a2)–C(b2)	1.442(6)	C(6)–O(1)	1.333(5)
C(a3)–C(m1)	1.373(6)	O(1)–C(7)	1.448(5)
C(a3)–C(b3)	1.476(5)	C(8)–C(9)	1.517(6)
C(a4)–C(m2)	1.374(6)	C(9)–C(10)	1.513(6)
C(a4)–C(b4)	1.428(6)	C(10)–O(4)	1.204(6)
C(a5)–C(m2)	1.353(6)	C(10)–O(3)	1.335(6)
C(a5)–C(b5)	1.453(6)	O(3)–C(11)	1.444(7)
C(a6)–C(m3)	1.362(6)		
C(a6)–C(b6)	1.453(6)		

[a]The estimated standard deviations of the least significant digits are given in parentheses.

Table S5. Bond Angles for [Fe(deut)(NO)][a]

angle	degree	angle	degree
N(5)–Fe(1)–N(4)	94.92(13)	C(m3)–C(a7)–C(b7)	124.3(4)
N(5)–Fe(1)–N(1)	92.47(14)	N(4)–C(a7)–C(b7)	110.6(3)
N(4)–Fe(1)–N(1)	89.60(12)	N(4)–C(a8)–C(m4)	125.0(3)
N(5)–Fe(1)–N(2)	100.29(13)	N(4)–C(a8)–C(b8)	111.5(3)
N(4)–Fe(1)–N(2)	164.79(12)	C(m4)–C(a8)–C(b8)	123.5(3)
N(1)–Fe(1)–N(2)	89.92(13)	C(b2)–C(b1)–C(a1)	106.3(4)
N(5)–Fe(1)–N(3)	102.33(14)	C(b2)–C(b1)–C(8)	127.4(4)
N(4)–Fe(1)–N(3)	88.34(13)	C(a1)–C(b1)–C(8)	126.1(4)
N(1)–Fe(1)–N(3)	165.17(12)	C(b1)–C(b2)–C(a2)	107.6(3)
N(2)–Fe(1)–N(3)	88.25(14)	C(b1)–C(b2)–C(12)	128.2(4)
C(a1)–N(1)–C(a2)	105.8(3)	C(a2)–C(b2)–C(12)	124.1(4)
C(a1)–N(1)–Fe(1)	126.3(2)	C(b4)–C(b3)–C(a3)	106.4(4)
C(a2)–N(1)–Fe(1)	127.0(3)	C(b4)–C(b3)–C(1)	129.9(4)
C(a3)–N(2)–C(a4)	106.1(3)	C(a3)–C(b3)–C(1)	123.7(4)
C(a3)–N(2)–Fe(1)	126.7(3)	C(b3)–C(b4)–C(a4)	108.8(4)
C(a4)–N(2)–Fe(1)	126.6(3)	C(b6)–C(b5)–C(a5)	108.6(4)
C(a6)–N(3)–C(a5)	105.0(3)	C(b6)–C(b5)–C(2)	128.7(4)
C(a6)–N(3)–Fe(1)	127.0(3)	C(a5)–C(b5)–C(2)	122.7(4)
C(a5)–N(3)–Fe(1)	127.4(3)	C(b5)–C(b6)–C(a6)	106.8(4)
C(a8)–N(4)–C(a7)	104.6(3)	C(b8)–C(b7)–C(a7)	107.4(3)
C(a8)–N(4)–Fe(1)	126.7(2)	C(b8)–C(b7)–C(3)	127.1(4)
C(a7)–N(4)–Fe(1)	127.9(3)	C(a7)–C(b7)–C(3)	125.5(4)
O(5)–N(5)–Fe(1)	143.1(3)	C(b7)–C(b8)–C(a8)	106.0(3)
N(1)–C(a1)–C(m4)	125.0(3)	C(b7)–C(b8)–C(4)	127.6(3)
N(1)–C(a1)–C(b1)	110.3(3)	C(a8)–C(b8)–C(4)	126.4(4)
C(m4)–C(a1)–C(b1)	124.7(4)	C(a3)–C(m1)–C(a2)	125.3(4)
N(1)–C(a2)–C(m1)	124.4(4)	C(a5)–C(m2)–C(a4)	126.1(4)
N(1)–C(a2)–C(b2)	109.9(3)	C(a6)–C(m3)–C(a7)	125.1(4)
C(m1)–C(a2)–C(b2)	125.6(4)	C(a8)–C(m4)–C(a1)	124.7(4)
N(2)–C(a3)–C(m1)	125.5(4)	C(b8)–C(4)–C(5)	112.3(3)
N(2)–C(a3)–C(b3)	109.4(3)	C(6)–C(5)–C(4)	115.5(3)
C(m1)–C(a3)–C(b3)	125.1(4)	O(2)–C(6)–O(1)	122.7(4)
C(m2)–C(a4)–N(2)	125.1(4)	O(2)–C(6)–C(5)	124.5(4)
C(m2)–C(a4)–C(b4)	125.6(4)	O(1)–C(6)–C(5)	112.8(3)

