

Supporting information of

The Role of Porphyrin Peripheral Substituents in Determining the Reactivities of Ferrous Nitrosyl Species

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Table of content

1. Synthetic characterization data.....	Page 1-11
2. Cyclic voltammetric data of FeTPP-NO, FeTPC-NO and FeDEsC-NO: scan rate dependence.....	Page 12-13
3. Resonance Raman and EPR spectra of 5C-{FeNO} ⁷ adducts.....	Page 14-15
4. FTIR and EPR data of six-coordinate {FeNO} ⁷ adducts.....	Page 16-18
5. FTIR data of five-coordinate {FeNO} ⁶ adducts.....	Page 19
6. FTIR data of six-coordinate {FeNO} ⁶ adducts.....	Page 20
7. FTIR data of five-coordinate {FeNO} ⁸ adducts.....	Page 21
8. Estimation of K _d from the titration of 6C-{FeNO} ⁷ by nitrite.....	Page 22-24
9. Ring ruffling.....	Page 25-27
10. Identification of {FeHNO} ⁸ intermediate from {FeNO} ⁷ species.....	Page 27-29
11. References.....	Page 29
12. Coordinates of DFT optimized structures.....	Page 29-117

1. Synthetic characterization data

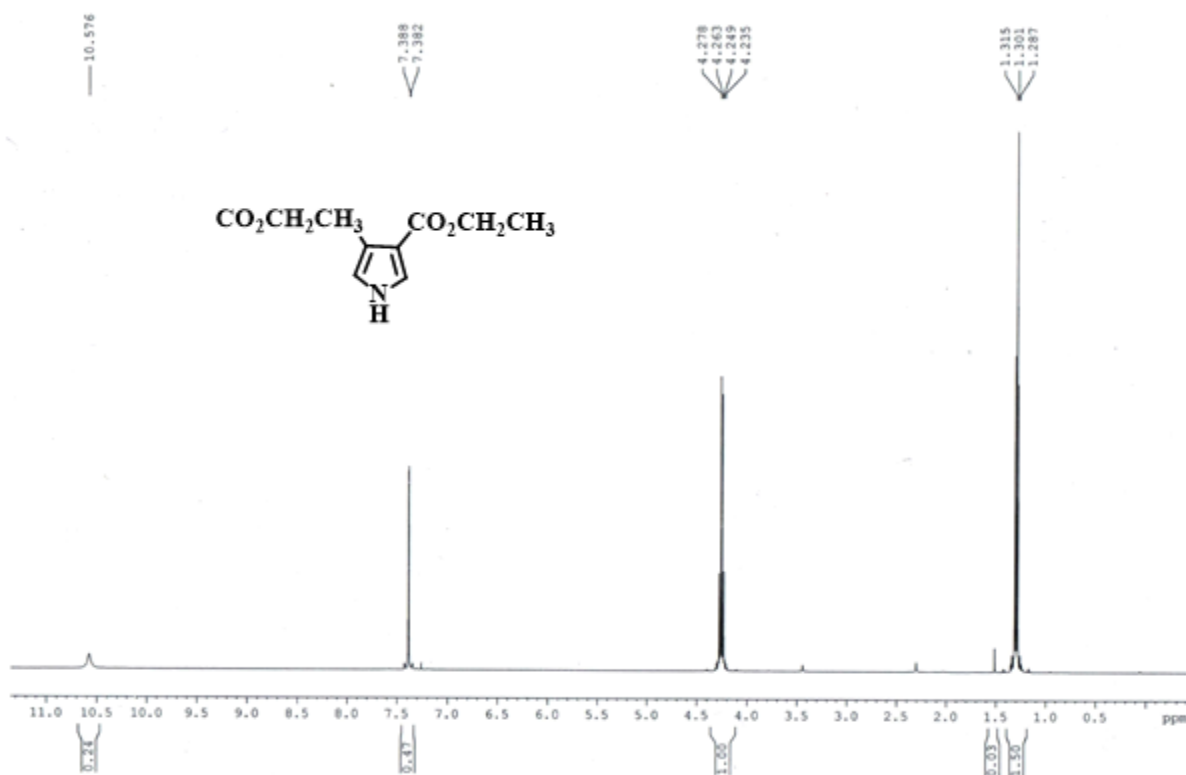


Figure S1. ¹H NMR of DEspyr.

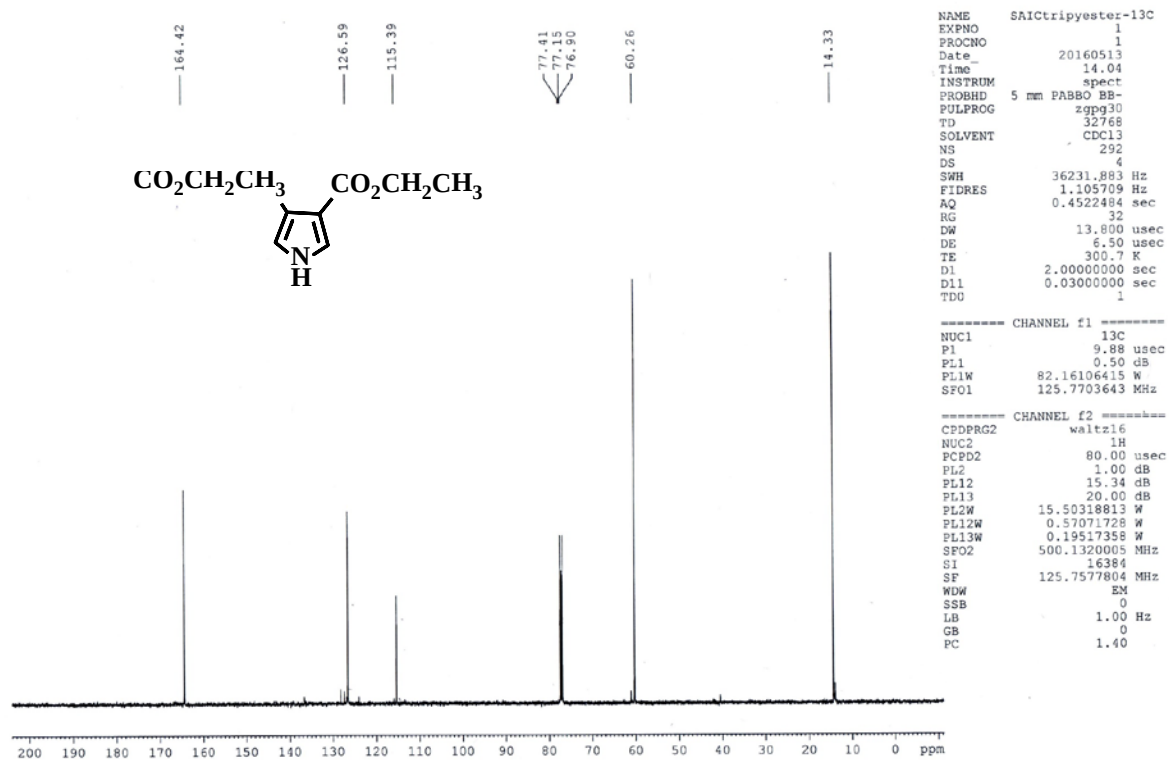


Figure S2. ^{13}C NMR of DEspyr.

