Supporting Information

A Mononuclear Nonheme Iron(IV)-Oxo Complex Which Is More Reactive Than Cytochrome P450 Model Compound I

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Experimental Section

Materials. Commercially available chemicals were used without further purification unless otherwise indicated. Solvents were dried according to published procedures and distilled under Ar prior to use.[1] Fe(TDCPP)Cl (TDCPP = *meso*-tetrakis(2,6-dichlorophenyl)porphinato dianion) was obtained from Frontier Scientific Inc. (Logan, UT, USA). *m*-Chloroperbenzoic acid (*m*-CPBA) was purified by washing with phosphate buffer (pH 7.4), followed by water and then dried under reduced pressure.[2] Ligands (Me_3NTB = tris(*N*-methylbenzimidazol-2-ylmethyl)amine, N4Py = *N*,*N*-bis(2-pyridylmethyl)-*N*-bis(2-pyridyl)methylamine and Bn-tpen = *N*-benzyl-*N,N′,N′*-tris(2-pyridylmethyl)-1,2-diaminoethane) and iron(II) complexes, $[Fe^{II}(N4Py)](CF_3SO_3)_2$ and $[Fe^{II}(Bn\text{-}TPEN)](CF_3SO_3)_2$, were prepared by literature methods.[3] The tripodal Me_3NTB (Me_3NTB = tris(*N*-methylbenzimidazol-2-ylmethyl)amine) ligand was synthesized in a modified procedure. Nitrilotriacetic acid (99%, 5 g, 26 mmol) was added a solution of *N*-methyl-1,2-phenylenediamine (97%, 9 mL, 81 mmol) in a 50 ml of propylene glycol at ambient temperature. The resulting mixture was refluxed for 24h, and then cooled to room temperature. A 50 mL of ice cold water was added to generate a pick precipitation. The solid was dissolved in hot methanol and filtered over activated carbon. The solution was allowed to evaporated slowly to give white solid (yield, 6.5 g, 54%).[4] The preparation of $[Fe^{II}(Me_3NTB)(CH_3CN)](CF_3SO_3)_2$ (**2**) was carried out in dry box. Equimolar amounts of Me_3NTB (0.45 mmol, 200 mg) and $Fe(CF_3SO_3)_2{\cdot}2CH_3CN$ (0.68 mmol, 290 mg) were dissolved in CH_3CN and stirred at ambient temperature for overnight. The resulting solution was filtered and added to a large volume of Et_2O. The product was obtained as white solid power in 85% yield (330 mg). Colorless plate crystals suitable for X-ray analysis were obtained by diffusion of dry Et_2O into a saturated CH_3CN solution of **2**. $^{57}Fe(II)(Me_3NTB)(CF_3SO_3)_2$ was prepared analogously using $^{57}Fe(CF_3SO_3)_2{\cdot}2CH_3CN$ in a glove box. Anal. Calcd for $C_{31}H_{30}F_6FeN_8O_6S_2$: C, 44.08; H, 3.58; N, 13.27. Found C, 44.02; H, 3.71; N, 13.29

Instrumentation. UV-vis spectra were recorded on a Hewlett Packard 8453 diode array spectrophotometer equipped with a UNISOKU Scientific Instruments Cryostat USP-203A for low-temperature experiments or on a Hi-Tech Scientific (U.K.) SF-61 DX2 cryogenic stopped-flow spectrometer equipped with a Xe arc lamp and a KinetaScan diode array rapid scanning unit. Electrospray ionization mass spectra (ESI MS) were collected on a Thermo Finnigan (San Jose, CA, USA) LCQ^{TM} Advantage MAX quadrupole ion trap instrument, by

infusing samples directly into the source using a manual method. The spray voltage was set at 3.7 kV and the capillary temperature at 100 °C. Product analysis for oxidation reactions was performed with an Agilent Technologies 6890N gas chromatograph (GC), Thermo Finnigan (Austin, Texas, USA) FOCUS DSQ (dual stage quadrupole) mass spectrometer interfaced with Finnigan FOCUS gas chromatograph (GC-MS), or DIONEX Summit Pump Series P580 equipped with a variable wavelength UV-200 detector (HPLC). Products for HPLC analysis were separated on Hypersil GOLD column (4.6 x 250 mm), and product yields were determined with a UV Detector at 215 and 254 nm. ^{1}H NMR spectra were measured with Bruker model digital AVANCE III 400 FT-NMR spectrometer. Elemental analysis were perforemed with ans EA1110 or EA1112(CE Instrument, Italy) for C, H and N.

X-ray Structural Analysis. Single crystals of **2** were grown by slow diffusion of ether into an acetonitrile solution and mounted on a glass fiber tip with epoxy cement. The diffraction data for **2** were collected at 170 K on a Bruker SMART AXS diffractometer equipped with a monochromator in the Mo Kα (λ = 0.71073 Å) incident beam. The CCD data were integrated and scaled using the Bruker-SAINT software package, and the structure was solved and refined using SHEXTL V 6.12.[5] Hydrogen atoms were located in the calculated positions. Crystal data for **2**: $C_{31}H_{30}F_6FeN_8O_6S_2$, *Monoclinic*, *P2(1)/n*, Z = 4, a = 13.9439(14), b = 11.1989(12), c = 23.710(3) Å, α = 90, β = 95.497(6), γ = 90°, V = 3685.5(7) Å^3, μ = 0.607 mm^{-1}, d_{calc} = 1.522 g/cm^3, R_1 = 0.0623, wR_2 = 0.1737 for 7231 unique reflections, 518 variables. The crystallographic data for **2** are listed in Table S1, and Table S2 lists the selected bond distances and angles. CCDC 801232 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

Mössbauer Analysis. Mössbauer spectra were recorded at 4.2 K and 80 K, either on a lowfield Mössbauer spectrometer equipped with a Janis SVT-400 cryostat or on a strong-field Mössbauer spectrometer equipped with an Oxford Instruments Spectromag 4000 cryostat containing an 8T split-pair superconducting magnet. Both spectrometers were operated in a constant acceleration mode in transmission geometry. The isomer shifts are

referenced against that of a room-temperature metallic iron foil. Analysis of the data was performed with the program WMOSS (WEB Research).

Kinetic Studies and Product Analysis. Reactions were run at least in triplicate, and data reported represent the average of these reactions. All reactions were followed by monitoring UV-vis spectral changes of reaction solutions with a Hewlett Packard 8453 spectrophotometer equipped with cryostat system or a Hi-Tech Scientific SF-61 DX2 cryogenic stopped-flow spectrophotometer. $[Fe^{IV}(O)(Me_3NTB)]^{2+}$ (**3**) was prepared by reacting $[Fe^{II}(Me_3NTB)](CF_3SO_3)_2$ (**2**) (2 mM) with 1 equiv of *m*-CPBA in CH_3CN at –40 ^oC. Subsequently, appropriate amounts of substrates were added to reaction solutions at the given temperatures, and pseudo-first-order fitting of the kinetic data allowed us to determine k_{obs} values. For the stopped-flow experiments, the intermediate was generated by rapidly mixing a solution of $Fe^{II}(Me_3NTB)(CF_3SO_3)_2$ and 1 equiv of *m*-CPBA in CH_3CN (final mixing concentration of 2 mM) in the initial push of a double-mixing experiment at –40 °C. After a specified time delay (age time 10 seconds) that coincides with the maximal concentration of the intermediate, a solution containing substrate was introduced by a second push to initiate the reaction at the same low temperature. All reaction traces were collected at 770 nm, using a 1cm optical path length at given temperature. The raw kinetic data were treated with KinetAsyst 3 (Hi-Tech Scientific) and Specfit/32 Global Analysis System software from Spectrum Software Associates.

For the reactions of $[Fe^{IV}(O)(N4Py)]^{2+}$ (**4**) and $[Fe^{IV}(O)(Bn\text{-}TPEN)]^{2+}$ (**5**), the intermediates (1 mM) were prepared by reacting $[Fe^{II}(N4Py)(CF_3SO_3)_2]$ and $[Fe^{II}(Bn\text{-}TPEN)(CF_3SO_3)_2]$ with excess of solid PhIO in CH_3CN at 0 ^oC.[6] $[Fe^{III}(TDCPP)(CF_3SO_3)]$ were prepared by stirring equimolar amount of $[Fe^{III}(TDCPP)Cl]$ and $Ag(CF_3SO_3)$, followed by filtration through a 0.45μM filter. The resulting solution was used immediately. $[(TDCPP)^{+\cdot}Fe^{IV}(O)]$ (**7**) was prepared by treating $[Fe^{III}(TDCPP)(CF_3SO_3)]$ (1 mM) with *m*-CPBA (4 mM) in a solvent mixture of CH_3CN and CH_2Cl_2 (*v*/*v* = 1:1) at –40 ^oC. Subsequently, appropriate amounts of substrates were added to the reaction solutions at –40 ^oC. After the completion of reactions, pseudo-first-order fitting of the kinetic data allowed us to determine k_{obs} values.

Products formed in the oxidation of substrates by **2**, which were carried out under Ar atmosphere, were analyzed by ^1H NMR, GC, GC-MS, or HPLC. Quantitative analyses were made on the basis of comparisons of peak integration between products and authentic

samples. Products formed in controlled reactions, which were carried out under the same reaction conditions but without the Fe(II) catalyst, were also analyzed. In the oxidation of 1,4-cyclohexadiene, benzene, which was the desaturated product, was obtained as a sole product.[7,8] In the case of cyclooctane, products from desaturated and hydroxylated reactions were obtained, such as cyclooctanol and cyclooctanone for hydroxylation and cyclooctene and cyclooctene oxide for desaturation.[8] Product distributions (e.g., desaturation versus hydroxylation) were different depending on iron complexes, and results of product analysis, including DFT calculations, will be communicated in a separate paper.[8]

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Table S1. Crystal data and structure refinement for $[Fe^{II}(Me_3NTB)(CH_3CN)](OTf)_2$, **2**.

Empirical formula	$C_{31}H_{30}F_6FeN_8O_6S_2$
Formula weight	844.60
Temperature (K)	100
Wavelength (Å)	0.71073
Crystal system/space group	Monoclinic, *P2(1)/n*
Unit cell dimensions	
a (Å)	13.9439(14)
b (Å)	11.1989(12)
c (Å)	23.710(3)
α (°)	90.00
β (°)	95.497(6)
γ (°)	90.00
Volume (Å^3)	3685.5(7)
Z	4
Calculated density (g/cm^{-3})	1.522
Absorption coefficient (mm^{-1})	0.607
F(000)	1728
Reflections collected	29355
Independent reflections [*R*(int)]	7231 [0.0465]
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	7231/0/518
Goodness-of-fit on F^2	1.165
Final *R* indices [$I > 2$sigma(I)]	$R_1 = 0.0623$, $wR_2 = 0.1737$
R indices (all data)	$R_1 = 0.1060$, $wR_2 = 0.1991$
Largest difference peak and hole (e/Å^3)	0.731 and -0.590

Table S2. Selected bond distances and angles of $[Fe^{II}(Me_3NTB)(CH_3CN)](OTf)_2$, **2**.

		Distances (Å)	
Fe1-N2	2.036(3)	Fe1-N4	2.090(3)
Fe1-N6	2.068(3)	Fe1-N8	2.102(4)
Fe1-N1	2.299(3)		
		Angles (º)	
N2 Fe1 N6	109.39(12)	N2 Fe1 N4	112.26(13)
N6 Fe1 N4	123.79(13)	N2 Fe1 N8	106.56(14)
N4 Fe1 N8	100.96(14)	N6 Fe1 N8	101.52(13)
N2 Fe1 N1	77.69(12)	N4 Fe1 N1	75.96(12)
N6 Fe1 N1	77.93(11)	N8 Fe1 N1	175.56(13)

Table S3. Mössbauer parameters.

$Fe(Me_3NTB)(OTf)_2$	Fe Species	Percent	δ (mm/s)	ΔE_Q (mm/s)	Line width (mm/s)
Start	FeII	100 %	1.16	2.97	0.58
Inter	FeIII	35 %	0.48	1.42	0.35
	FeIV	57 %	0.02	1.53	0.27

Table S4. Mössbauer parameters of Fe^{IV} used in the simulation.

D (cm^{-1})	28 (2)
E/D	0 (E/D <0.2)
gx,gy,gz	2.3, 2.3, 2
Ax,Ay,Az (T)	-21 (2), -18 (2), 0
ΔE_Q ($mm.s^{-1}$)	1.53 (3)
η	0.37 (0.1< η <0.6)
δ ($mm.s^{-1}$)	0.02 (2)
Γ ($mm.s^{-1}$)	0.27 (2)

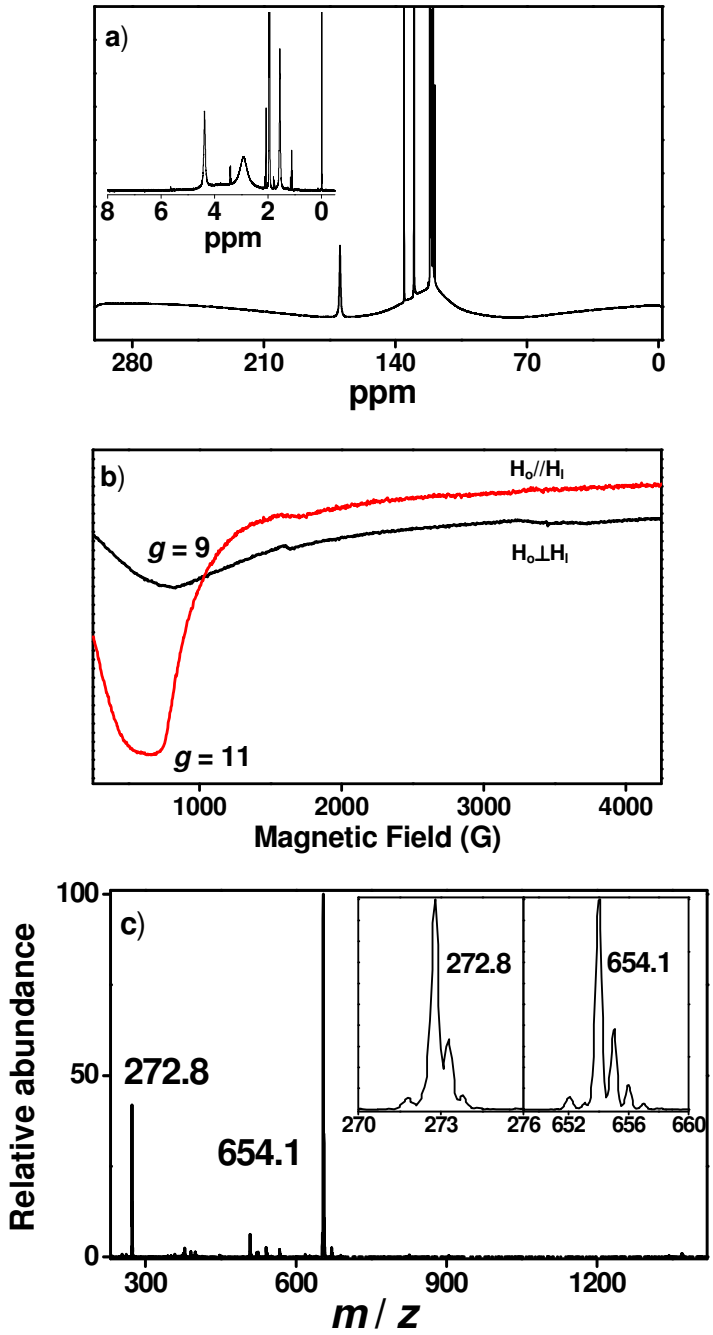

Figure S1. a) ^{1}H NMR spectrum of [Fe(II)(Me_3NTB)(CH_3CN)]$(OTf)_2$, **2**. b) X-band CW-EPR spectra of **2** recorded at 4 K. c) ESI MS spectra of **2**. Peaks at *m*/*z* = 272.9 and 654.1 correspond to $[Fe(II)(Me_3NTB)(CH_3CN)]^{2+}$ (calculated *m*/*z* of 273.1) and $[Fe(II)(Me_3NTB)(OTf)]^{+}$ (calculated *m*/*z* of 654.1), respectively. Insets show the observed isotope distribution patterns for $[Fe(II)(Me_3NTB)(CH_3CN)]^{2+}$ (left panel) and $[Fe(II)(Me_3NTB)(OTf)]^{+}$ (right panel).