Table S5. Continued

angle	degree	angle	degree
N(2)–C(a4)–C(b4)	109.3(4)	C(6)–O(1)–C(7)	115.5(3)
C(m2)–C(a5)–N(3)	124.5(4)	C(b1)–C(8)–C(9)	115.8(4)
C(m2)–C(a5)–C(b5)	126.3(4)	C(10)–C(9)–C(8)	113.8(4)
N(3)–C(a5)–C(b5)	109.3(4)	O(4)–C(10)–O(3)	122.5(5)
C(m3)–C(a6)–N(3)	125.4(4)	O(4)–C(10)–C(9)	125.7(4)
C(m3)–C(a6)–C(b6)	124.3(4)	O(3)–C(10)–C(9)	111.7(4)
N(3)–C(a6)–C(b6)	110.3(4)	C(10)–O(3)–C(11)	114.3(5)
C(m3)–C(a7)–N(4)	125.1(4)		

[a]The estimated standard deviations of the least significant digits are given in parentheses.

Table S6. Anisotropic Displacement Parameters (Å^2) for [Fe(deut)(NO)][a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0249(3)	0.0241(3)	0.0205(3)	−0.0003(2)	−0.0028(2)	−0.0149(2)
N(1)	0.0196(15)	0.0247(16)	0.0226(16)	−0.0031(13)	0.0044(12)	−0.0126(13)
N(2)	0.0333(18)	0.0307(18)	0.0218(16)	−0.0025(14)	−0.0022(14)	−0.0206(15)
N(3)	0.043(2)	0.0221(17)	0.0310(18)	0.0012(14)	−0.0155(16)	−0.0189(16)
N(4)	0.0179(15)	0.0258(17)	0.0238(16)	−0.0052(13)	0.0008(12)	−0.0114(13)
N(5)	0.0253(16)	0.0259(17)	0.0223(16)	−0.0016(13)	−0.0016(13)	−0.0151(14)
O(5)	0.0273(15)	0.0387(16)	0.0296(15)	−0.0064(12)	−0.0046(12)	−0.0169(13)
C(A1)	0.0177(18)	0.026(2)	0.029(2)	−0.0056(16)	−0.0013(15)	−0.0094(16)
C(A2)	0.0251(19)	0.028(2)	0.026(2)	−0.0058(16)	0.0030(16)	−0.0163(17)
C(A3)	0.043(2)	0.028(2)	0.025(2)	−0.0022(17)	−0.0063(18)	−0.023(2)
C(A4)	0.049(3)	0.033(2)	0.0205(19)	−0.0027(16)	−0.0018(17)	−0.031(2)
C(A5)	0.038(2)	0.029(2)	0.033(2)	−0.0042(18)	−0.0089(18)	−0.0192(19)
C(A6)	0.0212(19)	0.028(2)	0.041(2)	−0.0121(18)	−0.0052(17)	−0.0106(17)
C(A7)	0.0202(19)	0.029(2)	0.032(2)	−0.0130(17)	0.0009(16)	−0.0139(17)
C(A8)	0.025(2)	0.025(2)	0.0216(18)	−0.0047(15)	0.0006(15)	−0.0157(17)
C(B1)	0.0200(19)	0.031(2)	0.041(2)	−0.0065(18)	−0.0035(17)	−0.0093(17)
C(B2)	0.021(2)	0.033(2)	0.037(2)	−0.0122(18)	0.0068(17)	−0.0143(18)
C(B3)	0.037(2)	0.039(2)	0.024(2)	−0.0105(17)	0.0077(17)	−0.028(2)
C(B4)	0.041(2)	0.036(2)	0.029(2)	−0.0021(18)	−0.0071(19)	−0.022(2)
C(B5)	0.025(2)	0.032(2)	0.047(3)	−0.0137(19)	−0.0123(19)	−0.0105(18)
C(B6)	0.025(2)	0.034(2)	0.040(2)	−0.0090(19)	−0.0058(18)	−0.0121(18)
C(B7)	0.023(2)	0.038(2)	0.033(2)	−0.0176(18)	0.0089(17)	−0.0213(19)
C(B8)	0.026(2)	0.031(2)	0.0223(19)	−0.0070(16)	0.0042(15)	−0.0198(18)
C(M1)	0.033(2)	0.041(2)	0.030(2)	−0.0170(19)	0.0131(18)	−0.027(2)
C(M2)	0.034(2)	0.027(2)	0.038(2)	−0.0017(18)	−0.0179(19)	−0.0126(18)
C(M3)	0.021(2)	0.029(2)	0.044(2)	−0.0158(19)	−0.0046(18)	−0.0092(17)
C(M4)	0.0252(19)	0.0216(19)	0.0223(19)	0.0016(15)	−0.0041(15)	−0.0105(16)
C(1)	0.029(2)	0.044(3)	0.035(2)	−0.001(2)	−0.0004(18)	−0.017(2)
C(2)	0.036(2)	0.041(3)	0.040(3)	−0.004(2)	−0.009(2)	−0.013(2)
C(3)	0.029(2)	0.053(3)	0.035(2)	−0.015(2)	0.0095(19)	−0.024(2)
C(4)	0.034(2)	0.035(2)	0.024(2)	−0.0053(17)	0.0047(17)	−0.0239(19)
C(5)	0.051(3)	0.036(2)	0.027(2)	−0.0022(18)	−0.0025(19)	−0.029(2)
C(6)	0.033(2)	0.031(2)	0.035(2)	−0.0062(18)	−0.0041(18)	−0.0169(19)
O(1)	0.0375(16)	0.0317(16)	0.0365(16)	−0.0023(13)	−0.0108(13)	−0.0178(14)