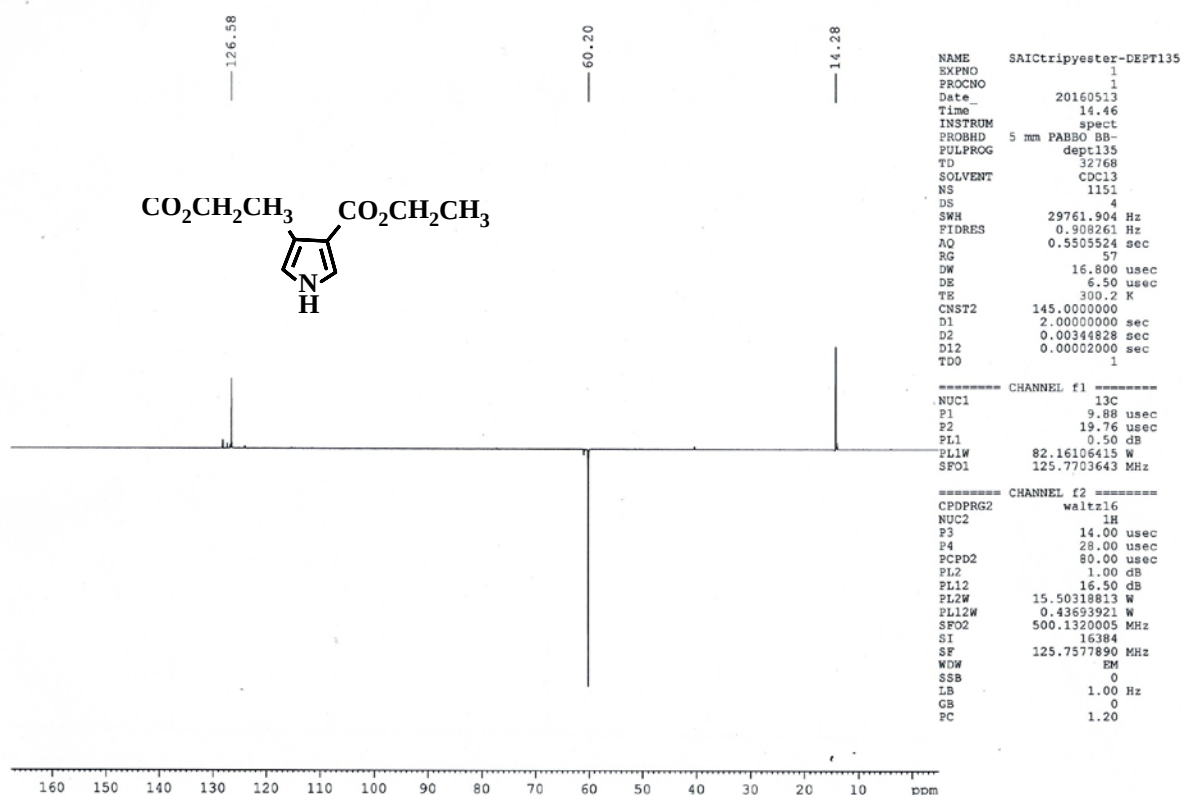


Figure S3. DEPT-135 NMR of DEspyr.

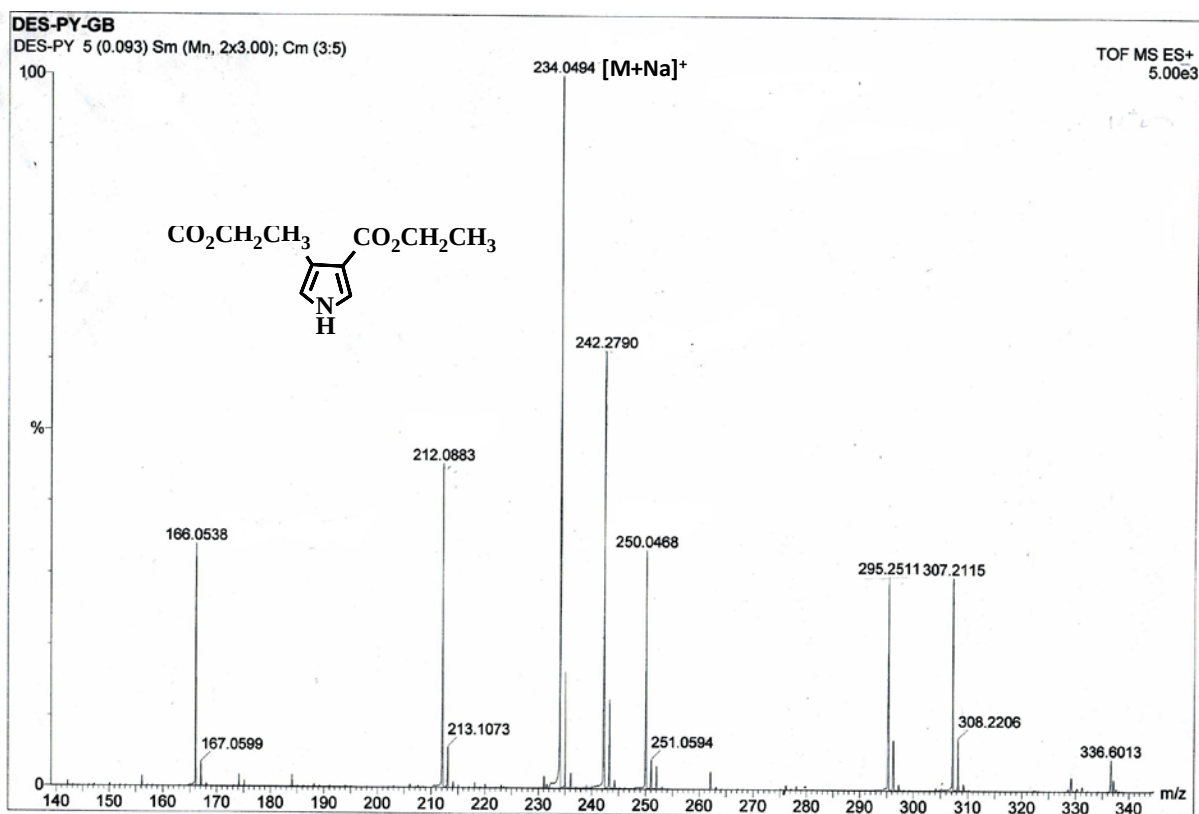


Figure S4. HRMS data of DESpyr.