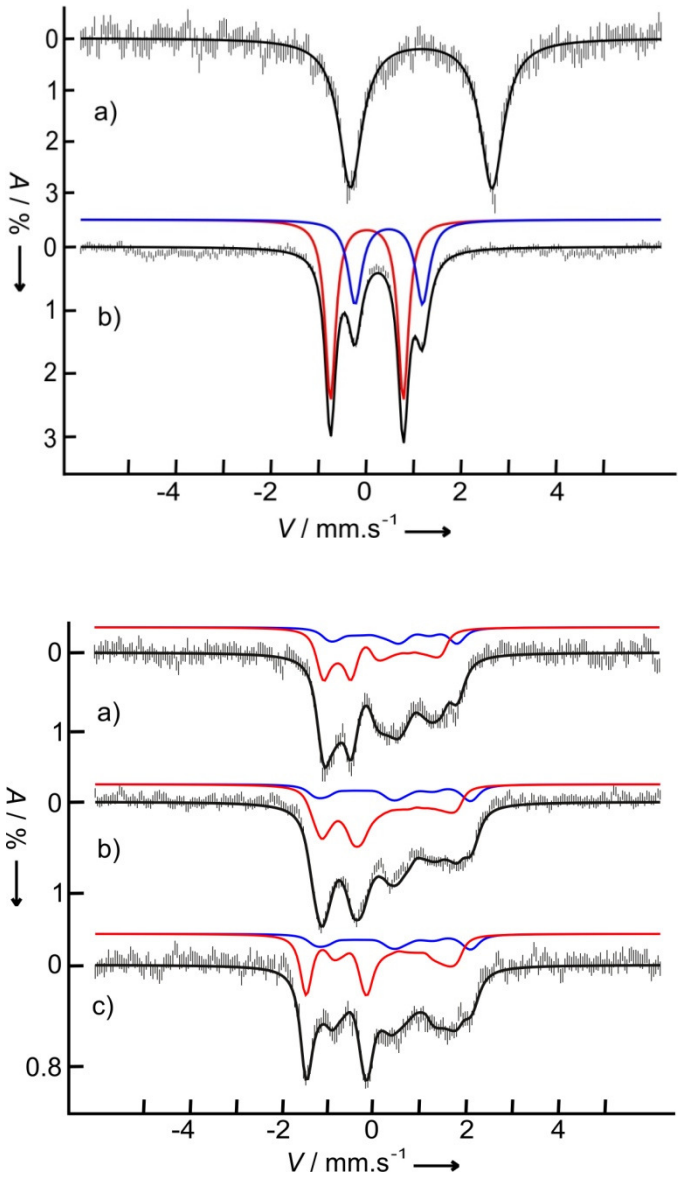

Figure S2. Top: Mössbauer spectra at 4.2 K with a magnetic field of 60 mT applied parallel to γ radiation. a) $Fe(Me_3NTB)(OTf)_2$. b) After the generation of the intermediate **3** by *m*-CPBA; composite simulation in black compound **3** (Fe^{IV} species, parameters in Table S3) in red and decay product (Fe^{III} species) in blue.

Bottom: Mössbauer spectra of $Fe(Me_3NTB)(OTf)_2$ complex after reaction with *m*-CPBA, in black composite simulation with Fe^{IV} $S = 1$ parameters in Table S4, Fe^{IV} component in red and Fe^{III} component in blue. a) Spectra at 4.2 K with a magnetic field of 5 T applied parallel to γ radiation. b) Spectra at 4.2 K with a magnetic field of 7 T applied parallel to γ radiation. c) Spectra at 80 K with a magnetic field of 7 T applied parallel to γ radiation.

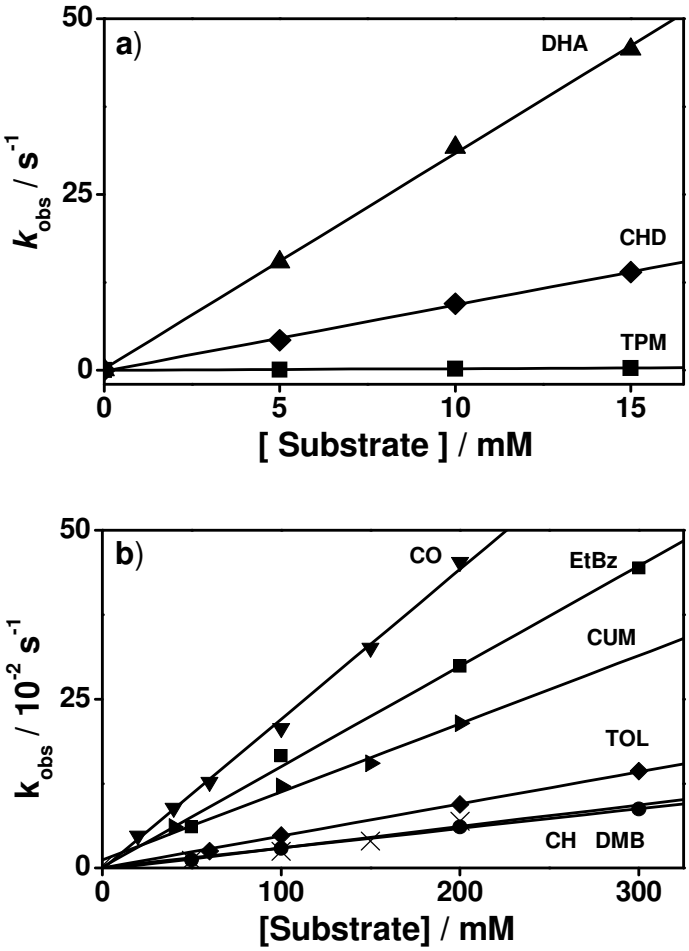

Figure S3. Plots of the pseudo-first-order rate constants, k_{obs} (s^{-1}), against substrate concentrations to determine second-order rate constants, k_2, for the reactions of $[Fe^{IV}(O)(Me_3NTB)]^{2+}$ (**3**) with a) 9,10-dihydroantrance (▲, DHA), 1,4-cyclohexadiene (♦, CHD), and triphenylmethane (■, TPM), and b) cumene (►, CUM), ethylbenzene (■, EtBz), toluene (♦, TOL), cyclooctane (▼, CO), 2,3-dimethylbutane (●, DMB), and cyclohexane (×, CH) in CH_3CN at –40 °C. Reaction conditions: $[Fe^{IV}(O)(Me_3NTB)]^{2+}$ = 1 mM and [substrate] = 5 – 300 mM. See Table S5 for the determined k_2 values.

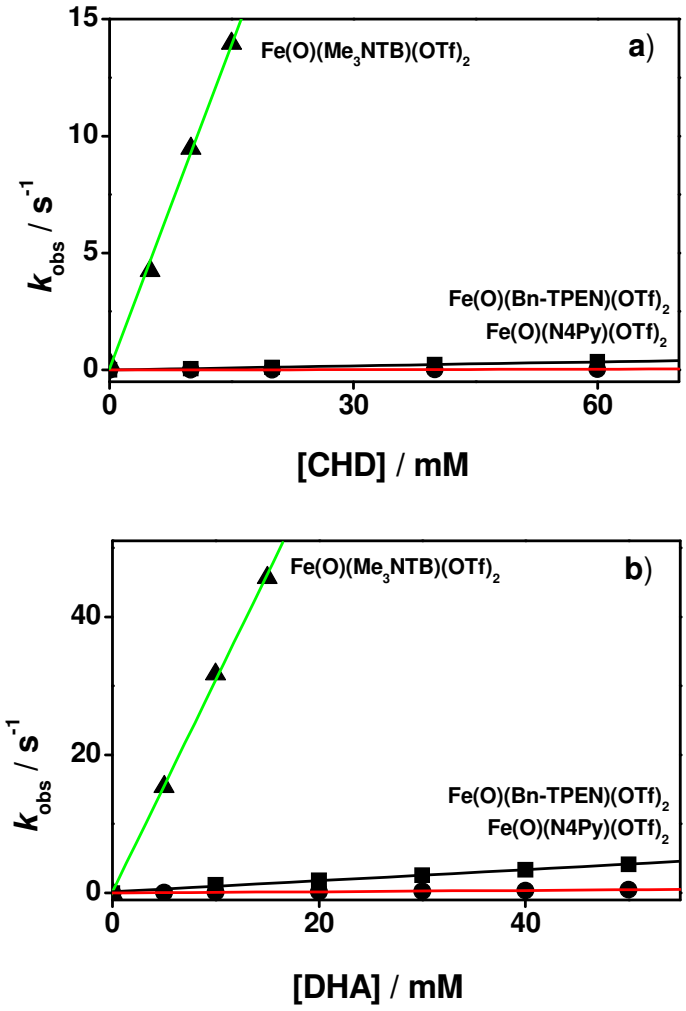

Figure S4. Plots of the pseudo-first-order rate constants, k_{obs}, against substrate concentrations to determine second-order rate constants, k_2, for the reaction of $[Fe^{IV}(O)(Me_3NTB)]^{2+}$ (▲, green solid line), $[Fe^{IV}(O)(Bn\text{-}TPEN)]^{2+}$ (■, black solid line), and $[Fe^{IV}(O)(N4Py)]^{2+}$ (●, red solid line) with a) 1,4-cyclohexadiene (CHD) and b) 9,10-dihydroantrance (DHA). Reaction conditions: $[Fe^{IV}(O)(L)]^{2+}$ = 1 mM and [substrate] = 5 – 60 mM in CH_3CN at –40 °C. Second-order rate constants are listed in Table 3 in text.

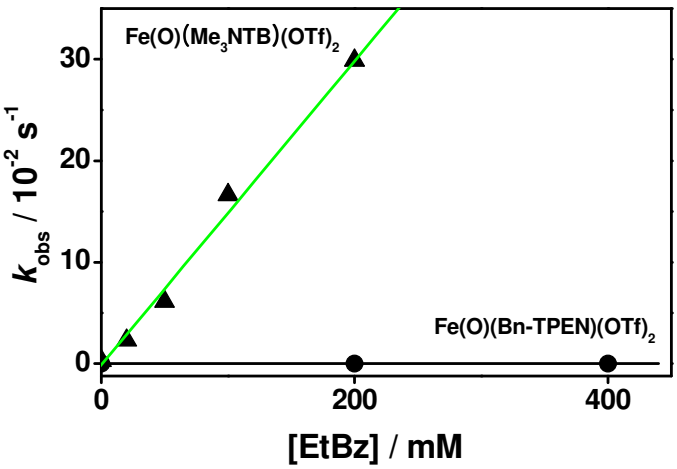

Figure S5. Plot of the pseudo-first-order rate constants, k_{obs}, against substrate concentrations to determine second-order rate constants, k_2, for the reactions of $[Fe^{IV}(O)(Me_3NTB)]^{2+}$ (▲, green solid line, k_2 = 1.5 M^{-1} s^{-1}) and $[Fe^{IV}(O)(Bn\text{-}TPEN)]^{2+}$ (●, black solid line, k_2 = 5.8 x 10^{-2} M^{-1} s^{-1}) with ethylbenzene (EtBz). Reaction conditions: $[Fe^{IV}(O)(L)]^{2+}$ = 1 mM and [EtBz] = 5 – 400 mM in CH_3CN at -40 °C.

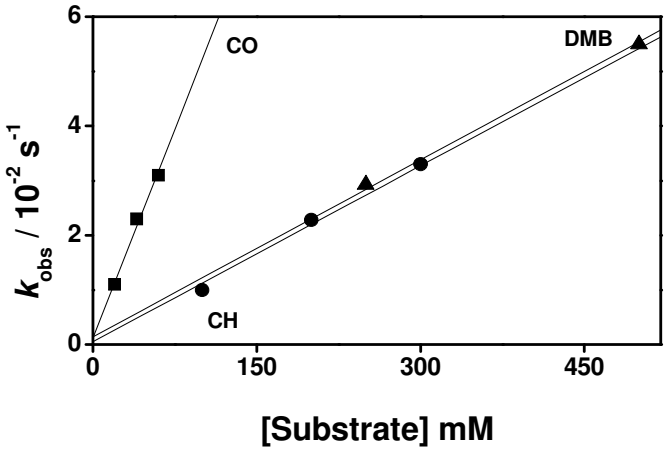

Figure S6. Plot of the pseudo-first-order rate constants, k_{obs}, against substrate concentrations to determine second-order rate constants, k_2, for the reactions of $[(TDCPP)^{+\cdot}Fe^{IV}(O)]$ (**7**) with cyclooctane (■, CO; k_2 = 5.1 x 10^{-1} M^{-1} s^{-1}), 2,3-dimethylbutane (▲, DMB; k_2 = 7.6 x 10^{-2} M^{-1} s^{-1}), and cyclohexane (●, CH; k_2 = 1.1 x 10^{-1} M^{-1} s^{-1}) in a solvent mixture of CH_3CN and CH_2Cl_2 (*v*/*v* = 1:1) at –40 °C. Reaction conditions: $[(TDCPP)^{+\cdot}Fe^{IV}(O)]$ = 1 mM and [substrate] = 20 – 500 mM.

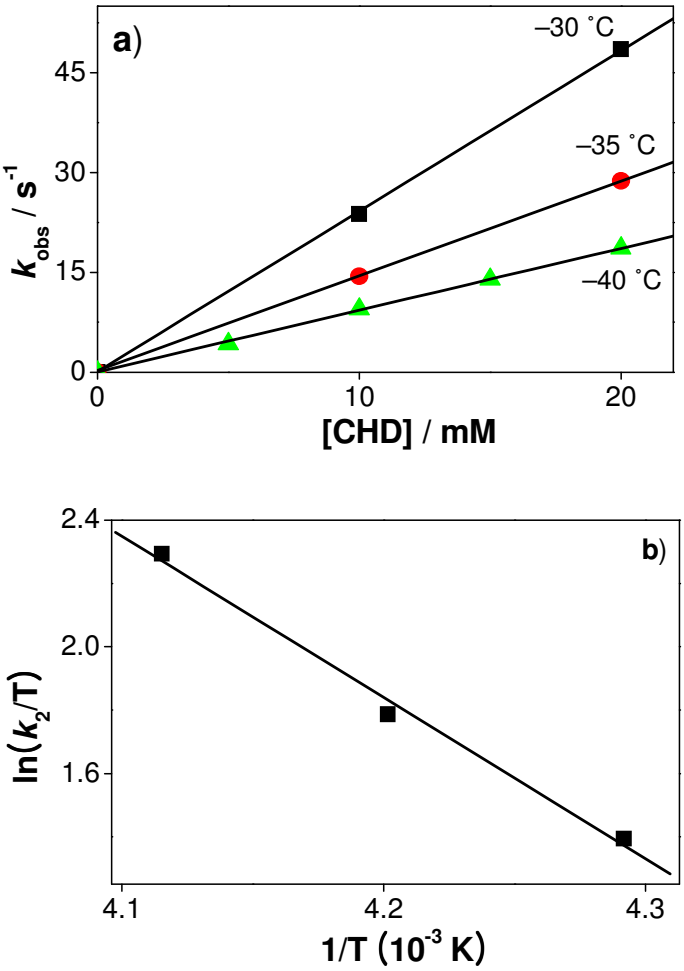

Figure S7. A) Plot of the pseudo-first-order rate constants, k_{obs}, against substrate concentrations to determine second-order rate constants for the reactions of $[Fe^{IV}(O)(Me_3NTB)]^{2+}$ (**3**) with 1,4-cyclohexadiene (CHD) at different temperature. B) Determination of activation parameters by plotting second-order rate constants k_2 of **3** against 1/T. Reaction conditions: $[Fe^{IV}(O)(Me_3NTB)]^{2+}$ = 1 mM and [CHD] = 5 – 20 mM in CH_3CN.

Density Functional Theory Calculations

Methods

Density functional theory (DFT)[9] was applied at B3LYP/LACV3P*+//B3LYP/LACVP level[10-13] using Gaussian 09.[14] The high molecular charge (2+) made it necessary to perform the optimizations in solvent to avoid artificial results.[15,16] The solvent (acetonitrile) effects were included using CPCM model with UFF cavity, per G09 default. The relative free energies of complexes were corrected with -1.89 kcal/mol due to change of standard states (either added to the complexed states or subtracted from the non-complexed states, depending on the reference state).[17,18] Dispersion effects were calculated using DFT-D3 program.[19]

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Energies

Table S5. $[Fe^{IV}O(Me_3NTB)]^{2+}$ in kcal/mol.

	Δlacvp	Δlacv3p^{*+}	ΔZ_0	$\Delta E_{Thermal}$	Dispersion	**ΔH**[a]	-TΔS[b]	**ΔG**[c]
$^3[Fe^{IV}O(Me_3NTB)]^{2+}$ (π^*,π^{*}')	9.65	+3.07	+0.61	-0.21	-2.35	**10.78**	+1.30	**12.08**
$^3[Fe^{IV}O(Me_3NTB)]^{2+}$ (π^*,π^{*}'(↓),δ, δ')	14.23	+2.88	-0.62	+0.16	+0.00	**16.66**	-0.05	**16.61**
$^5[Fe^{IV}O(Me_3NTB)]^{2+}$ (π^*,π^{*}',δ, δ')	0.00	+0.00	+0.00	+0.00	+0.00	**0.00**	+0.00	**0.00**

[a] Sum of the four previous columns. [b] T=298.15 K. [c] ΔG=ΔH-TΔS.