Table S6. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(7)	0.064(3)	0.034(2)	0.039(3)	0.003(2)	−0.026(2)	−0.022(2)
O(2)	0.075(2)	0.052(2)	0.0449(19)	0.0116(16)	−0.0223(17)	−0.048(2)
C(8)	0.028(2)	0.042(3)	0.046(3)	−0.007(2)	−0.008(2)	−0.014(2)
C(9)	0.030(2)	0.043(3)	0.041(2)	−0.008(2)	−0.0039(19)	−0.013(2)
C(10)	0.036(2)	0.031(2)	0.044(3)	0.004(2)	−0.013(2)	−0.006(2)
O(3)	0.046(2)	0.038(2)	0.111(3)	−0.014(2)	−0.009(2)	−0.0167(17)
C(11)	0.067(4)	0.046(4)	0.153(7)	−0.003(4)	−0.006(4)	−0.032(3)
O(4)	0.043(2)	0.055(2)	0.0440(19)	0.0100(17)	−0.0089(16)	−0.0164(18)
C(12)	0.023(2)	0.039(2)	0.044(3)	−0.009(2)	0.0066(18)	−0.0130(19)

[a]The estimated standard deviations of the least significant digits are given in parentheses. The anisotropic displacement factor exponent takes the form: $-2\ \pi\ [h^2\ U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}]$.

Table S7. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(deut)(NO)][a]

atom	x	y	z	U(eq)
H(B4	0.2847	0.2643	1.8265	0.040
H(B6	0.8702	0.1630	1.4093	0.038
H(M1	−0.0147	0.6083	1.6135	0.038
H(M2	0.5217	0.1781	1.7064	0.038
H(M3	0.7823	0.3338	1.2356	0.037
H(M4	0.2422	0.7347	1.1219	0.028
H(1A)	0.0284	0.3939	1.8884	0.055
H(1B)	−0.0481	0.4598	1.7803	0.055
H(1C)	−0.0012	0.5403	1.8414	0.055
H(2A)	0.8813	0.0202	1.6088	0.059
H(2B)	0.7481	−0.0023	1.6480	0.059
H(2C)	0.7694	0.1002	1.7040	0.059
H(3A)	0.7370	0.5207	0.9508	0.056
H(3B)	0.7971	0.3908	1.0330	0.056
H(3C)	0.8043	0.5183	1.0560	0.056
H(4A)	0.3818	0.7149	0.9595	0.035
H(4B)	0.5341	0.6504	0.9060	0.035
H(5A)	0.4136	0.8702	1.0281	0.042
H(5B)	0.5701	0.7976	1.0012	0.042
H(7A)	0.3897	1.0318	0.6748	0.065
H(7B)	0.4027	0.9104	0.6214	0.065
H(7C)	0.5322	0.9232	0.6389	0.065
H(8A)	−0.1136	0.8427	1.2016	0.046
H(8B)	0.0250	0.8227	1.1234	0.046
H(9A)	−0.1377	1.0437	1.1549	0.046
H(9B)	−0.0845	1.0138	1.2747	0.046
H(11A)	0.2291	1.1190	1.1408	0.133
H(11B)	0.1223	1.2638	1.1322	0.133
H(11C)	0.1546	1.1785	1.0309	0.133
H(12A)	−0.1927	0.8912	1.4266	0.055
H(12B)	−0.1585	0.7952	1.5412	0.055
H(12C)	−0.2058	0.7573	1.4427	0.055

[a] U(eq) is defined as one third of the trace of the orthogonalized $\mathbf{U}_{ij}$ tensor the estimated standard deviations of the least significant digits are given in parentheses.

Supporting Information