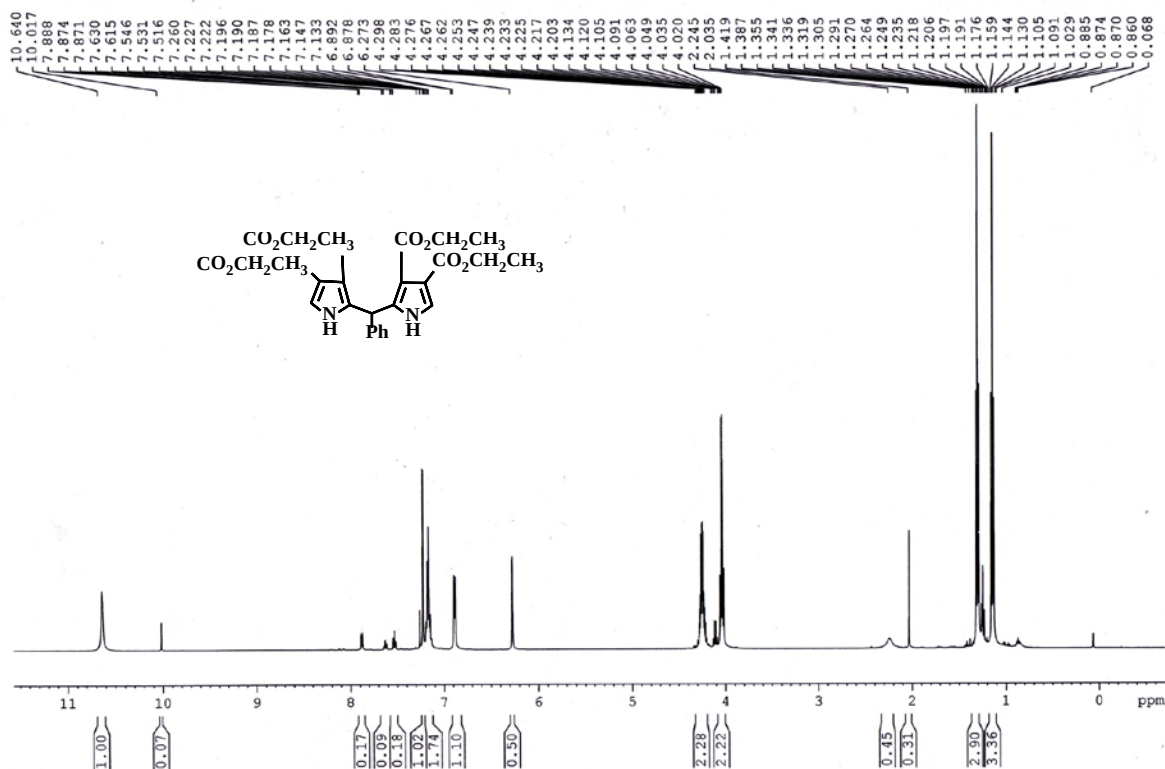


Figure S5. ¹H NMR of TESbpyr.

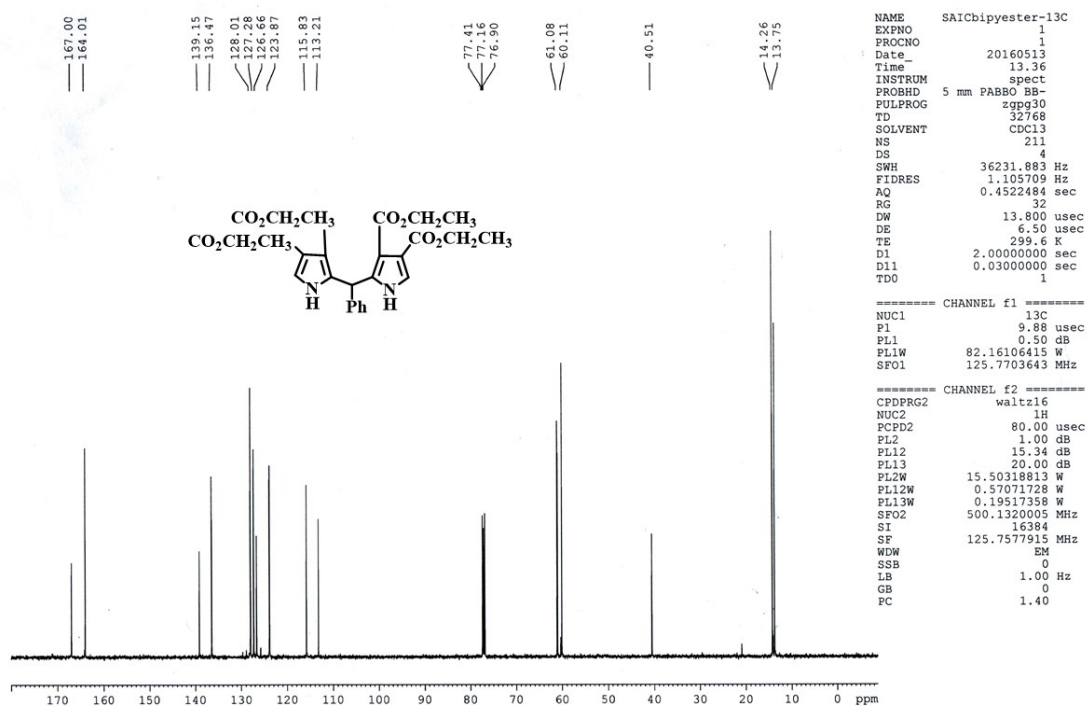


Figure S6. ¹³C NMR of TESbpyr.