Table S6. $^5[Fe^{IV}O(Me_3NTB)]^{2+}$ with 1,4-cyclohexadiene in kcal/mol.

	Δlacvp	Δlacv3p^{*+}	ΔZ_0	$\Delta E_{Thermal}$	Dispersion	**ΔH**[a]	-TΔS[b]	ΔG_{corr} [c]	**ΔG**[d]
Reactants, inf separated	1.20	-0.99	-0.15	-1.60	+4.61	**3.06**	-7.02	+1.89	**-1.62**
Reactants, 20 Å separated	1.04	-1.00	+0.08	-0.57	+4.60	**4.15**	+0.55	+1.89	**7.05**
Reactants, complexed	0.00	+0.00	+0.00	+0.00	+0.00	**0.00**	+0.00		**0.00**
Transition state	2.71	+0.51	-1.80	-0.51	-1.51	**-0.60**	+3.05		**2.88**
Intermediate	-23.07	-0.96	-2.56	0.36	-2.43	**-28.66**	+0.44		**-27.30**

[a] Sum of the four previous columns. [b] T=298.15 K. [c] Correction factor for standard state change, RTln(24.5), added for non-complexed structures. [d] $\Delta G=\Delta H-T\Delta S+\Delta G_{corr}$.

Table S7. $^5[Fe^{IV}O(Me_3NTB)]^{2+}$ with cyclohexane in kcal/mol.

	Δlacvp	Δlacv3p^{*+}	ΔZ_0	$\Delta E_{Thermal}$	Dispersion	**ΔH**[a]	-TΔS[b]	ΔG_{corr} [c]	**ΔG**[d]
Reactants, inf separated	0.16	+0.05	-0.44	-1.53	-0.02	**-1.79**	-2.06		**-3.85**
Reactants, 20 Å separated	0.00	+0.00	+0.00	+0.00	+0.00	**0.00**	+0.00		**0.00**
Reactants, complexed	-0.34	+0.16	+0.16	-0.07	-2.51	**-2.60**	+5.87	-1.89	**1.37**
Transition state	8.63	+1.42	-4.03	-0.26	-6.24	**-0.48**	+8.11	-1.89	**5.74**
Intermediate	1.25	-1.25	-3.03	+0.36	-5.53	**-8.21**	+6.17	-1.89	**-3.93**

[a] Sum of the four previous columns. [b] T=298.15 K. [c] Correction factor for standard state change, RTln(24.5), subtracted for complexed structures. [d] $\Delta G=\Delta H-T\Delta S+\Delta G_{corr}$.

Table S8. $[Fe^{IV}O(Me_3NTB)(CH_3CN)]^{2+}$ in kcal/mol.

	Δlacvp	Δlacv3p^{*+}	ΔZ_0	$\Delta E_{Thermal}$	Dispersion	**ΔH**[a]	-TΔS[b]	ΔG_{corr} [c]	**ΔG**[d]
$^5[Fe^{IV}O(Me_3NTB)]^{2+}$ + CH_3CN (inf sep)	10.14	-7.82	-1.98	-0.45	+6.54	**6.43**	-12.42	+1.75	**-4.23**
$^5[Fe^{IV}O(Me_3NTB)]^{2+}$ + CH_3CN (20 Å apart)	10.03	-7.80	-1.83	+0.62	+6.53	**7.55**	-6.54	+1.75	**2.75**
$^3[Fe^{IV}O(Me_3NTB)(CH_3CN)]^{2+}$ (π^*, π^{*}')	0.00	+0.00	+0.00	+0.00	+0.00	**0.00**	+0.00		**0.00**
$^5[Fe^{IV}O(Me_3NTB)(CH_3CN)]^{2+}$ (π^*, π^{*}', δ, σ^*_{xy})	6.92	-4.20	-1.19	+0.59	+0.45	**2.57**	-2.53		**0.05**
$^3[Fe^{IV}O(Me_3NTB)(CH_3CN)]^{2+}$ (stereoisomer)	6.03	-1.03	-0.06	0.02	-0.77	**4.19**	-0.11		**4.07**

[a] Sum of the four previous columns. [b] T=298.15 K. [c] Correction factor for standard state change, RTln(19.1), added for non-complexed structures (19.1 is the molarity of acetonitrile). [d] $\Delta G=\Delta H-T\Delta S+\Delta G_{corr}$.

Table S9. $[Fe^{IV}O(Me_3NTB)(CH_3CN)]^{2+}$ with 1,4-cyclohexadiene in kcal/mol.

	2S+1	Δlacvp	Δlacv3p^{*+}	ΔZ_0	ΔE(Thermal)	Dispersion	**ΔH**[a]	-TΔS[b]	ΔG_{corr} [c]	**ΔG**[d]
Reactants, inf separated	3	-5.69	+3.32	+0.93	-2.17	+4.26	**0.65**	-4.81	+1.89	**-2.27**
Reactants, 20 Å separated	3	-5.83	+3.28	+1.09	-1.10	+4.32	**1.74**	+2.40	+1.89	**6.04**
Reactants, complexed	3	-7.10	+4.66	+1.22	-0.64	-1.23	**-3.10**	+3.48		**0.38**
Transition state	3	2.05	+7.18	-2.34	-1.17	-3.96	**1.76**	+5.96		**7.72**
Intermediate	3	-20.33	+2.87	-0.74	-0.35	-2.17	**-20.72**	+2.32		**-18.39**
Reactants, inf separated	5	1.23	-0.88	-0.26	-1.57	+4.70	**3.22**	-7.34	+1.89	**-2.22**
Reactants, 20 Å separated	5	1.14	-0.90	-0.19	-1.02	+4.62	**3.64**	+1.73	+1.89	**7.26**
Reactants, complexed	5	0.00	+0.00	+0.00	+0.00	+0.00	**0.00**	+0.00		**0.00**
Transition state	5	2.56	+0.26	-2.12	-0.28	-1.26	**-0.83**	+1.13		**0.30**
Intermediate	5	-24.03	+1.87	-2.76	0.37	-3.03	**-31.33**	0.94		**-30.39**

[a] Sum of the four previous columns. [b] T=298.15 K. [c] Correction factor for standard state change, RTln(24.5), added for non-complexed structures. [d] $\Delta G=\Delta H-T\Delta S+\Delta G_{corr}$.

Table S10. $[Fe^{IV}O(Me_3NTB)(CH_3CN)]^{2+}$ with cyclohexane in kcal/mol.

	2S+1	Δlacvp	Δlacv3p^{*+}	ΔZ_0	ΔE(Thermal)	Dispersion	**ΔH**[a]	-TΔS[b]	ΔG_{corr} [c]	**ΔG**[d]
Reactants, inf separated	3	0.13	+0.00	-0.24	-1.68	+0.03	**-1.76**	-0.52		**-2.28**
Reactants, 20 Å separated	3	0.00	+0.00	+0.00	+0.00	+0.00	**0.00**	+0.00		**0.00**
Reactants, complexed	3	-0.49	+0.43	+0.37	-0.21	-2.76	**-2.65**	+6.57	-1.89	**2.03**
Transition state	3	17.18	+2.79	-4.19	-0.58	-8.17	**7.03**	+10.60	-1.89	**15.74**
Intermediate	3	11.42	-1.44	-2.07	+0.07	-6.00	**1.99**	+8.25	-1.89	**8.35**
Reactants, inf separated	5	7.05	-4.20	-1.43	-1.09	+0.47	**0.81**	-3.05		**-2.23**
Reactants, 20 Å separated	5	6.94	-4.19	-1.20	-0.01	+0.37	**1.92**	+0.20		**2.12**
Reactants, complexed	5	6.38	-3.67	-1.05	+0.45	-3.27	**-1.16**	+4.72	-1.89	**1.67**
Transition state	5	15.19	-2.63	-4.89	+0.10	-8.52	**-0.74**	+7.50	-1.89	**4.87**
Intermediate	5	6.91	-5.64	-4.30	+0.85	-7.35	**-9.54**	+5.11	-1.89	**-6.32**

[a] Sum of the four previous columns. [b] T=298.15 K. [c] Correction factor for standard state change, RTln(24.5), subtracted for complexed structures. [d] $\Delta G=\Delta H-T\Delta S+\Delta G_{corr}$.

Mulliken spin density distribution

Table S11. $[Fe^{IV}O(Me_3NTB)]^{2+}$.

	Fe	O	4 x ligated N	Rest
$^3[Fe^{IV}O(Me_3NTB)]^{2+}$ ($\pi^*,\pi^{*\prime}$)	1.20	0.81	-0.03	0.03
$^3[Fe^{IV}O(Me_3NTB)]^{2+}$ ($\pi^*,\pi^{*\prime}(\downarrow),\delta, \delta'$)	2.55	-0.79	0.13	0.11
$^5[Fe^{IV}O(Me_3NTB)]^{2+}$ ($\pi^*,\pi^{*\prime},\delta, \delta'$)	3.10	0.72	0.17	0.00

Table S12. $^5[Fe^{IV}O(Me_3NTB)]^{2+}$ with 1,4-cyclohexadiene.

	Fe	O	4 x ligated N	Substrate	Rest
Reactants, 20 Å separated	3.11	0.72	0.17	0.00	0.00
Reactants, complexed	3.11	0.74	0.16	0.00	-0.01
Transition state	3.54	0.42	0.24	-0.21	0.02
Intermediate	4.18	0.43	0.33	-0.98	0.04

Table S13. $^5[Fe^{IV}O(Me_3NTB)]^{2+}$ with cyclohexane.

	Fe	O	4 x ligated N	Substrate	Rest
Reactants, 20 Å separated	3.10	0.72	0.17	0.00	0.01
Reactants, complexed	3.11	0.74	0.16	-0.00	-0.01
Transition state	3.79	0.18	0.32	-0.34	0.05
Intermediate	4.20	0.31	0.31	-0.84	0.02

Table S14. $[Fe^{IV}O(Me_3NTB)(CH_3CN)]^{2+}$.

	Fe	O	4 x ligated N	CH_3CN	Rest
$^3[Fe^{IV}O(Me_3NTB)(CH_3CN)]^{2+}$ (π^*, $\pi^{*\prime}$)	1.12	0.97	-0.02	-0.00	-0.06
$^5[Fe^{IV}O(Me_3NTB)(CH_3CN)]^{2+}$ (π^*, $\pi^{*\prime}$, δ, σ^*_{xy})	2.97	0.71	0.09	0.18	0.05
$^3[Fe^{IV}O(Me_3NTB)(CH_3CN)]^{2+}$ (stereoisomer)	1.27	0.94	-0.11	-0.05	-0.05

Table S15. $[Fe^{IV}O(Me_3NTB)(CH_3CN)]^{2+}$ with 1,4-cyclohexadiene.

	2S+1	Fe	O	4 x ligated N	CH_3CN	Substrate	Rest
Reactants, 20 Å separated	3	1.12	0.97	-0.02	-0.01	0.00	-0.06
Reactants, complexed	3	1.08	1.00	-0.04	0.00	0.00	-0.05
Transition state	3	0.86	0.80	-0.04	0.03	0.38	-0.03
Intermediate	3	0.89	0.19	-0.06	0.01	0.99	-0.02
Reactants, 20 Å separated	5	2.97	0.72	0.09	0.17	0.00	0.05
Reactants, complexed	5	3.07	0.74	0.00	0.16	0.00	0.02
Transition state	5	3.50	0.42	0.12	0.13	-0.19	0.02
Intermediate	5	4.24	0.40	0.11	0.17	-0.96	0.03

Table S16. $[Fe^{IV}O(Me_3NTB)(CH_3CN)]^{2+}$ with cyclohexane.

	2S+1	Fe	O	4 x ligated N	CH_3CN	Substrate	Rest
Reactants, 20 Å separated	3	1.12	0.97	-0.02	-0.00	0.00	-0.06
Reactants, complexed	3	1.11	0.98	-0.04	0.01	0.00	-0.06
Transition state	3	0.86	0.69	-0.07	0.05	0.49	-0.02
Intermediate	3	0.89	0.21	-0.06	0.03	0.95	-0.02
Reactants, 20 Å separated	5	2.97	0.72	0.09	0.17	0.00	0.05
Reactants, complexed	5	3.08	0.74	-0.00	0.17	0.00	0.01
Transition state	5	3.86	0.14	0.17	0.12	-0.31	0.02
Intermediate	5	4.23	0.36	0.18	0.13	-0.92	0.02

Geometries

Table S17. $[Fe^{IV}O(Me_3NTB)]^{2+}$ distances and angles (Å and °).

	D(Fe-O)	D(Fe-N_{eq1})	D(Fe-N_{eq2})	D(Fe-N_{eq3})	D(Fe-N_{ax})	A(N_{eq}-Fe-N_{eq})[a]
$^3[Fe^{IV}O(Me_3NTB)]^{2+}$ ($\pi^*,\pi^{*'}$)	1.63	1.89	1.94	1.95	2.15	160.59
$^3[Fe^{IV}O(Me_3NTB)]^{2+}$ ($\pi^*,\pi^{*'}(\downarrow),\delta,\delta'$)	1.72	1.96	1.97	2.01	2.12	120.39
$^5[Fe^{IV}O(Me_3NTB)]^{2+}$ ($\pi^*,\pi^{*'},\delta,\delta'$)	1.65	1.98	1.98	1.98	2.15	118.59

[a] The largest angle of the three possible ones.

Table S18. $^5[Fe^{IV}O(Me_3NTB)]^{2+}$ with 1,4-cyclohexadiene distances and angles (Å and °).

	D(Fe-O)	D(Fe-N_{eq1})	D(Fe-N_{eq2})	D(Fe-N_{eq3})	D(Fe-N_{ax})	D(O-H)	D(FeOH-C_6H_7)	A(Fe-O-H)
Reactants, 20 Å separated	1.65	1.98	1.98	1.98	2.15	19.83	1.10	170.30
Reactants, complexed	1.65	1.98	1.98	1.99	2.14	2.80	1.10	168.99
Transition state	1.69	2.01	2.01	2.02	2.27	1.72	1.14	177.01
Intermediate	1.78	2.04	2.04	2.04	2.42	0.98	2.21	178.17

Table S19. $^5[Fe^{IV}O(Me_3NTB)]^{2+}$ with cyclohexane distances and angles (Å and °).

	D(Fe-O)	D(Fe-N_{eq1})	D(Fe-N_{eq2})	D(Fe-N_{eq3})	D(Fe-N_{ax})	D(O-H)	D(FeOH-C_6H_{11})	A(Fe-O-H)
Reactants, 20 Å separated	1.65	1.98	1.98	1.98	2.15	20.42	1.10	164.75
Reactants, complexed	1.65	1.98	1.98	1.99	2.15	2.92	1.10	170.92
Transition state	1.73	2.03	2.03	2.03	2.34	1.40	1.20	177.06
Intermediate	1.78	2.05	2.04	2.05	2.42	1.00	1.88	169.49

Table S20. $[Fe^{IV}O(Me_3NTB)(CH_3CN)]^{2+}$ distances angles (Å and °).

	D(Fe-O)	D(Fe-N_{eq1})	D(Fe-N_{eq2})	D(Fe-N_{eq3})	D(Fe-N_{ax})	D(Fe-$NCCH_3$)	A(N_{eq}-Fe-N_{eq})[a]
$^3[Fe^{IV}O(Me_3NTB)(CH_3CN)]^{2+}$	1.65	1.93	1.96	1.96	2.17	2.01	90.59
$^5[Fe^{IV}O(Me_3NTB)(CH_3CN)]^{2+}$	1.65	2.07	1.99	1.99	2.17	2.36	94.94
$^3[Fe^{IV}O(Me_3NTB)(CH_3CN)]^{2+}$ (stereoisomer)	1.67	2.03	1.98	1.98	2.04	1.98	92.20

[a] The largest angle of the four possible ones.

Table S21. $[Fe^{IV}O(Me_3NTB)(CH_3CN)]^{2+}$ with 1,4-cyclohexadiene distances and angles (Å and °).

	D (Fe-O)	D (Fe-N_{eq1})	D (Fe-N_{eq2})	D (Fe-N_{eq3})	D (Fe-N_{ax})	D (Fe-$NCCH_3$)	D (O-H)	D (FeOH-C_6H_7)	A (Fe-O-H)
S=1									
Reactants, 20Å separated	1.65	1.93	1.96	1.96	2.17	2.01	20.55	1.10	161.82
Reactants, complexed	1.66	1.93	1.96	1.96	2.17	2.01	2.79	1.10	173.81
Transition state	1.74	1.95	1.97	1.97	2.17	2.00	1.39	1.24	124.73
Intermediate	1.81	1.95	1.97	1.97	2.14	2.00	0.98	2.48	115.09
S=2									
Reactants, 20Å separated	1.65	2.07	1.99	1.99	2.18	2.36	20.30	1.10	165.59
Reactants, complexed	1.65	2.07	1.99	1.99	2.18	2.36	2.64	1.10	174.43
Transition state	1.69	2.06	2.05	2.06	2.29	2.30	1.73	1.14	169.99
Intermediate	1.81	2.07	2.09	2.09	2.44	2.27	0.98	2.18	146.57

Table S22. $[Fe^{IV}O(Me_3NTB)(CH_3CN)]^{2+}$ with cyclohexane distances and angles (Å and °).

	D (Fe-O)	D (Fe-N_{eq1})	D (Fe-N_{eq2})	D (Fe-N_{eq3})	D (Fe-N_{ax})	D (Fe-$NCCH_3$)	D (O-H)	D (FeOH-C_6H_{11})	A (Fe-O-H)
S=1									
Reactants, 20Å separated	1.66	1.93	1.96	1.96	2.17	2.01	19.92	1.10	159.23
Reactants, complexed	1.66	1.93	1.96	1.96	2.17	2.01	2.82	1.10	154.07
Transition state	1.78	1.95	1.97	1.97	2.16	2.00	1.20	1.35	121.97
Intermediate	1.81	1.95	1.97	1.97	2.14	2.00	0.99	2.19	115.66
S=2									
Reactants, 20Å separated	1.65	2.07	1.99	1.99	2.17	2.36	19.71	1.10	152.54
Reactants, complexed	1.65	2.07	1.99	1.99	2.17	2.36	2.91	1.10	164.16
Transition state	1.73	2.06	2.08	2.08	2.37	2.27	1.41	1.20	165.91
Intermediate	1.79	2.08	2.10	2.09	2.44	2.27	1.00	1.94	160.75

Coordinates

The coordinates are given in xyz-format, and the specific charge/multiplicity pair for each of the calculations is given in parenthesis in the comment line of the structure.

```
63
[FeO(NTB)] (+2/3) 2-radical
Fe 0.55917 -0.35751 0.79360
O 0.67523 1.06997 1.57554
C -2.42537 1.95559 -3.10662
C -2.39111 3.26089 -2.61381
C -2.14587 -1.16159 -3.68490
C -1.74365 0.98571 -2.36563
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N -1.57682 -0.39612 -2.56704
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C -1.05281 1.30841 -1.17291
C -1.02170 2.61812 -0.68406
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C -0.39658 -2.27879 -1.28458
N -0.49893 0.11446 -0.69618
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N 3.78067 -1.22665 -1.47938
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N 0.51691 -2.33064 -0.06413
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C -0.05454 -3.24292 1.00159
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C 3.11112 2.12778 -0.37362
C -1.05835 -2.43558 1.75950
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C -3.43046 0.84638 3.81161
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H 3.98851 -3.15776 -2.28910
H 4.80321 -1.87081 -3.19343
H 5.49293 -2.45130 -1.65313
H 5.91068 0.41266 -2.58827
H 5.94344 2.86109 -2.14764
H 4.20280 3.93339 -0.76178
H 2.34940 2.59093 0.23999
H 0.75945 -3.54360 1.66813
H -0.47583 -4.14901 0.55777
H -1.95896 -4.92444 2.13515
H -2.37589 -4.50026 3.80869
H -3.59319 -4.34527 2.51175
H -4.37773 -2.42724 4.27636
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H -3.73302 1.84004 4.12233
H -1.76411 1.55182 2.61160

63
[FeO(NTB)] (+2/3) 4-radical
Fe 0.01318 0.07860 0.08145
O -0.02120 1.68518 0.70497
C -2.99971 1.75732 -4.24057
C -2.83369 3.13374 -4.07194
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C -1.21867 -2.08382 -1.50604
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N 0.03279 -1.90836 -0.67045
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C 0.04036 -2.84817 0.51708
C 4.62301 2.24700 0.97474
C 3.31022 1.79627 0.83201
C -0.74205 -2.19620 1.60772
N -0.86497 -0.85557 1.62383
N -1.34806 -2.76331 2.68148
C -1.41601 -4.18940 3.02791
C -1.59246 -0.51698 2.77531
C -2.00630 0.72051 3.27983
C -1.89905 -1.72103 3.45214
C -2.72722 0.70932 4.47448
C -2.62009 -1.73599 4.64910
C -3.02917 -0.49746 5.14705
H -3.59789 1.35742 -5.04994
H -3.31366 3.81238 -4.76776
H -1.95629 4.74019 -2.92549
H -0.81822 3.23520 -1.28269
H -2.71966 -2.43614 -3.81548
H -4.07768 -1.30205 -3.97135
H -2.70371 -1.22099 -5.10935
H -2.02901 -2.40077 -0.84145
H -1.07402 -2.86976 -2.25287
H 1.05276 -1.77777 -2.53299
H 1.58856 -3.12928 -1.53152
H 3.82217 -3.03483 -2.14458
H 4.87414 -1.73961 -2.75797
H 5.26746 -2.57019 -1.22702
H 6.36581 -0.16810 -0.74637
H 6.71673 1.92917 0.54585
H 4.81415 3.15878 1.52913
H 2.47091 2.33410 1.25616
H 1.07978 -2.98316 0.83324
H -0.34973 -3.82860 0.22878
H -1.06736 -4.79003 2.18938
H -0.79012 -4.39214 3.89977
H -2.45067 -4.45799 3.24741
H -2.85143 -2.65721 5.16973
H -3.59134 -0.45998 6.07324
H -3.06418 1.64786 4.89999
H -1.76606 1.64047 2.76248

63
[FeO(NTB)] (+2/5)
Fe -0.00830 0.11008 0.03773
O -0.02665 1.65053 0.62628
C -3.08932 1.74142 -4.27709
C -2.96537 3.12008 -4.09244
C -2.99607 -1.43139 -4.14659
C -2.42731 0.92636 -3.35574
C -2.20914 3.66152 -3.02761
N -2.33670 -0.47611 -3.24530
C 4.46288 -2.21885 -1.81331
C -1.66951 1.46189 -2.28884
C -1.54815 2.84348 -2.11027
C -1.56563 -0.75094 -2.16572
C -1.22087 -2.07796 -1.57542
N -1.14333 0.38112 -1.56363
C 1.28112 -2.04743 -1.55461
N 3.66995 -1.22456 -1.07623
C 2.32247 -1.16582 -0.94880
C 5.53034 0.28848 -0.18251
N 0.02096 -1.89356 -0.72874
C 4.21050 -0.12614 -0.37695
N 1.94597 -0.10012 -0.20991
C 5.71564 1.44182 0.58278
C 3.11393 0.58013 0.16889
C 0.02550 -2.83261 0.45908
C 4.62312 2.15177 1.13176
C 3.30626 1.73336 0.93601
C -0.72696 -2.16667 1.56311
N -0.85169 -0.82263 1.57237
N -1.29279 -2.72126 2.66241
C -1.34071 -4.14323 3.03095
C -1.54007 -0.47450 2.74500
C -1.94073 0.76668 3.24916
C -1.82164 -1.67218 3.44173
C -2.62246 0.76571 4.46696
C -2.50393 -1.67791 4.66073
C -2.89929 -0.43511 5.16008
H -3.67126 1.33265 -5.09384
H -3.46239 3.79201 -4.78281
H -2.14272 4.73846 -2.92272
H -0.96959 3.25072 -1.29079
H -2.67464 -2.44419 -3.90999
H -4.07972 -1.36339 -4.02960
H -2.72167 -1.20407 -5.17820
H -2.03194 -2.41335 -0.92083
H -1.05879 -2.85522 -2.32789
H 1.06033 -1.71524 -2.57426
H 1.57745 -3.09933 -1.60565
H 3.80985 -3.00063 -2.19745
H 4.97288 -1.73693 -2.65010
H 5.19779 -2.66667 -1.14204
H 6.37073 -0.25128 -0.60126
H 6.72265 1.80192 0.76004
H 4.81520 3.04280 1.71867
H 2.46468 2.27308 1.35147
H 1.06586 -2.99065 0.76126
H -0.38952 -3.80498 0.17833
H -0.97856 -4.75174 2.20418
H -0.71356 -4.32010 3.90738
H -2.37160 -4.42460 3.25243
H -2.71793 -2.59456 5.19642
H -3.43188 -0.39016 6.10319
H -2.94849 1.70744 4.89370
H -1.72285 1.68216 2.71378

77
[FeO(NTB)]+CHD React (+2/5)
Fe -0.09767 0.05240 -0.07632
O -0.16829 1.61407 0.44978
C -2.99250 1.47614 -4.59018
C -2.88849 2.86241 -4.45763
C -2.87339 -1.68845 -4.32840
C -2.36377 0.70629 -3.60865
C -2.18288 3.45449 -3.38505
N -2.26500 -0.68969 -3.43789
C 4.48139 -2.24627 -1.68509
C -1.65771 1.29259 -2.53288
C -1.55515 2.68143 -2.40736
C -1.54019 -0.91206 -2.31541
C -1.20862 -2.20884 -1.65556
N -1.15423 0.24759 -1.74182
C 1.28932 -2.12094 -1.55231
N 3.64544 -1.25074 -0.99891
C 2.29319 -1.21021 -0.92565
C 5.44658 0.30441 -0.05799
N -0.00137 -1.97369 -0.77367
C 4.14155 -0.13263 -0.29777
N 1.87216 -0.13781 -0.22156
C 5.58465 1.47167 0.69603
C 3.01386 0.56591 0.19244
C -0.01618 -2.87827 0.44004
C 4.46102 2.17245 1.19127
C 3.15863 1.73237 0.95030
C -0.79794 -2.19056 1.50919
N -0.93721 -0.84803 1.48226
N -1.37234 -2.72364 2.61452
C -1.41010 -4.13664 3.01679
C -1.64243 -0.47798 2.63885
C -2.05514 0.77121 3.11275
C -1.92048 -1.66135 3.36144
C -2.74727 0.79164 4.32458
C -2.61390 -1.64531 4.57402
C -3.02307 -0.39485 5.04196
H -3.53504 1.02793 -5.41338
H -3.36129 3.50046 -5.19552
H -2.12982 4.53545 -3.32216
H -1.01493 3.12778 -1.58222
H -2.52829 -2.68460 -4.05666
H -3.96135 -1.64921 -4.24174
H -2.57792 -1.48032 -5.35814
H -2.04029 -2.52177 -1.01589
H -1.01273 -3.01741 -2.36577
H 1.09982 -1.81235 -2.58565
H 1.60485 -3.16831 -1.57275
H 3.85481 -3.03887 -2.09054
H 5.02585 -1.76904 -2.50260
H 5.18817 -2.67897 -0.97473
H 6.31061 -0.22914 -0.43443
H 6.57850 1.84949 0.90743
H 4.61702 3.07397 1.77292
H 2.29573 2.26655 1.32848
H 1.01805 -3.01864 0.77103
H -0.41545 -3.86267 0.17878
H -1.03795 -4.76139 2.20669
H -0.78695 -4.28762 3.90093
H -2.43993 -4.42161 3.23854
H -2.82467 -2.55144 5.12855
H -3.56395 -0.33275 5.97940
H -3.07955 1.74195 4.72670
H -1.83676 1.68077 2.56764
H -0.68716 4.31553 0.98640
C -0.56071 5.03768 1.81041
C -1.66476 4.85265 2.82511
C -1.44503 4.55869 4.11573
C -0.06713 4.37544 4.70797
C 1.03776 4.58771 3.69942
C 0.81788 4.88636 2.40997
H -0.65522 6.02648 1.33072
H -2.68383 4.97712 2.46324
H -2.28619 4.44761 4.79781
H 0.01802 3.36931 5.15252
H 0.06827 5.06248 5.56040
H 2.05739 4.49525 4.06897
H 1.66017 5.03784 1.73710

77
[FeO(NTB)]+CHD TS (+2/5)
Fe -0.06389 0.17807 0.01157
O -0.10512 1.76581 0.57758
C -3.04283 1.64173 -4.46360
C -2.92464 3.02468 -4.30990
C -2.94012 -1.52525 -4.25876
C -2.40197 0.84977 -3.50729
C -2.19360 3.59245 -3.24109
N -2.30905 -0.54793 -3.36157
C 4.43338 -2.28385 -1.75620
C -1.67158 1.41106 -2.43490
C -1.55506 2.79705 -2.28870
C -1.56416 -0.79514 -2.25359
C -1.23304 -2.11884 -1.64369
N -1.16043 0.35082 -1.66833
C 1.26107 -2.06406 -1.58611
N 3.64138 -1.27650 -1.03731
C 2.28948 -1.18873 -0.94559
C 5.50957 0.18658 -0.08061
N -0.00874 -1.94431 -0.78823
C 4.18668 -0.19751 -0.31525
N 1.91618 -0.12276 -0.20774
C 5.69888 1.32641 0.70361
C 3.09032 0.52587 0.20779
C -0.01122 -2.86022 0.40425
C 4.60689 2.05220 1.23275
C 3.28744 1.66456 0.99552
C -0.75437 -2.18784 1.51299
N -0.88897 -0.84623 1.54182
N -1.30767 -2.76392 2.61138
C -1.34074 -4.19047 2.96074
C -1.57146 -0.52388 2.72696
C -1.97724 0.70615 3.25394
C -1.83757 -1.73262 3.41012
C -2.64767 0.68277 4.47777
C -2.50811 -1.76137 4.63567
C -2.90878 -0.52935 5.15704
H -3.60495 1.21224 -5.28375
H -3.40578 3.67915 -5.02789
H -2.12934 4.67180 -3.16122
H -0.99462 3.22245 -1.46618
H -2.58561 -2.52720 -4.02308
H -4.02564 -1.49211 -4.14196
H -2.67440 -1.29089 -5.29111
H -2.05733 -2.44108 -0.99848
H -1.07854 -2.90172 -2.39348
H 1.05870 -1.71066 -2.60281
H 1.57771 -3.10957 -1.66000
H 3.77807 -3.05947 -2.14850
H 4.96523 -1.81362 -2.58626
H 5.15078 -2.73848 -1.07050
H 6.34935 -0.36633 -0.48336
H 6.70822 1.66262 0.91231
H 4.80171 2.93084 1.83739
H 2.44656 2.21523 1.39745
H 1.02777 -3.02566 0.70858
H -0.43372 -3.83629 0.14471
H -0.98413 -4.78600 2.12223
H -0.70240 -4.37574 3.82752
H -2.36673 -4.48323 3.19076
H -2.70907 -2.68759 5.16004
H -3.43240 -0.50221 6.10598
H -2.97600 1.61717 4.91922
H -1.77258 1.63373 2.73484
H -0.21810 3.35962 1.20353
C -0.32322 4.41825 1.62435
C -1.63251 4.51380 2.34185
C -1.72653 4.68632 3.67518
C -0.52506 4.83410 4.57097
C 0.77850 4.88239 3.81895
C 0.86430 4.71078 2.48524
H -0.31850 5.02709 0.70646
H -2.53406 4.42727 1.73974
H -2.70312 4.74421 4.15026
H -0.50339 4.01072 5.30756
H -0.63143 5.73971 5.19201
H 1.67394 5.08551 4.40163
H 1.83060 4.77539 1.99019

77
[FeO(NTB)]+CHD Interm (+2/5)
Fe -0.08748 0.31874 0.09377
O -0.14694 1.99272 0.70952
C -3.11134 1.55771 -4.43800
C -3.04605 2.94483 -4.29021
C -2.89710 -1.59895 -4.21693
C -2.44887 0.79416 -3.47330
C -2.34536 3.54311 -3.21801
N -2.30476 -0.59727 -3.32067
C 4.46340 -2.18545 -1.67775
C -1.74751 1.38470 -2.39777
C -1.68547 2.77513 -2.25759
C -1.55810 -0.81308 -2.20484
C -1.18824 -2.13166 -1.60494
N -1.20128 0.34713 -1.62049
C 1.29764 -2.01985 -1.53040
N 3.65354 -1.18872 -0.96490
C 2.29836 -1.11576 -0.88366
C 5.49924 0.29324 0.00389
N 0.02395 -1.94187 -0.75178
C 4.18207 -0.10424 -0.24045
N 1.90690 -0.05386 -0.15190
C 5.67155 1.43525 0.78897
C 3.07356 0.60707 0.27268
C 0.02837 -2.82563 0.45336
C 4.56799 2.14973 1.30871
C 3.25429 1.74858 1.06103
C -0.77218 -2.16360 1.52872
N -0.92714 -0.82528 1.56428
N -1.37567 -2.76065 2.59072
C -1.41629 -4.19208 2.91640
C -1.67315 -0.52759 2.71884
C -2.12227 0.69049 3.24003
C -1.95799 -1.74727 3.37407
C -2.85463 0.64317 4.42738
C -2.68962 -1.80022 4.56334
C -3.13399 -0.58049 5.07791
H -3.65100 1.10356 -5.26001
H -3.54552 3.57800 -5.01482
H -2.32174 4.62438 -3.14145
H -1.14942 3.22618 -1.43264
H -2.48942 -2.58364 -3.99517
H -3.98165 -1.62236 -4.08771
H -2.65667 -1.34352 -5.25050
H -2.00730 -2.48011 -0.96629
H -1.02275 -2.90180 -2.36652
H 1.09684 -1.67166 -2.54955
H 1.65546 -3.05282 -1.60540
H 3.82190 -2.96853 -2.07764
H 4.99748 -1.70802 -2.50239
H 5.18048 -2.63270 -0.98670
H 6.34744 -0.25153 -0.39236
H 6.67582 1.78171 1.00543
H 4.74850 3.03070 1.91453
H 2.40630 2.29290 1.45690
H 1.06420 -2.93989 0.79129
H -0.34425 -3.82792 0.21494
H -1.05882 -4.77579 2.07000
H -0.78585 -4.39670 3.78476
H -2.44554 -4.48261 3.13406
H -2.90325 -2.73549 5.06629
H -3.70594 -0.57195 5.99890
H -3.21828 1.56687 4.86348
H -1.90103 1.62678 2.74310
H -0.19097 2.92020 1.01967
C -0.31119 5.05282 1.58441
C -1.50070 4.83524 2.34256
C -1.44819 4.52459 3.67841
C -0.14344 4.39537 4.41913
C 1.06552 4.66382 3.56260
C 0.95963 4.97561 2.23018
H -0.37547 5.35257 0.54357
H -2.46340 4.92594 1.84739
H -2.36329 4.37233 4.24368
H -0.06749 3.38937 4.87645
H -0.13990 5.06827 5.29827
H 2.04001 4.61163 4.03953
H 1.85645 5.17396 1.64985

81
[FeO(NTB)]+CHX React (+2/5)
Fe -0.00676 -0.35128 -
0.31540
O -0.05163 1.23553 0.13601
C -2.79995 0.91209 -4.93778
C -2.67261 2.30095 -4.86549
C -2.74624 -2.23883 -4.52989
C -2.20396 0.17655 -3.91056
C -1.97645 2.92843 -3.80691
N -2.13398 -1.21180 -3.67503
C 4.55162 -2.84045 -1.67875
C -1.50676 0.79849 -2.84926
C -1.38123 2.18950 -2.78351
C -1.43176 -1.39583 -2.53139
C -1.13312 -2.66735 -1.81016
N -1.03590 -0.21819 -2.00333
C 1.36316 -2.62771 -1.64702
N 3.72423 -1.78633 -1.07514
C 2.37224 -1.70967 -1.04092
C 5.53915 -0.22259 -0.17574
N 0.05774 -2.41304 -0.91034
C 4.23023 -0.64237 -0.42478
N 1.96007 -0.59076 -0.40729
C 5.68696 0.98294 0.51349
C 3.10835 0.10893 -0.00487
C -0.00995 -3.25398 0.34734
C 4.56904 1.73825 0.93641
C 3.26304 1.31458 0.68632
C -0.81920 -2.49971 1.34860
N -0.92657 -1.15758 1.25026
N -1.45905 -2.96650 2.44790
C -1.54888 -4.35818 2.91170
C -1.67943 -0.71776 2.35051
C -2.09312 0.56061 2.73739
C -2.01831 -1.85791 3.11523
C -2.84592 0.65581 3.90859
C -2.77133 -1.76731 4.28836
C -3.17922 -0.48759 4.67051
H -3.33449 0.43647 -5.75078
H -3.11936 2.91325 -5.64051
H -1.90464 4.01002 -3.79169
H -0.84855 2.66228 -1.96819
H -2.45958 -3.22924 -4.18035
H -3.83396 -2.14829 -4.49496
H -2.39825 -2.10978 -5.55626
H -1.98329 -2.94317 -1.17792
H -0.93194 -3.50745 -2.48107
H 1.20701 -2.36488 -2.69852
H 1.65467 -3.68135 -1.60975
H 3.91609 -3.64277 -2.04940
H 5.12598 -2.42768 -2.51069
H 5.23138 -3.24375 -0.92582
H 6.39898 -0.79678 -0.49814
H 6.68422 1.34911 0.72923
H 4.73270 2.66908 1.46749
H 2.40202 1.88861 1.00458
H 1.01012 -3.39097 0.72096
H -0.41381 -4.24561 0.12395
H -1.20643 -5.03150 2.12764
H -0.92991 -4.49557 3.80107
H -2.58843 -4.59178 3.14696
H -3.02730 -2.63980 4.87666
H -3.76559 -0.36805 5.57439
H -3.18413 1.62958 4.24452
H -1.83184 1.43224 2.15087
H -0.38073 3.89675 1.29513
C -0.47002 4.84335 1.84547
C -1.90475 5.01125 2.38752
C -1.67880 7.54438 2.20466
H -3.11964 6.47937 3.44776
H -1.45261 6.37167 4.01501
C -0.24394 7.37707 1.66334
```