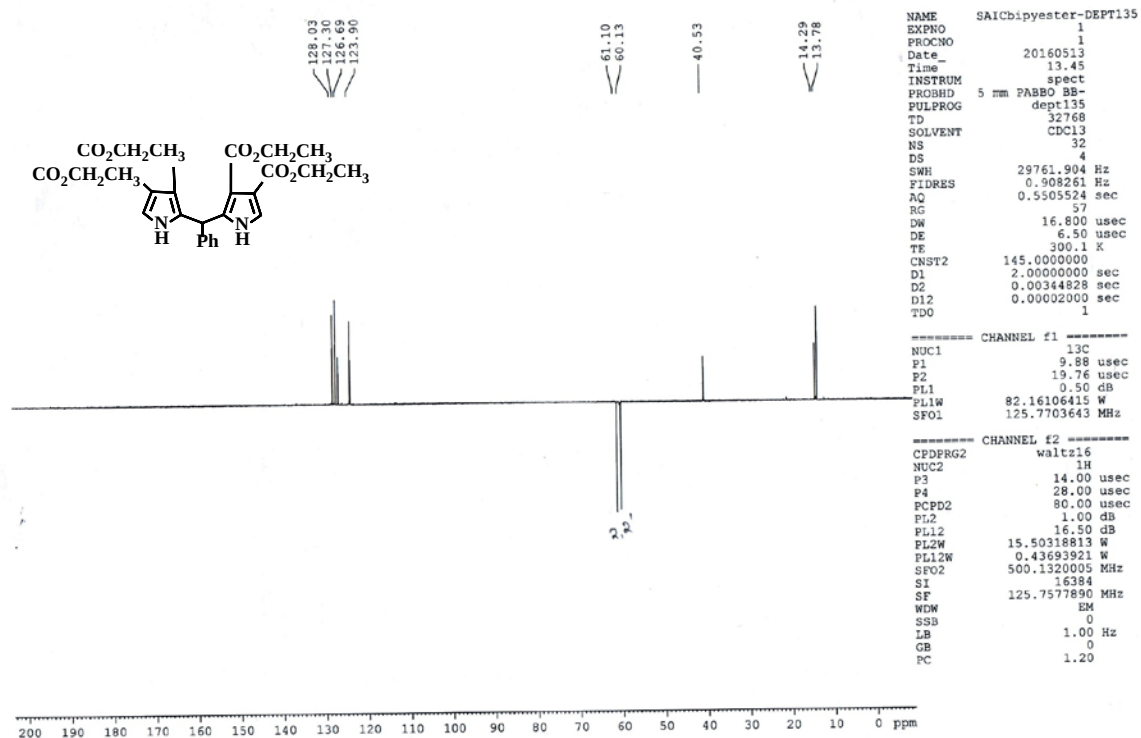


Figure S7. DEPT-135 NMR of TESbpyr.

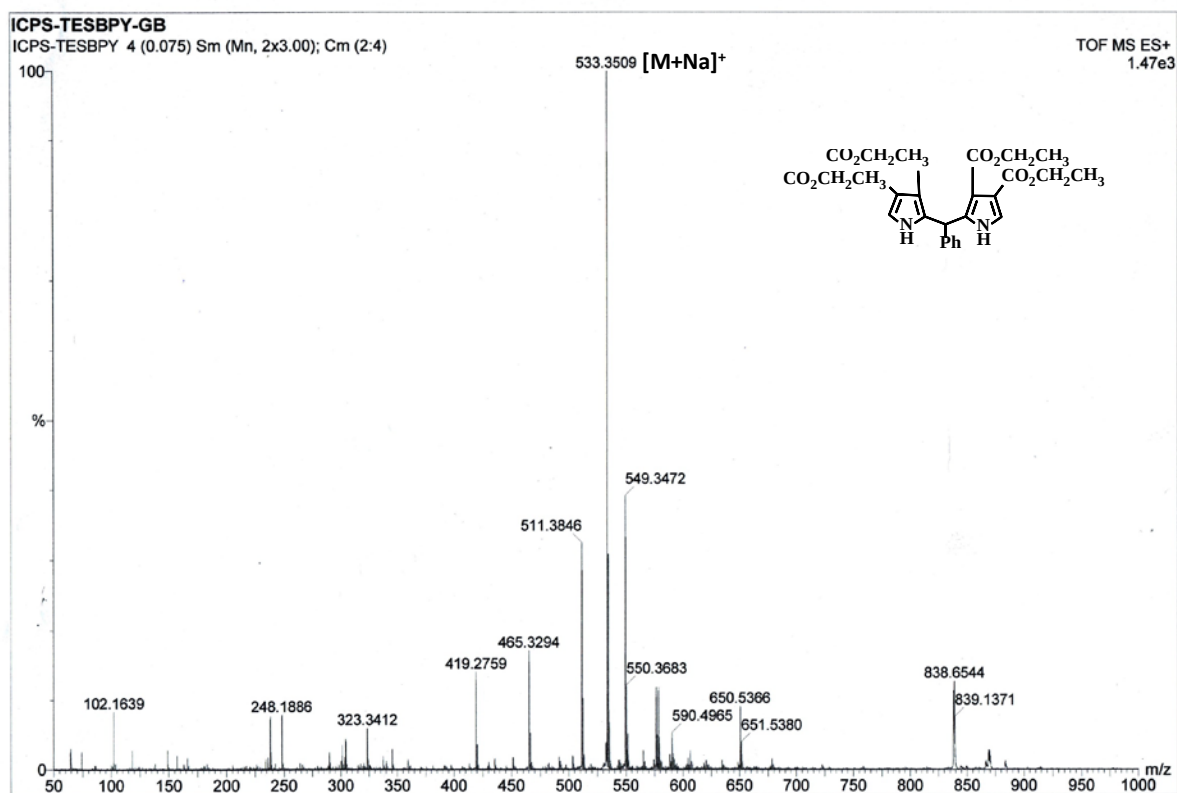


Figure S8. HRMS data of TESbpyr.

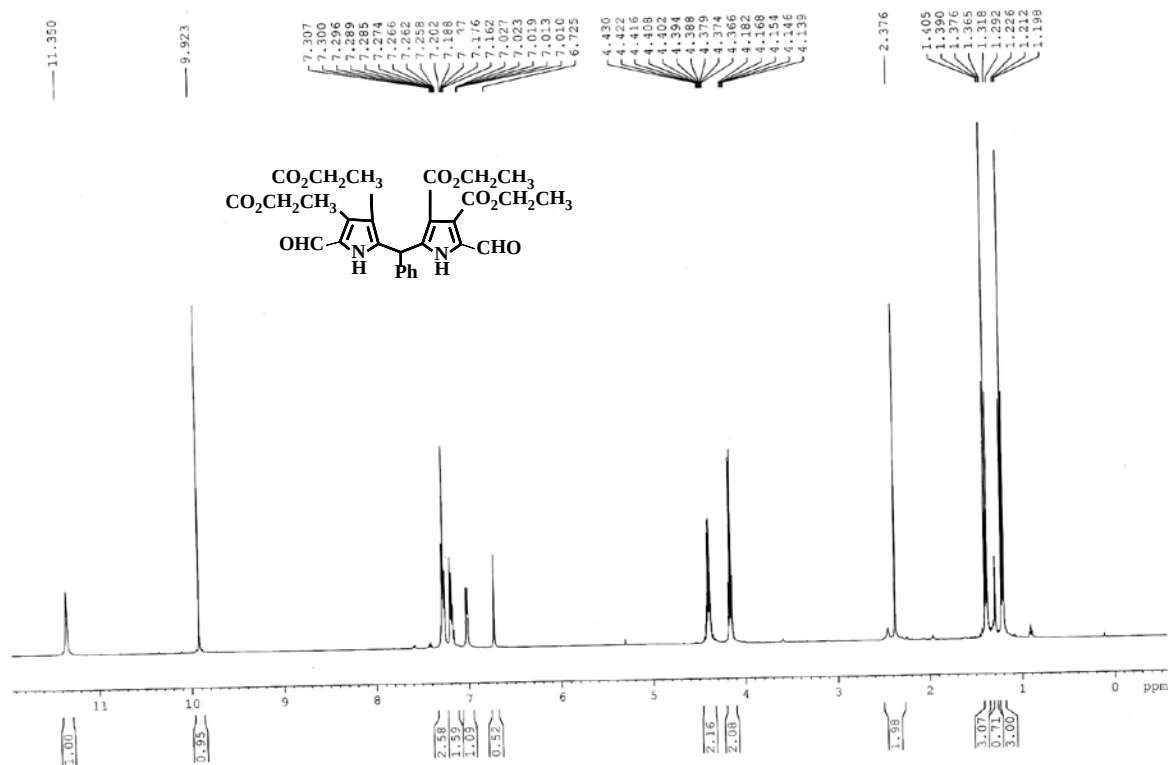


Figure S9. ¹H NMR of TESbpyr-dial.

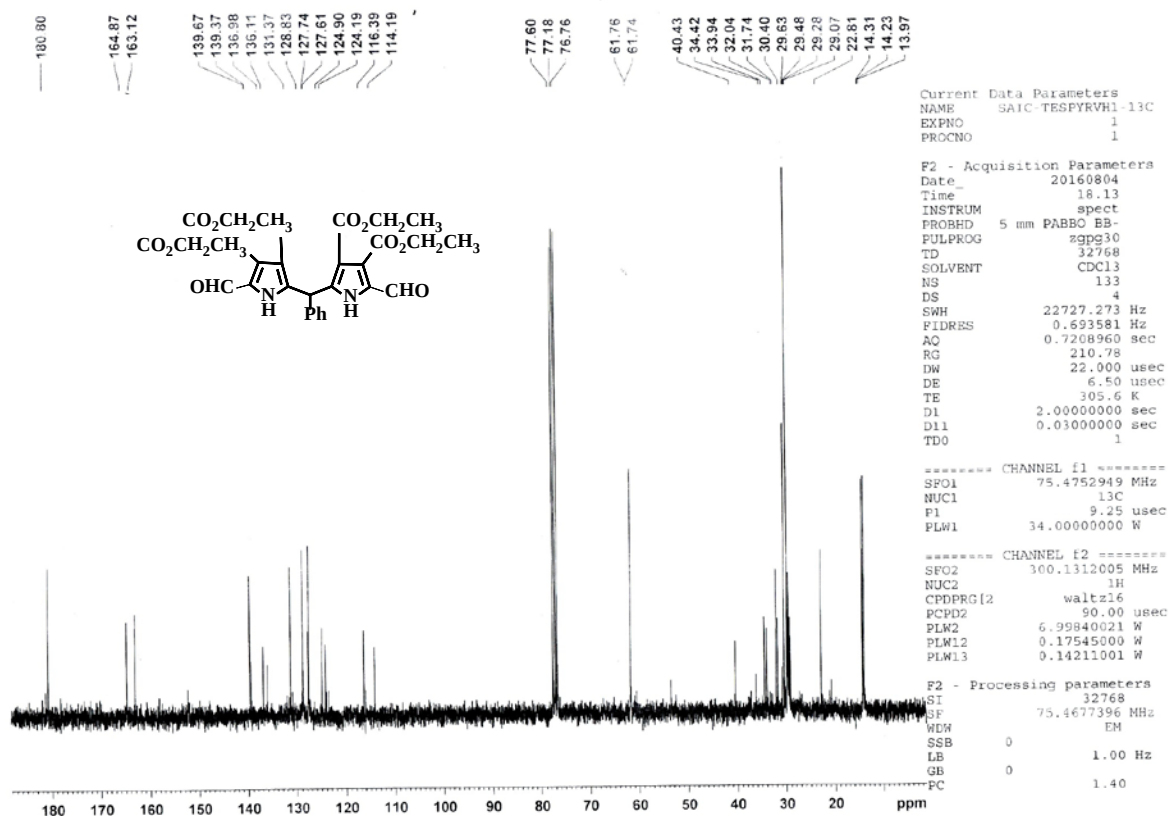


Figure S10. ¹³C NMR of TESbpyr-dial.