H -2.37932 7.60406 1.35726
H -1.76833 8.49069 2.75468
C -0.06810 6.02587 0.93973
H 0.00430 8.20485 0.98568
H 0.46669 7.43175 2.50262
H -0.69674 6.01702 0.03567
H 0.97063 5.90909 0.60270

81
[FeO(NTB)]+CHX TS (+2/5)
Fe -0.16709 0.00774 -0.01916
O -0.30985 1.63448 0.53874
C -3.00409 1.23219 -4.66439
C -2.93057 2.62155 -4.54392
C -2.82232 -1.92275 -4.37055
C -2.37223 0.48393 -3.66768
C -2.25045 3.23719 -3.46813
N -2.24371 -0.90564 -3.48218
C 4.46917 -2.26708 -1.75690
C -1.69348 1.09260 -2.58772
C -1.62112 2.48468 -2.47558
C -1.52740 -1.10320 -2.34469
C -1.17857 -2.40710 -1.70129
N -1.17650 0.06821 -1.77605
C 1.30559 -2.25708 -1.56685
N 3.62342 -1.30996 -1.03093
C 2.26816 -1.30285 -0.93349
C 5.40628 0.26230 -0.08512
N 0.01030 -2.18888 -0.81630
C 4.10745 -0.19923 -0.31444
N 1.83474 -0.25590 -0.20223
C 5.53132 1.41334 0.69575
C 2.97203 0.45985 0.20912
C -0.00081 -3.07227 0.39316
C 4.40053 2.07430 1.22792
C 3.10544 1.60903 0.99499
C -0.83696 -2.41974 1.44742
N -1.02686 -1.08440 1.46156
N -1.43849 -3.01581 2.51013
C -1.44293 -4.44290 2.85785
C -1.79492 -0.78889 2.60073
C -2.28162 0.42466 3.09694
C -2.05627 -2.00566 3.27096
C -3.02570 0.37801 4.27661
C -2.80026 -2.05853 4.45251
C -3.28066 -0.84252 4.94304
H -3.52666 0.76528 -5.49024
H -3.40677 3.24309 -5.29379
H -2.21859 4.31961 -3.41473
H -1.09866 2.94627 -1.64794
H -2.44847 -2.90845 -4.09923
H -3.91131 -1.91659 -4.28473
H -2.53411 -1.70753 -5.40103
H -2.01449 -2.73905 -1.07603
H -0.98754 -3.19740 -2.43526
H 1.11800 -1.95463 -2.60284
H 1.69279 -3.28159 -1.59255
H 3.85163 -3.04978 -2.19388
H 5.00572 -1.75152 -2.55640
H 5.18429 -2.72024 -1.06759
H 6.27576 -0.24228 -0.48828
H 6.51990 1.80851 0.90041
H 4.54512 2.96324 1.83157
H 2.23498 2.10806 1.40094
H 1.02855 -3.16890 0.75503
H -0.35200 -4.07999 0.14604
H -1.07293 -5.03010 2.01920
H -0.80634 -4.61851 3.72809
H -2.46437 -4.75514 3.08152
H -2.99635 -2.99069 4.96809
H -3.86262 -0.83438 5.85770
H -3.41789 1.29856 4.69409
H -2.07986 1.35487 2.58174
H -0.38431 2.93432 1.04672
C -0.42041 4.03703 1.52646
C -1.87490 4.49800 1.54837
H -0.02714 3.87356 2.53977
C -1.95502 5.95740 2.08053
H -2.29224 4.46767 0.53207
H -2.48810 3.83903 2.17451
C -1.04797 6.89945 1.26627
H -2.99794 6.29702 2.04485
H -1.64784 5.97230 3.13606
C 0.40853 6.39858 1.23664
H -1.42853 6.97002 0.23649
H -1.08653 7.91229 1.68853
C 0.49111 4.94076 0.70126
H 1.02952 7.04950 0.60818
H 0.83054 6.43290 2.25127
H 0.17310 4.93285 -0.35105
H 1.52849 4.58780 0.73228

81
[FeO(NTB)]+CHX Interm (+2/5)
Fe -0.06154 0.05972 -0.05265
O -0.09434 1.74476 0.52317
C -3.00318 1.27643 -4.64384
C -2.90034 2.66422 -4.52629
C -2.87049 -1.87988 -4.35454
C -2.36802 0.51656 -3.65793
C -2.18900 3.26710 -3.46353
N -2.26113 -0.87450 -3.47410
C 4.45718 -2.53301 -1.78135
C -1.65838 1.11208 -2.59067
C -1.55680 2.50310 -2.48144
C -1.52772 -1.08511 -2.34803
C -1.19363 -2.39989 -1.71791
N -1.14595 0.07836 -1.78669
C 1.29438 -2.33218 -1.63550
N 3.65870 -1.51096 -1.09206
C 2.30412 -1.42302 -1.00908
C 5.52120 -0.01981 -0.16969
N 0.01939 -2.22290 -0.86391
C 4.19977 -0.41252 -0.39866
N 1.92541 -0.33869 -0.30399
C 5.70602 1.14325 0.58093
C 3.09956 0.32309 0.09737
C 0.00543 -3.08837 0.35328
C 4.61055 1.88374 1.08134
C 3.29277 1.48694 0.84921
C -0.78110 -2.39708 1.42064
N -0.92514 -1.05723 1.43326
N -1.38282 -2.97092 2.49695
C -1.42887 -4.39562 2.84997
C -1.66425 -0.73482 2.58547
C -2.10484 0.49460 3.08610
C -1.95391 -1.93992 3.26480
C -2.83064 0.47598 4.27791
C -2.67941 -1.96550 4.45879
C -3.11303 -0.73353 4.95307
H -3.54959 0.81928 -5.45973
H -3.37754 3.29447 -5.26828
H -2.13475 4.34877 -3.41202
H -1.00970 2.95609 -1.66443
C -2.50008 -2.87107 -4.09903
H -3.95725 -1.86423 -4.24428
H -2.60407 -1.66076 -5.39015
H -2.02340 -2.71364 -1.07496
H -1.04554 -3.19005 -2.46260
H 1.10165 -2.00714 -2.66382
H 1.64160 -3.37035 -1.68516
H 3.80820 -3.32322 -2.15412
H 4.98890 -2.08338 -2.62300
H 5.17594 -2.96504 -1.08243
H 6.36343 -0.58303 -0.55270
H 6.71404 1.48690 0.78411
H 4.80100 2.78172 1.65845
H 2.44803 2.05022 1.22508
H 1.03874 -3.22020 0.69277
H -0.38830 -4.08612 0.12956
H -1.07118 -4.99657 2.01584
H -0.80044 -4.58540 3.72318
H -2.45933 -4.67910 3.07134
H -2.89663 -2.88969 4.98035
H -3.67958 -0.70404 5.87693
H -3.18691 1.41001 4.69766
H -1.88397 1.41709 2.56525
H -0.23781 2.63065 0.96609
C -0.58523 4.26318 1.83722
C -2.02379 4.55135 1.50485
H -0.36223 3.83639 2.81682
C -2.35510 6.03676 1.86307
H -2.20014 4.42033 0.42591
H -2.70619 3.87687 2.03374
C -1.35027 7.00267 1.20524
H -3.37946 6.26516 1.54323
H -2.32150 6.15691 2.95476
C 0.10484 6.65740 1.57835
H -1.46544 6.95780 0.11191
H -1.57606 8.03442 1.50480
C 0.43948 5.17299 1.21746
H 0.80687 7.32218 1.05970
H 0.25402 6.80493 2.65691
H 0.41553 5.08316 0.12015
H 1.45392 4.92414 1.54706

69
[FeO(NTB)(CH3CN)] (+2/3)
Fe 0.65349 -0.46844 0.90550
O 0.70207 1.03383 1.59776
C -2.39615 2.00293 -2.92517
C -2.37296 3.28729 -2.37938
C -2.08138 -1.07894 -3.63883
C -1.70722 1.00913 -2.22366
C -1.68596 3.56650 -1.17556
N -1.52820 -0.35848 -2.48555
C 4.52891 -2.34801 -2.27493
C -1.01806 1.28110 -1.01682
C -0.99964 2.57268 -0.47706
C -0.76996 -0.86870 -1.47456
C -0.32496 -2.28084 -1.30614
N -0.44724 0.07384 -0.58499
C 1.95996 -2.78193 -0.40997
N 3.77031 -1.32928 -1.53863
C 2.66896 -1.51176 -0.75573
C 5.10293 0.77411 -2.11882
N 0.53840 -2.40659 -0.05967
C 4.08212 0.03990 -1.50662
N 2.24927 -0.35202 -0.22890
C 5.11972 2.14810 -1.87491
C 3.11127 0.65414 -0.67806
C -0.09728 -3.33603 0.94844
C 4.15351 2.76677 -1.04686
C 3.13658 2.03299 -0.43681
C -1.09305 -2.52204 1.71150
N -0.91836 -1.19733 1.82750
N -2.20312 -2.93545 2.38678
C -2.72377 -4.30259 2.51102
C -1.96118 -0.69980 2.61614
C -2.26355 0.59758 3.04662
C -2.77848 -1.79867 2.97816
C -3.39842 0.75553 3.84160
C -3.91659 -1.64219 3.77579
C -4.21171 -0.34559 4.19944
H -2.92490 1.79122 -3.84664
H -2.89440 4.08913 -2.89001
H -1.69354 4.57868 -0.78671
H -0.47163 2.77994 0.44416
H -1.69382 -2.09667 -3.65870
H -3.17127 -1.11331 -3.57243
H -1.78657 -0.57370 -4.56075
H -1.18682 -2.94868 -1.21363
H 0.24543 -2.61758 -2.17704
H 1.98611 -3.52140 -1.21511
H 2.42251 -3.23744 0.47019
H 3.97292 -3.28411 -2.28834
H 4.67842 -2.01420 -3.30334
H 5.49824 -2.51387 -1.79896
H 5.84788 0.30506 -2.74999
H 5.89381 2.75633 -2.32923
H 4.20810 3.83727 -0.88323
H 2.39691 2.49788 0.20231
H 0.68272 -3.70084 1.62283
H -0.54154 -4.20534 0.45562
H -2.14939 -4.97541 1.87644
H -2.64621 -4.63913 3.54738
H -3.76882 -4.32582 2.19557
H -4.54118 -2.48189 4.05553
H -5.08508 -0.17800 4.81968
H -3.66555 1.74481 4.19616
H -1.63365 1.43405 2.77210
N 1.80043 -1.24126 2.36001
C 2.46141 -1.53941 3.27100
C 3.28237 -1.91376 4.40835
H 3.58353 -2.96241 4.32770
H 4.18105 -1.29118 4.44495
H 2.72103 -1.77899 5.33761