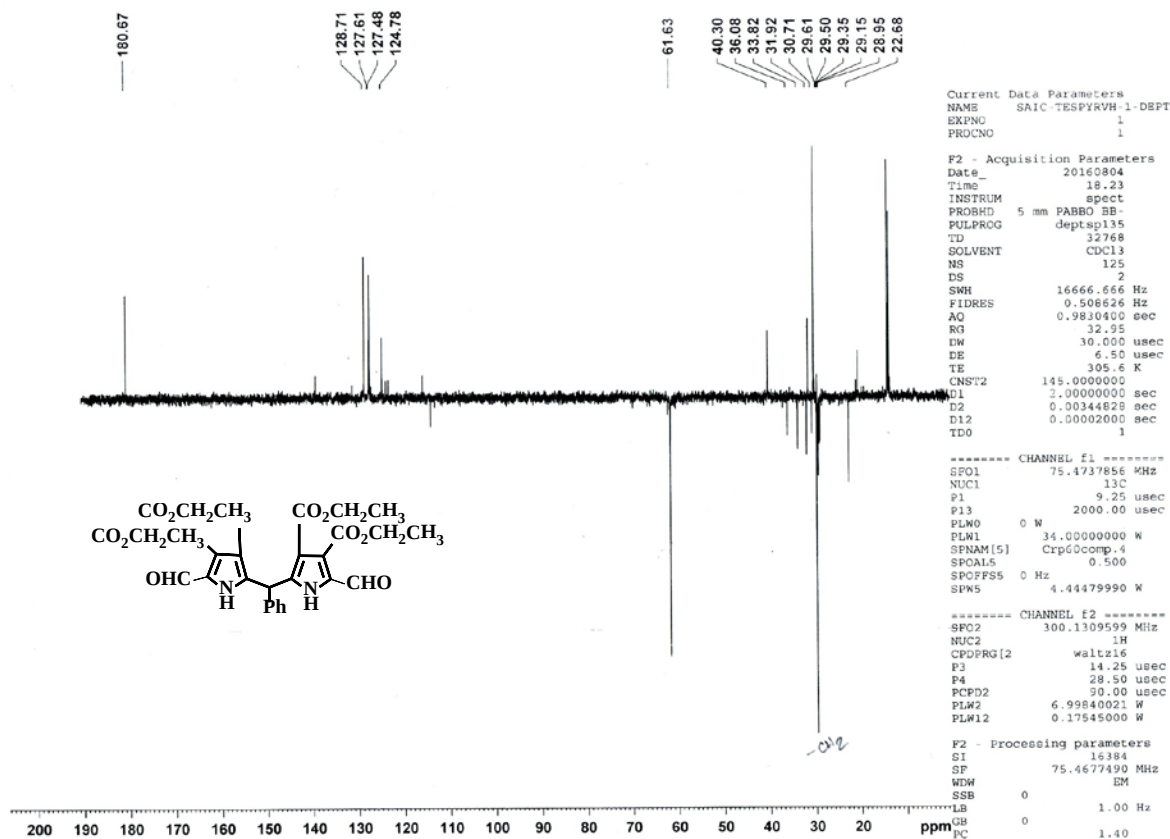


Figure S11. DEPT-135 NMR of TESbpyr-dial.

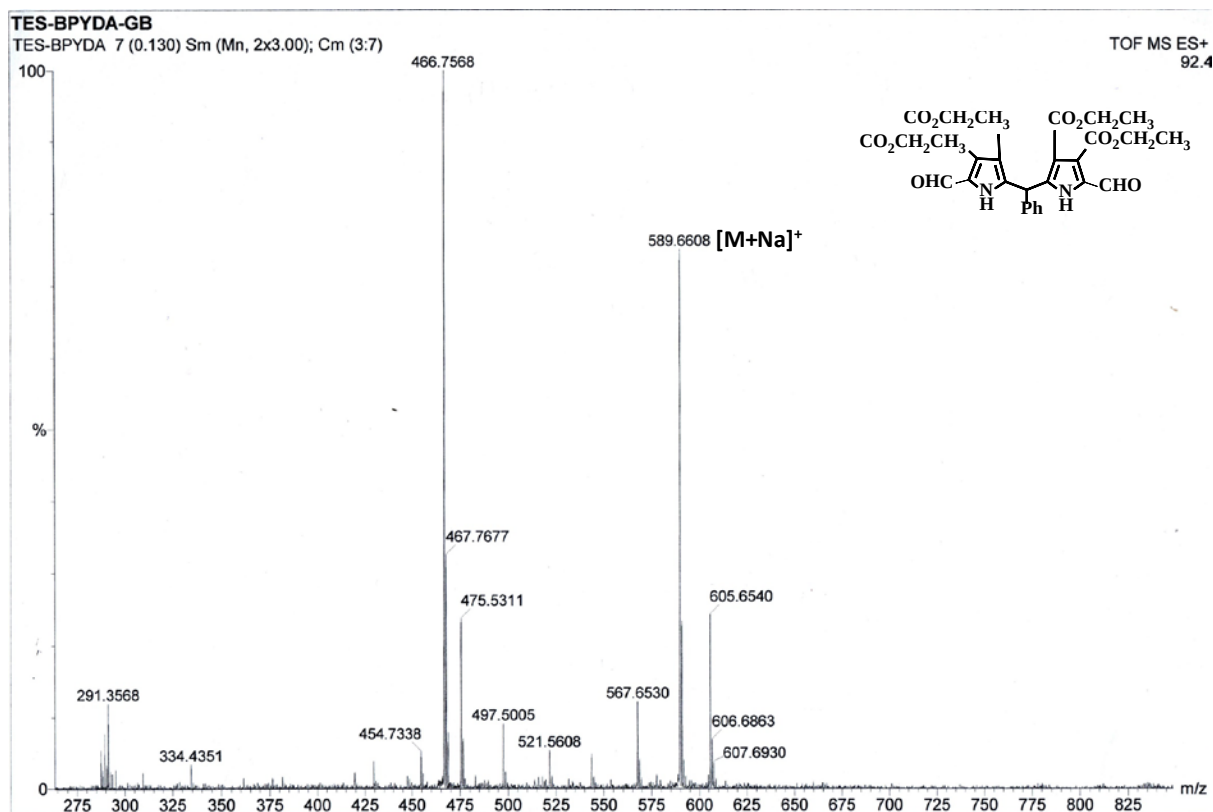


Figure S12. HRMS data of TESbpyr-dial.

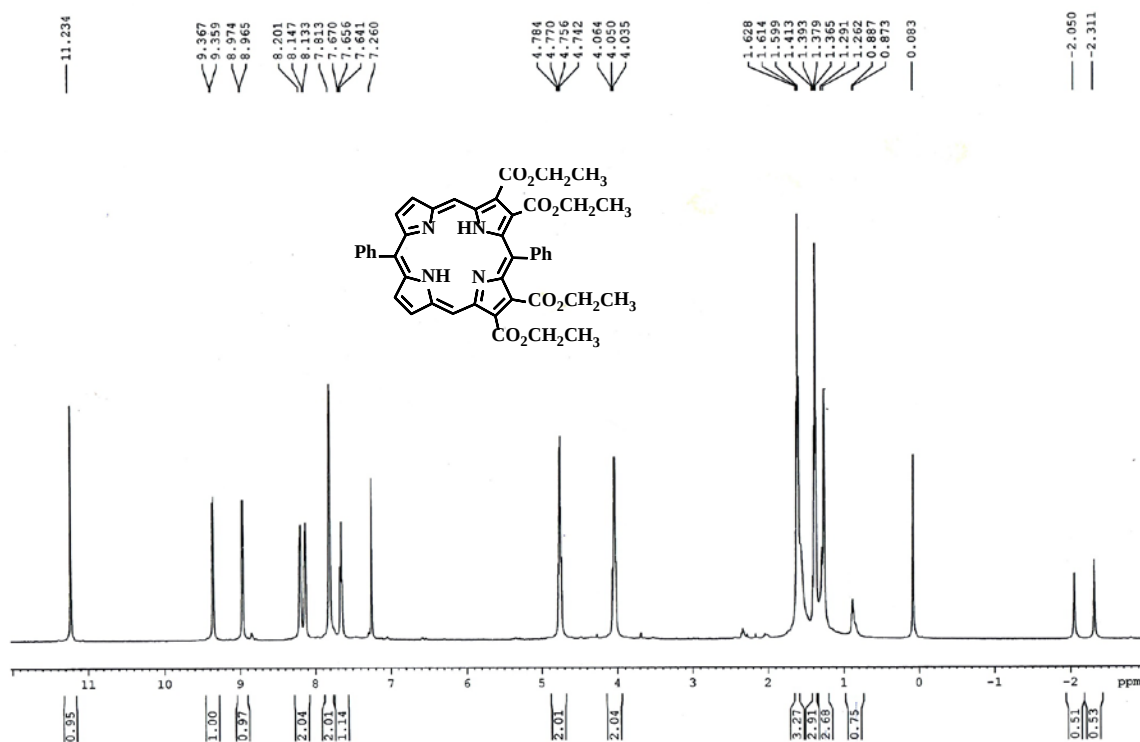


Figure S13. ¹H NMR of TESP.

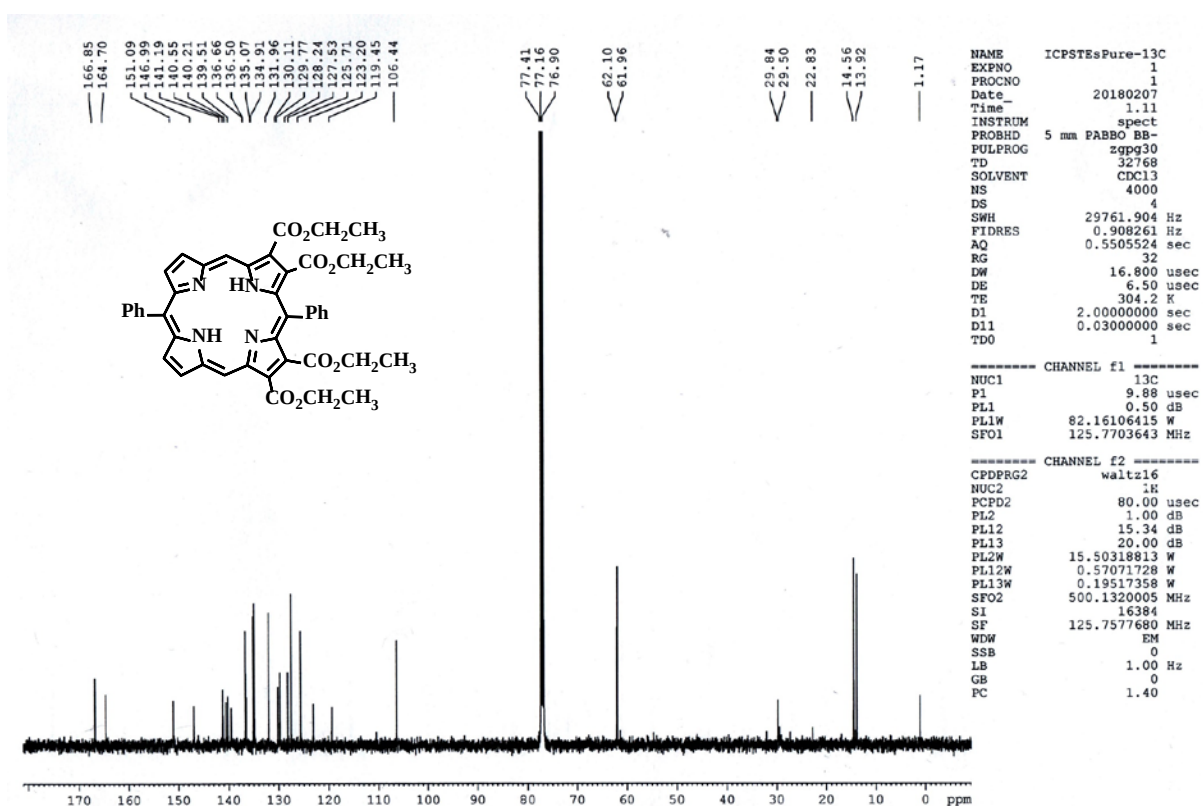


Figure S14. ¹³C NMR of TESP.

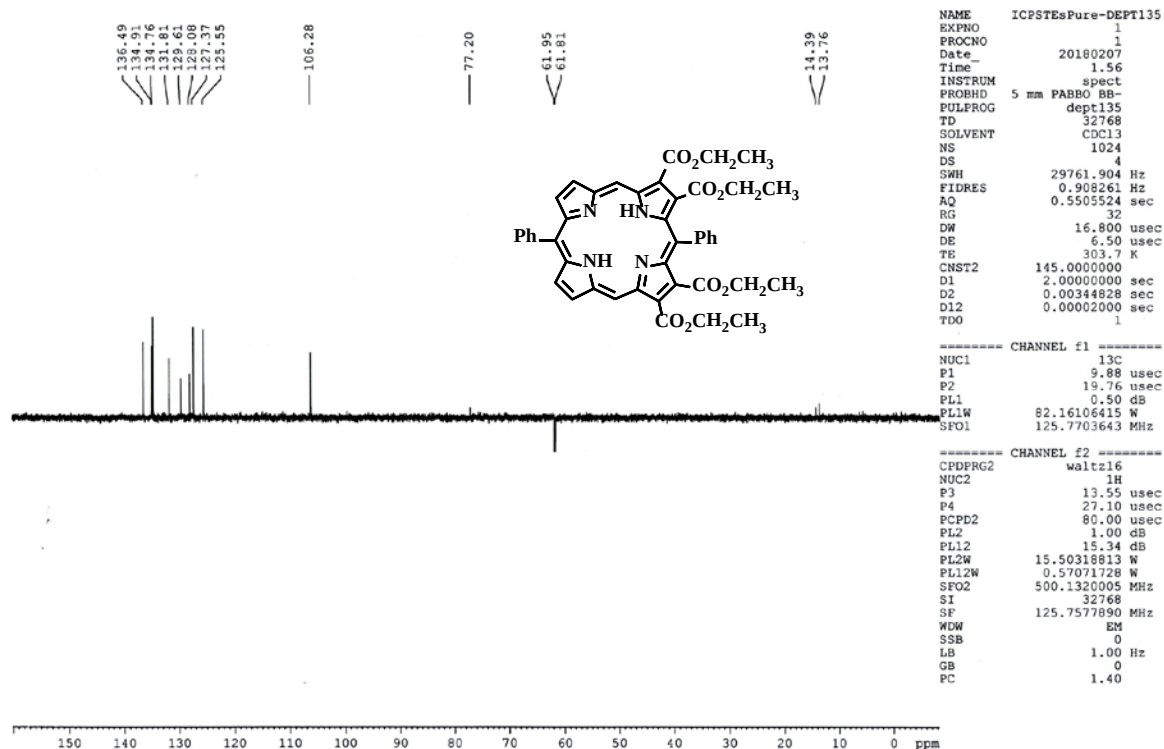


Figure S15. DEPT-135 NMR of TESP.