69
[FeO(NTB)(CH3CN)] (+2/5)
Fe 0.57050 -0.38406 0.86123
O 0.64527 1.09115 1.60340
C -2.49013 1.97693 -3.25028
C -2.48713 3.28627 -2.76331
C -2.14134 -1.13987 -3.79507
C -1.81671 1.02215 -2.48325
C -1.83608 3.62740 -1.55535
N -1.61834 -0.35808 -2.66802
C 4.47173 -2.28442 -2.30820
C -1.16442 1.35665 -1.27287
C -1.16526 2.67036 -0.79231
C -0.88465 -0.80517 -1.60718
C -0.45293 -2.21344 -1.36160
N -0.59525 0.18309 -0.75601
C 1.86563 -2.69436 -0.50822
N 3.74969 -1.27171 -1.52659
C 2.62467 -1.43824 -0.78200
C 5.21520 0.78195 -1.94905
N 0.44631 -2.31452 -0.13251
C 4.14061 0.07501 -1.40298
N 2.25768 -0.28774 -0.18792
C 5.30455 2.13605 -1.62023
C 3.18928 0.69208 -0.55697
C -0.14606 -3.27207 0.88364
C 4.35572 2.75885 -0.77653
C 3.28396 2.04967 -0.23299
C -1.11486 -2.49772 1.71548
N -0.93650 -1.17431 1.88985
N -2.17975 -2.94956 2.42860
C -2.69075 -4.32433 2.51315
C -1.93624 -0.72683 2.76395
C -2.21936 0.54460 3.27401
C -2.72759 -1.84691 3.11175
C -3.30894 0.65331 4.13882
C -3.82025 -1.74153 3.97669
C -4.09594 -0.46997 4.48353
H -2.99225 1.72165 -4.17563
H -2.99746 4.06020 -3.32574
H -1.86002 4.65708 -1.21620
H -0.66361 2.92182 0.13391
H -1.73961 -2.15178 -3.76356
H -3.23176 -1.18764 -3.74493
H -1.83910 -0.67262 -4.73447
H -1.32821 -2.85116 -1.20511
H 0.08036 -2.61544 -2.22807
H 1.87207 -3.39180 -1.34964
H 2.31752 -3.20553 0.34647
H 3.85339 -3.17312 -2.42307
H 4.69433 -1.88194 -3.29782
H 5.40237 -2.55528 -1.80434
H 5.94619 0.30872 -2.59308
H 6.12261 2.72415 -2.02053
H 4.46628 3.81275 -0.54726
H 2.55462 2.51849 0.41540
H 0.66356 -3.63933 1.51992
H -0.59636 -4.13504 0.38647
H -2.15663 -4.96070 1.80989
H -2.54855 -4.71215 3.52418
H -3.75312 -4.33323 2.26221
H -4.42592 -2.59849 4.24501
H -4.93413 -0.34083 5.15889
H -3.56006 1.62115 4.55799
H -1.61091 1.39917 3.00623
N 1.92127 -1.45528 2.47170
C 2.59191 -1.69513 3.39689
C 3.42431 -1.99424 4.55014
H 2.85040 -2.54919 5.29800
H 4.28615 -2.59727 4.24986
H 3.78685 -1.06696 5.00371

69
[FeO(NTB)(CH3CN)] (+2/3) iso
Fe 0.69842 -0.46661 0.99050
O 1.65658 -1.10959 2.19846
C -2.43064 1.93560 -3.01222
C -2.45548 3.24550 -2.53148
C -2.01134 -1.15377 -3.58191
C -1.72375 0.99993 -2.25216
C -1.79525 3.60163 -1.33425
N -1.50455 -0.37144 -2.44802
C 4.52554 -2.25864 -2.23057
C -1.05868 1.34356 -1.04898
C -1.09109 2.66281 -0.57940
C -0.74532 -0.80859 -1.40394
C -0.27099 -2.20463 -1.18791
N -0.45604 0.17486 -0.54569
C 2.02289 -2.65473 -0.26265
N 3.75830 -1.22382 -1.52616
C 2.69307 -1.39357 -0.69526
C 4.99142 0.87818 -2.28395
N 0.59005 -2.28051 0.06997
C 4.02042 0.15409 -1.58553
N 2.25028 -0.22197 -0.21412
C 4.96566 2.26539 -2.13866
C 3.05542 0.78583 -0.76079
C -0.02720 -3.21700 1.09280
C 4.00020 2.90520 -1.32733
C 3.03387 2.18023 -0.63095
C -1.09000 -2.42899 1.78313
N -0.96122 -1.09594 1.86709
N -2.22514 -2.86258 2.39692
C -2.70632 -4.24312 2.53163
C -2.07610 -0.61127 2.56364
C -2.47395 0.68456 2.91596
C -2.87650 -1.72944 2.90929
C -3.66849 0.81969 3.62255
C -4.07438 -1.59736 3.61817
C -4.45553 -0.30245 3.97060
H -2.93646 1.66204 -3.93027
H -2.99198 4.00551 -3.08825
H -1.83657 4.63029 -0.99394
H -0.58960 2.94900 0.33360
H -1.69921 -2.19266 -3.48431
H -3.10261 -1.11365 -3.60159
H -1.61352 -0.75169 -4.51634
H -1.11749 -2.88851 -1.07676
H 0.31565 -2.55627 -2.04127
H 2.05086 -3.44735 -1.01406
H 2.49035 -3.03078 0.65155
H 4.03188 -3.22277 -2.12018
H 4.58152 -2.01100 -3.29232
H 5.53380 -2.32483 -1.81541
H 5.72912 0.39063 -2.90958
H 5.70040 2.86692 -2.66178
H 4.01169 3.98640 -1.24718
H 2.29199 2.67608 -0.02065
H 0.75386 -3.49744 1.80456
H -0.39816 -4.12401 0.60939
H -2.04049 -4.91899 1.99763
H -2.72712 -4.52743 3.58605
H -3.71009 -4.32505 2.10987
H -4.68141 -2.45516 3.88102
H -5.37746 -0.15234 4.52091
H -4.00447 1.80931 3.91129
H -1.88144 1.54725 2.64502
N 0.79803 1.29599 1.88287
C 1.23005 3.37046 3.41763
H 2.14819 3.87934 3.10958
H 0.39509 4.07350 3.34340
H 1.33419 3.05574 4.46023

83
[FeO(NTB)(CH3CN)]+CHD React (+2/3)
Fe 1.05558 -0.94385 0.60848
O 1.33958 0.40992 1.51787
C -2.62288 2.21026 -1.96420
C -2.42024 3.37531 -1.22274
C -2.62104 -0.69488 -3.25314
C -1.84415 1.10177 -1.61894
C -1.47349 3.42791 -0.17416
N -1.79296 -0.19767 -2.14776
C 4.08986 -2.33547 -3.58130
C -0.89388 1.14706 -0.56973
C -0.69754 2.32024 0.16843
C -0.85614 -0.88722 -1.43785
C -0.44940 -2.30790 -1.62770
N -0.29971 -0.12267 -0.49468
C 1.92755 -3.02523 -1.31468
N 3.55311 -1.44221 -2.54726
C 2.62490 -1.73165 -1.59122
C 4.85189 0.70246 -3.04846
N 0.63009 -2.67793 -0.62141
C 3.93890 -0.10435 -2.36176
N 2.38659 -0.66975 -0.80747
C 4.99301 2.01485 -2.59521
C 3.19280 0.38015 -1.25958
C 0.14802 -3.75311 0.32464
C 4.25165 2.50349 -1.49358
C 3.34224 1.69733 -0.80954
C -0.61403 -3.06139 1.40933
N -0.33419 -1.78455 1.70969
N -1.58560 -3.56023 2.22541
C -2.15447 -4.91355 2.22568
C -1.15778 -1.41026 2.77736
C -1.27819 -0.20704 3.48269
C -1.95262 -2.53421 3.11150
C -2.21125 -0.16772 4.51839
C -2.88889 -2.49646 4.14970
C -3.00474 -1.29231 4.84562
H -3.35006 2.17140 -2.76624
H -3.00304 4.25941 -1.45599
H -1.34598 4.35066 0.38079
H 0.02604 2.36021 0.97160
H -2.29712 -1.69562 -3.53611
H -3.66974 -0.73175 -2.94923
H -2.51286 -0.03486 -4.11613
H -1.30534 -2.97713 -1.49937
H -0.06960 -2.47040 -2.64098
H 1.74589 -3.61717 -2.21604
H 2.52933 -3.63580 -0.63555
H 3.53307 -3.27107 -3.58641
H 3.99091 -1.86094 -4.55950
H 5.14274 -2.54860 -3.38252
H 5.42540 0.33214 -3.88945
H 5.68991 2.67589 -3.09813
H 4.39690 3.52964 -1.17474
H 2.77510 2.06134 0.03754
H 1.02050 -4.26014 0.74626
H -0.44658 -4.50407 -0.20302
H -1.76672 -5.47806 1.37940
H -1.88672 -5.43067 3.14995
H -3.24141 -4.85320 2.14149
H -3.49479 -3.35695 4.40663
H -3.71800 -1.21793 5.65887
H -2.32805 0.74708 5.08856
H -0.66461 0.64992 3.23649
N 2.43015 -1.99078 1.63142
C 3.25092 -2.45486 2.31457
C 4.27463 -3.03134 3.16730
H 4.51762 -2.33873 3.97875
H 3.92066 -3.97090 3.60145
H 5.18187 -3.22841 2.58885
H 1.74413 2.52605 3.29098
C 1.49667 3.39511 3.92360
C 1.00937 4.53616 3.06088
H 2.45241 3.67021 4.40152
C -0.18787 5.12294 3.21220
H 1.69011 4.88587 2.28676
C -1.19291 4.71296 4.26340
H -0.47374 5.94776 2.56177
C -0.70330 3.57658 5.13036
H -1.44933 5.58093 4.89436
H -2.14592 4.43472 3.78270
C 0.49426 2.99047 4.97949
H -1.37577 3.24180 5.91831
H 0.78816 2.17998 5.64402

83
[FeO(NTB)(CH3CN)]+CHD TS (+2/3)
Fe 0.74547 -0.54976 0.66395
O 0.65747 1.03915 1.37784
C -3.11282 1.62038 -2.62935
C -3.18768 2.88054 -2.03369
C -2.48066 -1.36000 -3.52610
C -2.20129 0.71601 -2.07588
C -2.37887 3.22214 -0.92536
N -1.87986 -0.60499 -2.42103
C 4.47876 -1.97548 -2.92075
C -1.38704 1.04967 -0.96548
C -1.46968 2.31771 -0.37538
C -0.91605 -1.02572 -1.54893
C -0.24936 -2.35974 -1.53789
N -0.59682 -0.07393 -0.67001
C 2.13008 -2.69142 -0.85550
N 3.68706 -1.05014 -2.10156
C 2.68269 -1.35323 -1.22752
C 4.73233 1.18849 -2.75946
N 0.71932 -2.45516 -0.36993
C 3.85504 0.34348 -2.07188
N 2.19643 -0.25196 -0.63975
C 4.62364 2.55468 -2.49485
C 2.90362 0.84268 -1.14843
C 0.26595 -3.48100 0.64185
C 3.67273 3.05938 -1.57643
C 2.79975 2.21495 -0.89070
N -0.63660 -1.47697 1.72493
N -1.71598 -3.35083 2.29042
C -2.10476 -4.76325 2.37676
C -1.63586 -1.11969 2.63704
C -2.00043 0.12063 3.17439
C -2.32137 -2.30414 3.00365
C -3.06101 0.13451 4.08009
C -3.38435 -2.29232 3.91260
C -3.74221 -1.05160 4.44250
H -3.73244 1.36110 -3.47948
H -3.88119 3.61375 -2.43059
H -2.46858 4.21299 -0.49339
H -0.84382 2.56505 0.47097
H -2.08597 -2.37518 -3.53831
H -3.56427 -1.40613 -3.39629
H -2.24772 -0.87856 -4.47886
H -0.98494 -3.16669 -1.46406
H 0.30005 -2.51849 -2.47157
H 2.14758 -3.40820 -1.68184
H 2.71030 -3.12187 -0.03446
H 4.08774 -2.98660 -2.81866
H 4.42082 -1.67822 -3.96984
H 5.52148 -1.96464 -2.59479
H 5.46203 0.80677 -3.46342
H 5.28395 3.24650 -3.00586
H 3.62399 4.12886 -1.40362
H 2.06881 2.58748 -0.18481
H 1.13773 -3.80261 1.21897
H -0.14677 -4.36573 0.14878
H -1.56164 -5.34155 1.63101
H -1.87367 -5.15716 3.36931
H -3.17538 -4.85966 2.18552
H -3.90686 -3.19805 4.19592
H -4.56123 -0.99557 5.15096
H -3.37227 1.07546 4.52028
H -1.46545 1.01859 2.89457

N 2.11587 -1.19856 1.96886
C 2.90467 -1.54313 2.75426
C 3.88760 -1.97513 3.73311
H 3.94089 -1.25608 4.55591
H 3.61157 -2.95252 4.13956
H 4.87531 -2.05169 3.26940
H 1.43896 1.47334 2.43711
C 2.08770 2.02364 3.34175
C 2.12881 3.45821 2.97524
H 3.04864 1.50956 3.22081
C 1.40977 4.39502 3.63042
H 2.75004 3.74120 2.12928
C 0.55009 4.07553 4.82448
H 1.45269 5.43544 3.31769
C 0.67395 2.64737 5.28477
H 0.79485 4.75904 5.65532
H -0.50705 4.30667 4.59843
C 1.39593 1.72237 4.61607
H 0.16650 2.38137 6.20881
H 1.46617 0.70788 5.00049

83
[FeO(NTB)(CH3CN)]+CHD Interm (+2/3)
Fe 0.75066 -0.61159 0.63219
O 0.69689 1.02068 1.40500
C -3.10228 1.69527 -2.56844
C -3.14481 2.94727 -1.95287
C -2.54008 -1.28125 -3.52056
C -2.20182 0.76525 -2.04010
C -2.31528 3.25570 -0.85007
N -1.91169 -0.55626 -2.41093
C 4.42211 -2.02461 -3.01202
C -1.36699 1.06547 -0.93482
C -1.41682 2.32618 -0.32463
C -0.94547 -1.00871 -1.55834
C -0.30165 -2.35311 -1.57274
N -0.59617 -0.07900 -0.66835
C 2.08257 -2.73797 -0.92800
N 3.66315 -1.10389 -2.15712
C 2.65964 -1.40681 -1.28342
C 4.75904 1.12619 -2.75935
N 0.68236 -2.47659 -0.41584
C 3.86538 0.28422 -2.08947
N 2.20463 -0.31126 -0.66196
C 4.69081 2.48566 -2.45044
C 2.93532 0.78069 -1.14275
C 0.22829 -3.52067 0.58181
C 3.76443 2.98660 -1.50524
C 2.87422 2.14590 -0.83751
C -0.72874 -2.84563 1.50835
N -0.62408 -1.52608 1.70819
N -1.72219 -3.38875 2.27043
C -2.13133 -4.79618 2.34563
C -1.59339 -1.16414 2.65003
C -1.91892 0.07339 3.21818
C -2.29213 -2.34216 3.01319
C -2.95765 0.09133 4.14881
C -3.33359 -2.32552 3.94661
C -3.65415 -1.08756 4.50598
H -3.73717 1.46072 -3.41452
H -3.82868 3.69989 -2.32980
H -2.38037 4.24168 -0.40258
H -0.77401 2.54337 0.51675
H -2.17657 -2.30778 -3.54398
H -3.62383 -1.29589 -3.38537
H -2.29763 -0.79775 -4.46993
H -1.04781 -3.14966 -1.49679
H 0.23495 -2.51071 -2.51368
H 2.06719 -3.44165 -1.76495
H 2.66423 -3.19502 -0.12234
H 4.02709 -3.03414 -2.90943
H 4.33501 -1.71414 -4.05531
H 5.47399 -2.02482 -2.71717
H 5.47173 0.74699 -3.48183
H 3.56539 3.17497 -2.94599
H 3.74950 4.05057 -1.29604
H 2.16431 2.51395 -0.10809
H 1.10376 -3.86432 1.14041
H -0.20039 -4.38829 0.07284
H -1.60794 -5.37294 1.58469
H -1.89085 -5.20526 3.32970
H -3.20601 -4.87450 2.16971
H -3.86729 -3.22575 4.22650
H -4.45534 -1.02820 5.23426
H -3.23949 1.02998 4.61305
H -1.37144 0.96448 2.93964
N 2.12107 -1.23803 1.94033
C 2.90958 -1.54320 2.74226
C 3.89018 -1.92646 3.74271
H 3.89229 -1.20210 4.56263
H 3.64989 -2.91379 4.14793
H 4.88991 -1.95980 3.30021
H 1.34044 1.15731 2.13611
C 2.57185 2.44385 3.86584
C 2.29726 3.66866 3.18960
H 3.47671 1.88849 3.64239
C 1.18071 4.41157 3.48030
H 2.99290 4.01743 2.43096
C 0.18513 3.98408 4.52749
H 0.98857 5.34416 2.95699
C 0.54451 2.68605 5.20324
H 0.06565 4.78399 5.28460
H -0.82633 3.91198 4.08164
C 1.67611 1.98178 4.87351
H -0.12590 2.32000 5.97586
H 1.90149 1.05384 5.39272

83

[FeO(NTB)(CH3CN)]+CHD React (+2/5)
Fe 0.82883 -0.54744 0.46934
O 1.00396 0.92625 1.19759
C -3.11301 1.70645 -2.88020
C -3.09958 2.99835 -2.34894
C -2.65150 -1.35315 -3.63327
C -2.22424 0.78780 -2.31504
C -2.23022 3.35785 -1.29338
N -1.97663 -0.56873 -2.59223
C 4.37725 -2.48429 -3.07308
C -1.35017 1.14150 -1.25978
C -1.34350 2.43730 -0.73257
C -0.99688 -0.98254 -1.73678
C -0.38193 -2.34245 -1.68849
N -0.59803 0.00414 -0.92896
C 1.96662 -2.86840 -1.00887
N 3.72416 -1.45765 -2.25024
C 2.68248 -1.61545 -1.39220
C 5.10799 0.60055 -2.87804
N 0.58799 -2.47306 -0.51755
C 4.10518 -0.10300 -2.20548
N 2.36046 -0.45213 -0.79526
C 5.21101 1.96436 -2.59667
C 3.23616 0.52717 -1.28375
C 0.06617 -3.43135 0.53500
C 4.34470 2.59990 -1.67731
C 3.34426 1.89432 -1.00772
C -0.76434 -2.65303 1.50158
N -0.53023 -1.34091 1.68743
N -1.73996 -3.10287 2.33445
C -2.26474 -4.46963 2.45361
C -1.39756 -0.89737 2.69545
C -1.58066 0.36359 3.27275
C -2.16598 -2.00983 3.11256
C -2.54702 0.46886 4.27398
C -3.13484 -1.90775 4.11446
C -3.31129 -0.64669 4.68751
H -3.78042 1.43837 -3.69031
H -3.77246 3.74424 -2.75713
H -2.25456 4.37303 -0.91305
H -0.67397 2.70344 0.07593
H -2.36680 -2.40117 -3.55001
H -3.73307 -1.27310 -3.50717
H -2.37045 -0.98506 -4.62294
H -1.14840 -3.11844 -1.60451
H 0.16514 -2.53599 -2.61673
H 1.89503 -3.59210 -1.82497
H 2.49925 -3.34804 -0.18319
H 3.81576 -3.41504 -3.01659
H 4.40682 -2.15148 -4.11218
H 5.39386 -2.65814 -2.71352
H 5.77550 0.11914 -3.58217
H 5.97514 2.55026 -3.09480
H 4.46323 3.66104 -1.48909
H 2.67942 2.37314 -0.30001
H 0.92405 -3.85876 1.06168
H -0.47989 -4.25630 0.07062
H -1.88655 -5.08364 1.63810
H -1.95472 -4.90751 3.40512
H -3.35461 -4.44389 2.39947
H -3.72151 -2.75989 4.43530
H -4.05189 -0.52034 5.46916
H -2.71587 1.43014 4.74617
H -0.99256 1.21606 2.95733
N 2.36869 -1.63038 1.89006
C 3.13512 -1.87580 2.73603
C 4.08874 -2.17990 3.78983
H 3.78885 -3.08716 4.32241
H 5.08561 -2.33382 3.36666
H 4.13522 -1.35331 4.50508
H 1.49081 3.18000 2.47352
C 1.49166 3.80346 3.38338
C 0.07011 4.11701 3.78815
H 2.00925 4.73119 3.08495
C -0.44662 3.80511 4.98655
H -0.54424 4.62924 3.04969
C 0.33158 3.10294 6.07494
H -1.47798 4.06640 5.21725
C 1.75469 2.79376 5.67196
H 0.32699 3.71530 6.99278
H -0.18689 2.17337 6.36481
C 2.27156 3.10866 4.47494
H 2.37241 2.29302 6.41531
H 3.30835 2.86346 4.25076

83
[FeO(NTB)(CH3CN)]+CHD TS (+2/5)
Fe 0.79401 -0.42408 0.60924
O 0.91234 1.08580 1.34876
C -3.05779 1.78180 -2.84347
C -3.06561 3.06868 -2.30022
C -2.56677 -1.26371 -3.61161
C -2.18353 0.86089 -2.25963
C -2.23016 3.42013 -1.21513
N -1.92128 -0.49032 -2.54409
C 4.37859 -2.41231 -2.98873
C -1.34482 1.20539 -1.17396
C -1.35858 2.49657 -0.63570
C -0.96869 -0.91447 -1.66239
C -0.36992 -2.28397 -1.61962
N -0.59976 0.06581 -0.83001
C 1.97500 -2.79859 -0.93535
N 3.72793 -1.38318 -2.16847
C 2.68438 -1.53508 -1.30378
C 5.11584 0.67109 -2.80131
N 0.59030 -2.44376 -0.45776
C 4.11268 -0.03137 -2.12709
N 2.36680 -0.37361 -0.70905
C 5.22050 2.03519 -2.52164
C 3.24508 0.60014 -1.20466
C 0.07307 -3.41432 0.57234
C 4.35551 2.67278 -1.60204
C 3.35570 1.96804 -0.93077
C -0.80304 -2.67702 1.53423
N -0.61946 -1.36793 1.76789
N -1.79336 -3.18980 2.32004
C -2.27484 -4.57552 2.37847
C -1.53610 -0.99098 2.75983
C -1.77755 0.24392 3.37207
C -2.28130 -2.13954 3.11714
C -2.77727 0.28770 4.34456
C -3.28446 -2.09963 4.08996
C -3.51878 -0.86398 4.69691
H -3.69905 1.51821 -3.67592
H -3.72824 3.81636 -2.72179
H -2.26895 4.43159 -0.82602
H -0.71400 2.75449 0.19474
H -2.22363 -2.29680 -3.58064
H -3.65002 -1.24802 -3.47370
H -2.31627 -0.83658 -4.58548
H -1.15481 -3.04369 -1.54455
H 0.16882 -2.48012 -2.55314
H 1.93345 -3.51476 -1.76167
H 2.50845 -3.27983 -0.11042
H 3.80383 -3.33596 -2.94948
H 4.42858 -2.07266 -4.02498
H 5.38788 -2.60466 -2.61730
H 5.78284 0.18853 -3.50535
H 5.98485 2.61987 -3.02115
H 4.47516 3.73422 -1.41540
H 2.69076 2.44701 -0.22283
H 0.92960 -3.82633 1.11418
H -0.44307 -4.25279 0.09498
H -1.84465 -5.15248 1.56174
H -1.98770 -5.03298 3.32817
H -3.36223 -4.58661 2.28157
H -3.85363 -2.97935 4.36495
H -4.28725 -0.78606 5.45790
H -2.99114 1.22640 4.84370
H -1.20502 1.12221 3.10141
N 2.29128 -1.45241 2.01362
C 3.04850 -1.75396 2.84883
C 3.99055 -2.12632 3.89054
H 3.66052 -3.04127 4.39106
H 4.98218 -2.29773 3.46182
H 4.06314 -1.32690 4.63400
H 1.18087 2.48443 2.32339
C 1.38043 3.38005 3.00041
C 0.07501 3.87006 3.54624
H 1.82265 4.10510 2.29869
C -0.24308 3.80976 4.85361
H -0.63569 4.28187 2.83315
C 0.69391 3.27455 5.90475
H -1.20809 4.17539 5.19732
C 2.04974 2.90434 5.36213
H 0.80556 4.01372 6.71633
H 0.23791 2.40103 6.40427
C 2.36091 2.96758 4.05346
H 2.79851 2.59115 6.08619
H 3.36124 2.70137 3.71928

83
[FeO(NTB)(CH3CN)]+CHD Interm (+2/5)
Fe 0.73230 -0.17449 0.64118
O 0.77520 1.49221 1.33656
C -3.14650 1.61785 -3.01223
C -3.21107 2.93112 -2.54034
C -2.53387 -1.44164 -3.60285
C -2.25128 0.76271 -2.36346
C -2.41038 3.37043 -1.46107
N -1.93384 -0.59012 -2.56938
C 4.39369 -2.33383 -2.89178
C -1.44702 1.19520 -1.28374
C -1.51759 2.51243 -0.81629
C -0.98283 -0.93295 -1.64876
C -0.34988 -2.28693 -1.53860
N -0.66630 0.10352 -0.86473
C 2.00384 -2.69277 -0.83218
N 3.70701 -1.28242 -2.13224
C 2.66670 -1.41957 -1.25660
C 5.02725 0.77854 -2.88032
N 0.60845 -2.38602 -0.38237
C 4.04778 0.08040 -2.16750
N 2.31087 -0.23961 -0.72879
C 5.08532 2.15902 -2.67667
C 3.15842 0.73215 -1.28099
C 0.11934 -3.30548 0.69331
C 4.19848 2.81697 -1.79286
C 3.22264 2.11631 -1.08300
C -0.78515 -2.55046 1.61735
N -0.65987 -1.22780 1.79468
N -1.76421 -3.07148 2.41648
C -2.18734 -4.47196 2.53279
C -1.60444 -0.84920 2.76046
C -1.90577 0.40120 3.31271
C -2.30506 -2.01068 3.16200
C -2.91914 0.44707 4.27158
C -3.32056 -1.96938 4.12226
C -3.61493 -0.71856 4.66900
H -3.76132 1.28583 -3.84018
H -3.89157 3.63027 -3.01373
H -2.49327 4.39931 -1.12833
H -0.89746 2.83525 0.01070
H -2.12461 -2.44868 -3.53982
H -3.61565 -1.49118 -3.45930
H -2.31594 -1.03404 -4.59277
H -1.12476 -3.05502 -1.43468
H 0.18697 -2.51215 -2.46759
H 2.01026 -3.44545 -1.62829
H 2.55346 -3.11415 0.01524
H 3.83186 -3.26426 -2.82979
H 4.46432 -2.03644 -3.93984
H 5.39682 -2.49541 -2.48963
H 5.71172 0.28104 -3.55676
H 5.83008 2.74068 -3.20844
H 4.28185 3.89064 -1.66533
H 2.53926 2.60860 -0.40162
H 0.98463 -3.66524 1.25902
H -0.37485 -4.18595 0.26841
H -1.73727 -5.06373 1.73770
H -1.87915 -4.87984 3.49858
H -3.27367 -4.53183 2.44179
H -3.85521 -2.85911 4.43231
H -4.39562 -0.63908 5.41733
H -3.18185 1.39747 4.72297
H -1.36559 1.28796 3.00370
N 2.24443 -1.06355 2.08527
C 3.00367 -1.37464 2.91477
C 3.94627 -1.76098 3.95042
H 3.72323 -2.77055 4.30788
H 4.96786 -1.74340 3.55988
H 3.88040 -1.06797 4.79446
H 1.15034 2.08371 2.02533
C 2.12744 3.40750 3.45628
C 0.85018 3.99928 3.69094
H 2.74526 3.75366 2.63392
C 0.07923 3.62729 4.76372
H 0.48955 4.76083 3.00525
C 0.53329 2.58558 5.75014
H -0.88936 4.08944 4.93143
C 1.90311 2.03416 5.45990
H 0.50085 2.99748 6.77703
H -0.20469 1.76013 5.79012
C 2.63420 2.43658 4.37156
H 2.30478 1.29929 6.15183
H 3.62248 2.01937 4.20032

87
[FeO(NTB)(CH3CN)]+CHX React (+2/3)
Fe 0.85879 -0.77400 0.52432
O 1.02931 0.67436 1.30713
C -2.91828 1.88911 -2.42867
C -2.81093 3.12759 -1.79408
C -2.69132 -1.11210 -3.44675
C -2.08428 0.86913 -1.96149
C -1.90175 3.33709 -0.73177
N -1.93857 -0.46793 -2.36363
C 4.16984 -2.37997 -3.36665
C -1.17103 1.07144 -0.89818
C -1.06994 2.31746 -0.26773
C -0.97938 -1.02648 -1.57286
C -0.47131 -2.42637 -1.62543
N -0.50143 -0.14462 -0.69116
C 1.92409 -2.97071 -1.15470
N 3.52797 -1.42289 -2.45690
C 2.56317 -1.67043 -1.52587
C 4.73730 0.73308 -3.10704
N 0.58122 -2.63614 -0.54713
C 3.83093 -0.05314 -2.38870
N 2.22713 -0.55292 -0.86472
C 4.78614 2.08914 -2.78075
C 3.00083 0.49292 -1.37920
C 0.12028 -3.64445 0.47974
C 3.96111 2.63973 -1.77178
C 3.05763 1.85403 -1.05656
C -0.72272 -2.90142 1.46577
N -0.52205 -1.58911 1.65522
N -1.69952 -3.37656 2.28985
C -2.19274 -4.75516 2.39789
C -1.40676 -1.16475 2.65235
C -1.62096 0.09132 3.23224
C -2.15425 -2.29564 3.06304
C -2.59640 0.17522 4.22561
C -3.13232 -2.21353 4.05927
C -3.34003 -0.95790 4.63189
H -3.61429 1.73105 -3.24355
H -3.43864 3.94788 -2.12374
H -1.85027 4.31551 -0.26718
H -0.37253 2.47321 0.54461
H -2.44433 -2.17207 -3.48846
H -3.76226 -1.00835 -3.26069
H -2.43942 -0.64947 -4.40369
H -1.28528 -3.14330 -1.48131
H -0.03024 -2.64073 -2.60355
H 1.81224 -3.65213 -2.00259
H 2.52770 -3.47897 -0.39717
H 3.72906 -3.36679 -3.23552
H 4.02452 -2.05982 -4.40048
H 5.23846 -2.43869 -3.14819
H 5.37295 0.31544 -3.87829
H 5.47457 2.73653 -3.31225
H 4.03567 3.69858 -1.55033
H 2.42706 2.26700 -0.27964
H 1.00144 -4.05604 0.97985
H -0.40751 -4.47662 0.00554
H -1.79724 -5.35398 1.57904
H -1.87654 -5.19455 3.34685
H -3.28279 -4.75631 2.33929
H -3.70192 -3.07882 4.37594
H -4.08868 -0.84819 5.40845
H -2.79071 1.13073 4.69997
N 2.25336 -1.63623 1.68421
C 3.07558 -1.99230 2.42787
C 4.09998 -2.44036 3.35388
H 4.96768 -2.81694 2.80452
H 4.41945 -1.60866 3.98891
H 3.71013 -3.23976 3.99066
H 1.71063 2.30515 3.50587
C 1.84062 3.11544 4.23545
C 2.71502 2.64162 5.41488
H 2.35781 3.93449 3.71145
C 2.86520 3.74425 6.48349
H 2.25052 1.75540 5.87491
H 3.70340 2.32815 5.05264
C 1.49090 4.24880 6.97033
H 3.45458 3.37207 7.33218
H 3.42742 4.58775 6.05375
C 0.61426 4.72084 5.79173
H 0.97437 3.43285 7.49930
H 1.62100 5.06268 7.69605
C 0.46580 3.61873 4.72242
H -0.37402 5.03250 6.15541
H 1.07632 5.60805 5.33173
H -0.09608 2.77372 5.15044
H -0.12343 3.99226 3.87398

87
[FeO(NTB)(CH3CN)]+CHX TS (+2/3)
Fe 0.68460 -0.50768 0.88066
O 0.73818 1.13910 1.54222
C -2.33269 2.03075 -2.98590
C -2.27319 3.32366 -2.46314
C -2.09463 -1.06580 -3.65195
C -1.66732 1.03136 -2.26919
C -1.57304 3.60447 -1.26719
N -1.52915 -0.34384 -2.50710
C 4.46003 -2.57423 -2.32502
C -0.96314 1.30345 -1.07001
C -0.90968 2.60508 -0.55425
C -0.77486 -0.85435 -1.48883
C -0.37206 -2.27980 -1.31600
N -0.41924 0.08989 -0.61575
C 1.89040 -2.88211 -0.43154
N 3.75461 -1.51961 -1.58762
C 2.65375 -1.64853 -0.79023
C 5.16029 0.52525 -2.20473
N 0.49023 -2.43980 -0.07380
C 4.11928 -0.16386 -1.57385
N 2.28551 -0.47055 -0.27037
C 5.22802 1.90123 -1.98035
C 3.18010 0.49571 -0.74298
C -0.17388 -3.34852 0.93545
C 4.29010 2.56581 -1.15513
C 3.25397 1.87682 -0.52519
C -1.13923 -2.50264 1.70081
N -0.91482 -1.18732 1.81472
N -2.27318 -2.87458 2.36440
C -1.95209 -0.64878 2.58338
C -2.21980 0.66426 2.98908
C -2.81349 -1.71474 2.94257
C -3.36148 0.87085 3.76326
C -3.95722 -1.50977 3.72137
C -4.21485 -0.19853 4.12463
H -2.86979 1.81745 -3.90236
H -2.77519 4.13024 -2.98615
H -1.55207 4.62352 -0.89625
H -0.36972 2.80255 0.36122
H -1.86028 -2.12655 -3.57226
H -3.18022 -0.94581 -3.66707
H -1.67209 -0.67970 -4.58258
H -1.25511 -2.91977 -1.22318
H 0.18421 -2.63488 -2.18902
H 1.87611 -3.62610 -1.23327
H 2.33674 -3.35589 0.44719
H 3.88392 -3.49754 -2.28891
H 4.57665 -2.27329 -3.36799
H 5.44351 -2.75040 -1.88287
H 5.88194 0.02179 -2.83669
H 6.01920 2.47509 -2.44990
H 4.38207 3.63663 -1.01053
H 2.52912 2.37185 0.10796
H 0.59542 -3.74128 1.60623
H -0.64857 -4.20240 0.44331
H -2.28859 -4.91546 1.85776
H -2.78788 -4.55935 3.52375
H -3.88642 -4.20814 2.16210
H -4.61492 -2.32417 4.00041
H -5.09159 0.00588 4.72908
H -3.60338 1.87362 4.09782
H -1.55706 1.47081 2.70360
N 1.82042 -1.25755 2.34328
C 2.50027 -1.65912 3.20031
C 3.35033 -2.16162 4.26606
H 3.85269 -3.07952 3.94678
H 4.11048 -1.41820 4.52372
H 2.75319 -2.37848 5.15651
H 1.35575 1.40451 2.53375
C 2.00639 1.90305 3.61143
C 1.18381 1.55893 4.84136
H 2.96387 1.37170 3.55485
C 1.77537 2.27606 6.08972
H 0.14712 1.89731 4.70297
H 1.15147 0.47646 5.01072
C 1.89277 3.79488 5.85523
H 1.14279 2.06750 6.96204
H 2.76972 1.85986 6.30612
C 2.71560 4.11253 4.59144
H 0.88515 4.22421 5.74961
H 2.35069 4.27436 6.73037

C 2.12717 3.39397 3.34271
H 2.74204 5.19450 4.40927
H 3.75499 3.78547 4.73820
H 1.13316 3.81483 3.13299
H 2.75728 3.58644 2.46660

87
[FeO(NTB)(CH3CN)]+CHX Interm (+2/3)
Fe 0.52367 -0.65340 0.89994
O 0.47566 0.95097 1.72693
C -2.54746 2.05970 -2.79299
C -2.56615 3.30230 -2.15736
C -2.13949 -0.95071 -3.72007
C -1.84601 1.03519 -2.15003
C -1.90697 3.51017 -0.92370
N -1.63024 -0.30451 -2.50563
C 4.48854 -2.17298 -2.37117
C -1.18291 1.23444 -0.91345
C -1.20773 2.48607 -0.28379
C -0.87253 -0.86465 -1.51667
C -0.39850 -2.27642 -1.45128
N -0.58616 0.01375 -0.55501
C 1.89665 -2.80753 -0.59345
N 3.69874 -1.23400 -1.56595
C 2.59017 -1.50396 -0.81690
C 4.99304 0.94004 -1.93842
N 0.46718 -2.48385 -0.21507
C 3.98122 0.13259 -1.40865
N 2.14103 -0.40695 -0.19475
C 4.97452 2.28783 -1.57597
C 2.98635 0.65154 -0.54346
C -0.13983 -3.52663 0.69871
C 3.98220 2.81157 -0.71378
C 2.97457 2.00503 -0.18475
C -1.16698 -2.82202 1.52353
N -1.02970 -1.51055 1.75600
N -2.26771 -3.32734 2.15282
C -2.74587 -4.71484 2.15414
C -2.08910 -1.11467 2.57905
C -2.42841 0.13159 3.11955
C -2.87652 -2.26372 2.83877
C -3.56969 0.18763 3.91911
C -4.02043 -2.20903 3.64180
C -4.35256 -0.96293 4.17578
H -3.05344 1.90192 -3.73798
H -3.09855 4.12602 -2.62020
H -1.94738 4.49212 -0.46459
H -0.69724 2.62385 0.65890
H -1.80908 -1.98817 -3.75268
H -3.23174 -0.92791 -3.72514
H -1.75995 -0.43265 -4.60377
H -1.24784 -2.96581 -1.41041
H 0.17845 -2.53796 -2.34341
H 1.93284 -3.46906 -1.46345
H 2.36113 -3.33904 0.24190
H 3.94799 -3.11257 -2.47716
H 4.65373 -1.74976 -3.36374
H 5.45102 -2.36597 -1.89124
H 5.75707 0.54454 -2.59680
H 5.74064 2.94988 -1.96396
H 4.00875 3.86541 -0.45945
H 2.20862 2.38849 0.47690
H 0.65083 -3.92007 1.34406
H -0.54510 -4.36388 0.12360
H -2.15527 -5.30889 1.45844
H -2.65189 -5.14292 3.15491
H -3.79171 -4.74217 1.84157
H -4.62206 -3.08697 3.84380
H -5.23168 -0.87466 4.80438
H -3.86617 1.13420 4.35747
H -1.81631 1.00110 2.91687
N 1.67058 -1.42266 2.34183
C 2.33757 -1.82093 3.21049
C 3.16886 -2.32289 4.29083
H 2.93054 -3.37103 4.49441
H 4.22620 -2.24751 4.02094
H 2.99510 -1.74095 5.20078
H 0.97405 1.00836 2.58149
C 1.83203 1.92332 4.37280
C 0.96210 3.15002 4.34590
H 1.53511 1.08231 4.99903
C 1.57106 4.26637 5.25032
H 0.90369 3.54834 3.31945
H -0.06223 2.92279 4.66220
C 3.04685 4.52857 4.88858
H 0.97992 5.18553 5.14720
H 1.50169 3.95338 6.30175
C 3.89184 3.24116 4.96401
H 3.10243 4.93983 3.86904
H 3.46622 5.29027 5.55910
C 3.28980 2.11981 4.06032
H 4.92743 3.44113 4.65982
H 3.92310 2.88429 6.00319
H 3.41381 2.43590 3.01109
H 3.85759 1.19087 4.18526

87
[FeO(NTB)(CH3CN)]+CHX React (+2/5)
Fe 0.46908 -0.54400 0.60694
O 0.49675 0.95470 1.30494
C -2.79123 1.57470 -3.48007
C -2.83354 2.89514 -3.02600
C -2.32381 -1.53800 -3.95336
C -2.06053 0.66946 -2.70553
C -2.17069 3.29478 -1.84266
N -1.80778 -0.70550 -2.86022
C 4.35536 -2.36158 -2.63101
C -1.39665 1.06251 -1.51935
C -1.44263 2.38702 -1.07187
C -1.03316 -1.09384 -1.80531
C -0.54238 -2.47703 -1.52982
N -0.76770 -0.07247 -0.98613
C 1.82251 -2.83253 -0.74520
N 3.60908 -1.35811 -1.86045
C 2.51554 -1.55250 -1.07666
C 4.96029 0.74797 -2.39399
N 0.40120 -2.50498 -0.33027
C 3.93858 0.00880 -1.79153
N 2.11314 -0.40217 -0.50592
C 4.99317 2.11506 -2.11167
C 2.98468 0.60767 -0.93543
C -0.11071 -3.46182 0.72883
C 4.04060 2.71988 -1.25918
C 3.02188 1.97854 -0.65914
C -1.08016 -2.71057 1.58067
N -0.96313 -1.37503 1.70847
N -2.08835 -3.19318 2.35343
C -2.51914 -4.58940 2.50575
C -1.94684 -0.95152 2.61242
C -2.27513 0.31947 3.09585
C -2.66300 -2.09882 3.02765
C -3.33145 0.39968 4.00406
C -3.72179 -2.02220 3.93649
C -4.04268 -0.75089 4.41665
H -3.30260 1.27474 -4.38673
H -3.38925 3.63187 -3.59534
H -2.23129 4.33094 -1.52879
H -0.93166 2.68261 -0.16396
H -1.87480 -2.52924 -3.90885
H -3.40914 -1.63431 -3.87204
H -2.06842 -1.08121 -4.91160
H -1.38967 -3.13814 -1.32182
H -0.02456 -2.89052 -2.40027
H 1.83046 -3.55112 -1.56860
H 2.32516 -3.30048 0.10582
H 3.79613 -3.29508 -2.66210
H 4.49533 -2.00112 -3.65153
H 5.32842 -2.54129 -2.16825
H 5.69317 0.29002 -3.04690
H 5.76879 2.72795 -2.55675
H 4.10556 3.78510 -1.06817
H 2.28945 2.43349 -0.00452
H 0.73741 -3.78083 1.34056
H -0.54261 -4.35449 0.26895
H -1.99512 -5.21816 1.78820
H -2.29689 -4.93909 3.51638
H -3.59245 -4.66008 2.32010
H -4.26900 -2.90036 4.25667
H -4.85714 -0.64337 5.12405
H -3.61554 1.36632 4.40456
H -1.72479 1.19511 2.77570
N 1.92338 -1.50785 2.19639
C 2.64504 -1.70126 3.09368
C 3.54247 -1.94149 4.21150
H 4.54928 -2.16672 3.84787
H 3.59098 -1.05569 4.85189
H 3.18686 -2.78642 4.80842
H 1.06848 3.22926 3.01999
C 1.26996 3.97029 3.80914
C 1.76237 3.23698 5.07419
H 0.31935 4.48110 4.01363
C 3.12917 2.56256 4.83636
H 1.85633 3.96109 5.89829
H 1.02162 2.49116 5.39249
C 4.17744 3.57484 4.32997
H 3.48126 2.08197 5.75906
H 3.00983 1.76368 4.08749
C 3.68631 4.31072 3.06600
H 4.37716 4.31299 5.12215
H 5.12899 3.06563 4.12657
C 2.31750 4.98247 3.30057
H 4.42647 5.05874 2.75181
H 3.59786 3.58798 2.23979
H 2.43378 5.78508 4.04530
H 1.96591 5.45930 2.37580

87
[FeO(NTB)(CH3CN)]+CHX TS (+2/5)
Fe 0.70444 -0.18351 0.76300
O 0.74360 1.40807 1.44413
C -2.88111 1.75004 -3.10765
C -2.93874 3.06699 -2.64569
C -2.33704 -1.33400 -3.63552
C -2.06412 0.87049 -2.39204
C -2.20716 3.48598 -1.51091
N -1.77762 -0.49312 -2.57060
C 4.39958 -2.31432 -2.70853
C -1.32881 1.28219 -1.25626
C -1.39265 2.60324 -0.79959
C -0.91316 -0.86348 -1.57988
C -0.36304 -2.24417 -1.39554
N -0.62035 0.16713 -0.77683
C 1.99061 -2.65550 -0.66687
N 3.71085 -1.25795 -1.95741
C 2.66707 -1.38929 -1.08658
C 5.02817 0.79853 -2.72051
N 0.59102 -2.33258 -0.22991
C 4.04927 0.10505 -2.00241
N 2.30877 -0.20556 -0.56626
C 5.07622 2.18225 -2.53820
C 3.15346 0.76334 -1.12729
C 0.08953 -3.25669 0.84143
C 4.17753 2.84804 -1.67260
C 3.20343 2.15124 -0.95673
C -0.85602 -2.50263 1.72263
N -0.75343 -1.17320 1.87501
N -1.86210 -3.01772 2.48906
C -2.27639 -4.42020 2.61575
C -1.74926 -0.78472 2.78323
C -2.10452 0.47527 3.27765
C -2.45067 -1.94665 3.18228
C -3.16452 0.53024 4.18347
C -3.51225 -1.89716 4.09069
C -3.85557 -0.63683 4.58444
H -3.44467 1.43284 -3.97682
H -3.56018 3.78468 -3.16969
H -2.28236 4.51812 -1.18681
H -0.82937 2.91367 0.07098
H -1.91188 -2.33496 -3.58123
H -3.42167 -1.40301 -3.52447
H -2.09687 -0.90224 -4.60955
H -1.18643 -2.95029 -1.24071
H 0.15188 -2.56515 -2.30768
H 1.99433 -3.40939 -1.46127
H 2.52626 -3.08181 0.18660
H 3.83828 -3.24464 -2.64063
H 4.47160 -2.02416 -3.75849
H 5.40198 -2.47204 -2.30324
H 5.71807 0.29518 -3.38699
H 5.81980 2.76063 -3.07508
H 4.24900 3.92471 -1.56516
H 2.50725 2.65140 -0.29552
H 0.94543 -3.59272 1.43450
H -0.37412 -4.14940 0.40855
H -1.75975 -5.02841 1.87550
H -2.03540 -4.79391 3.61378
H -3.35213 -4.49845 2.44631
H -4.04651 -2.78756 4.39937
H -4.67339 -0.55058 5.29115
H -3.46809 1.48853 4.59015
H -1.57227 1.36323 2.96085
N 2.16800 -1.09911 2.23227
C 2.91886 -1.41002 3.06962
C 3.85191 -1.79943 4.11292
H 4.76972 -2.19837 3.67123
H 4.10772 -0.93359 4.73075
H 3.40584 -2.56699 4.75202
H 0.97562 2.55211 2.23643
C 1.14156 3.55289 2.87946
C 0.82046 3.21395 4.33554
H 0.41189 4.24190 2.43586
C 1.85045 2.24760 4.95483
H 0.82369 4.15946 4.90516
H -0.19395 2.80639 4.42329
C 3.29404 2.75431 4.75887
H 1.63640 2.11138 6.02238
H 1.74400 1.26052 4.48170
C 3.60260 3.01736 3.27070
H 3.43119 3.68680 5.32721
H 4.00726 2.02757 5.16930
C 2.58632 3.99701 2.65012
H 4.61949 3.41319 3.15627
H 3.56647 2.06697 2.71824
H 2.70969 4.98985 3.11670
H 2.78298 4.13582 1.58019

87
[FeO(NTB)(CH3CN)]+CHX Interm (+2/5)
Fe 0.68853 -0.12125 0.72119
O 0.72027 1.53512 1.40007
C -2.96060 1.65511 -3.17400
C -3.02866 2.97908 -2.73369
C -2.38278 -1.42944 -3.65651
C -2.12603 0.79716 -2.45229
C -2.29004 3.42570 -1.61402
N -1.82407 -0.56519 -2.61070
C 4.37639 -2.31704 -2.76606
C -1.38434 1.23627 -1.33112
C -1.45817 2.56439 -0.89638
C -0.94462 -0.90814 -1.62131
C -0.37655 -2.28107 -1.42570
N -0.65729 0.13810 -0.83907
C 1.98372 -2.65609 -0.71004
N 3.68605 -1.25752 -2.02125
C 2.64600 -1.38597 -1.14366
C 4.99530 0.79743 -2.80288
N 0.58487 -2.35178 -0.27069
C 4.02065 0.10582 -2.07710
N 2.28620 -0.20031 -0.63176
C 5.04306 2.18194 -2.62632
C 3.12738 0.76703 -1.20156
C 0.09909 -3.25480 0.82014
C 4.14919 2.85032 -1.75767
C 3.17886 2.15575 -1.03440
C -0.83638 -2.49140 1.70558
N -0.73944 -1.16121 1.84379
N -1.82603 -3.00543 2.49585
C -2.22883 -4.40881 2.64454
C -1.71829 -0.77044 2.76969
C -2.06420 0.49175 3.26565
C -2.40664 -1.93192 3.19168
C -3.10486 0.54970 4.19349
C -3.44902 -1.87923 4.12199
C -3.78511 -0.61652 4.61500
H -3.52947 1.31681 -4.03174
H -3.66379 3.68063 -3.26321
H -2.37349 4.46250 -1.30705
H -0.88758 2.89429 -0.03735
H -1.94022 -2.42235 -3.59495
H -3.46473 -1.51539 -3.53104
H -2.16265 -1.00716 -4.63948
H -1.19232 -2.99445 -1.26068
H 0.13355 -2.60417 -2.34034
H 1.99766 -3.41589 -1.49930
H 2.53012 -3.06871 0.14366
H 3.81316 -3.24627 -2.69876
H 4.45357 -2.02989 -3.81650
H 5.37697 -2.47585 -2.35646
H 5.68298 0.29200 -3.47015
H 5.78353 2.75878 -3.16921
H 4.22167 3.92727 -1.65350
H 2.48737 2.65790 -0.36907
H 0.96230 -3.58146 1.40825
H -0.37057 -4.15595 0.41072
H -1.73179 -5.01992 1.89333
H -1.95694 -4.77492 3.63757
H -3.30871 -4.49356 2.50768
H -3.97366 -2.76901 4.44855
H -4.58791 -0.52796 5.33850
H -3.40085 1.50945 4.60240
N 2.17455 -1.02311 2.18795
C 2.93145 -1.35294 3.01258
C 3.87308 -1.76839 4.03810
H 4.75078 -2.23397 3.58028
H 4.20004 -0.90298 4.62188
H 3.40334 -2.48976 4.71304
H 0.95732 2.31007 1.98145
C 1.36000 3.87048 3.06889
C 0.84165 3.47029 4.42316
H 0.69597 4.43627 2.41369
C 1.68949 2.35511 5.07974
H 0.86747 4.36060 5.08268
H -0.21357 3.17469 4.36782
C 3.19495 2.68045 5.01545
H 1.37052 2.21443 6.11963
H 1.50131 1.40680 4.55617
C 3.65596 2.90661 3.56178
H 3.39852 3.58559 5.60764
H 3.77506 1.86805 5.47206
C 2.84341 4.03259 2.87986
H 4.72433 3.15256 3.53078
H 3.52487 1.97535 2.99221
H 3.14756 5.00020 3.32631
H 3.09756 4.10543 1.81500