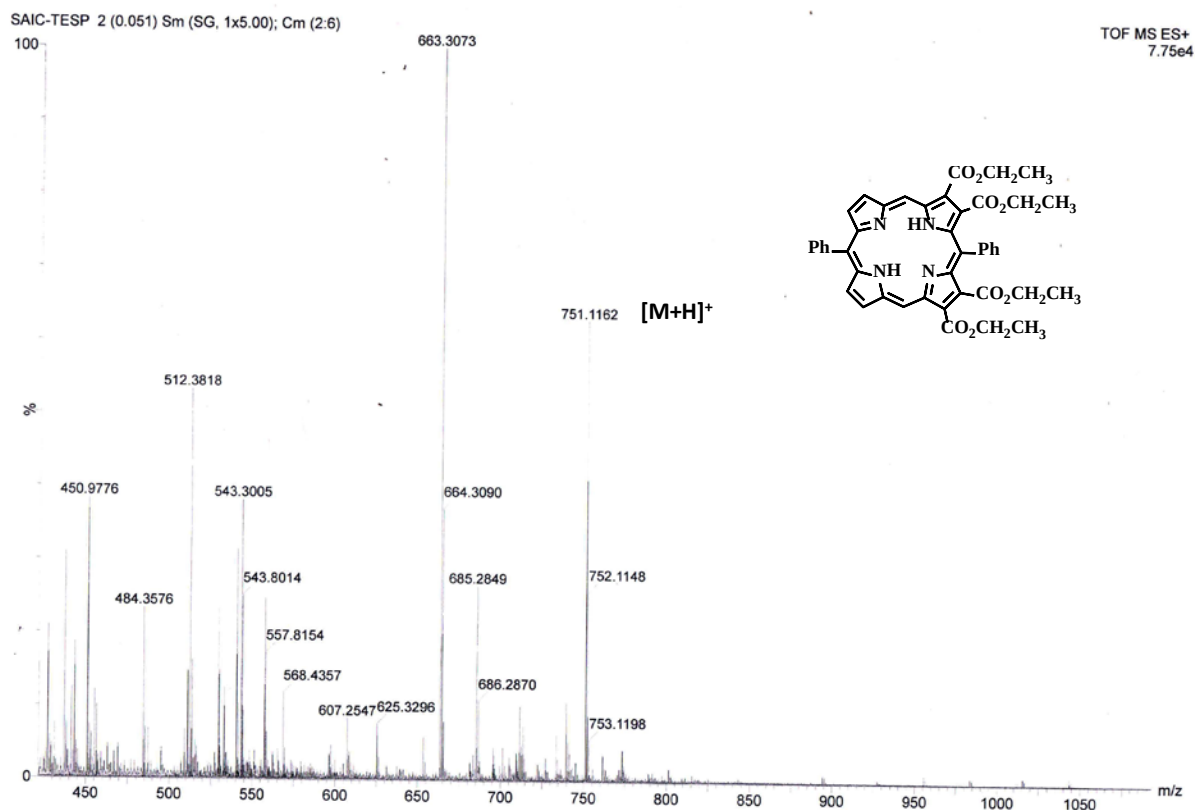


Figure S16. HRMS data of TESP.

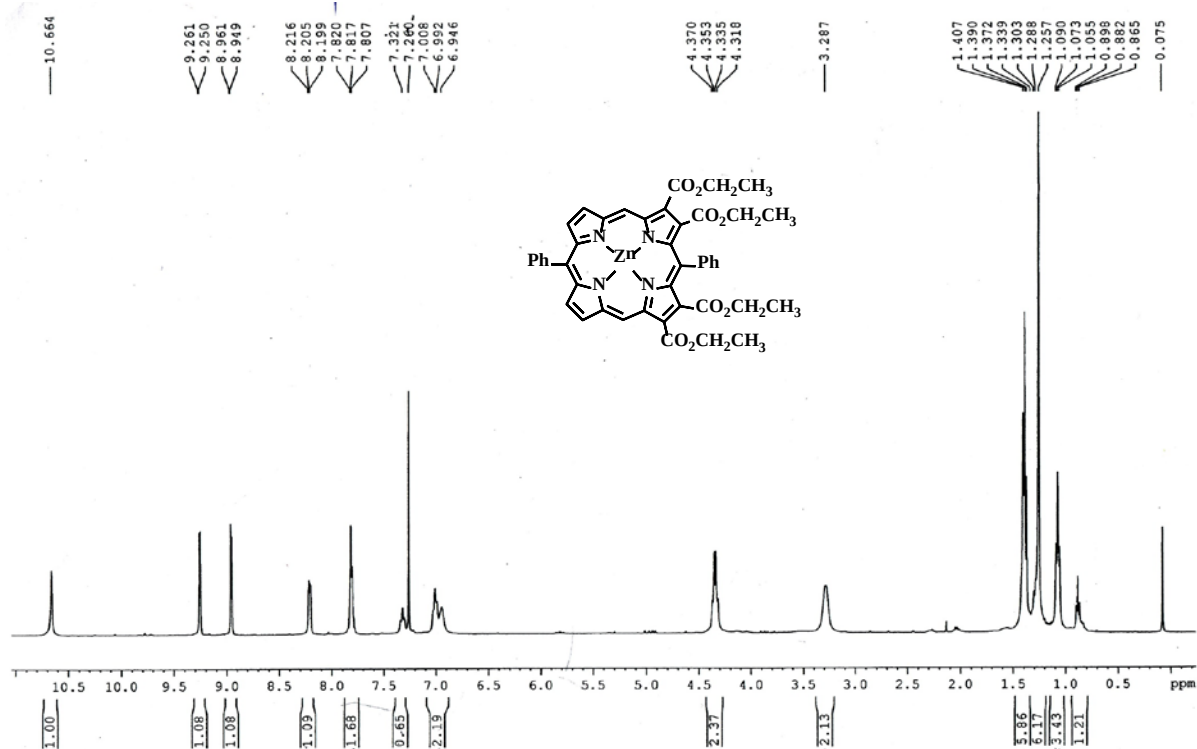


Figure S19. ¹H NMR of ZnTEsP.

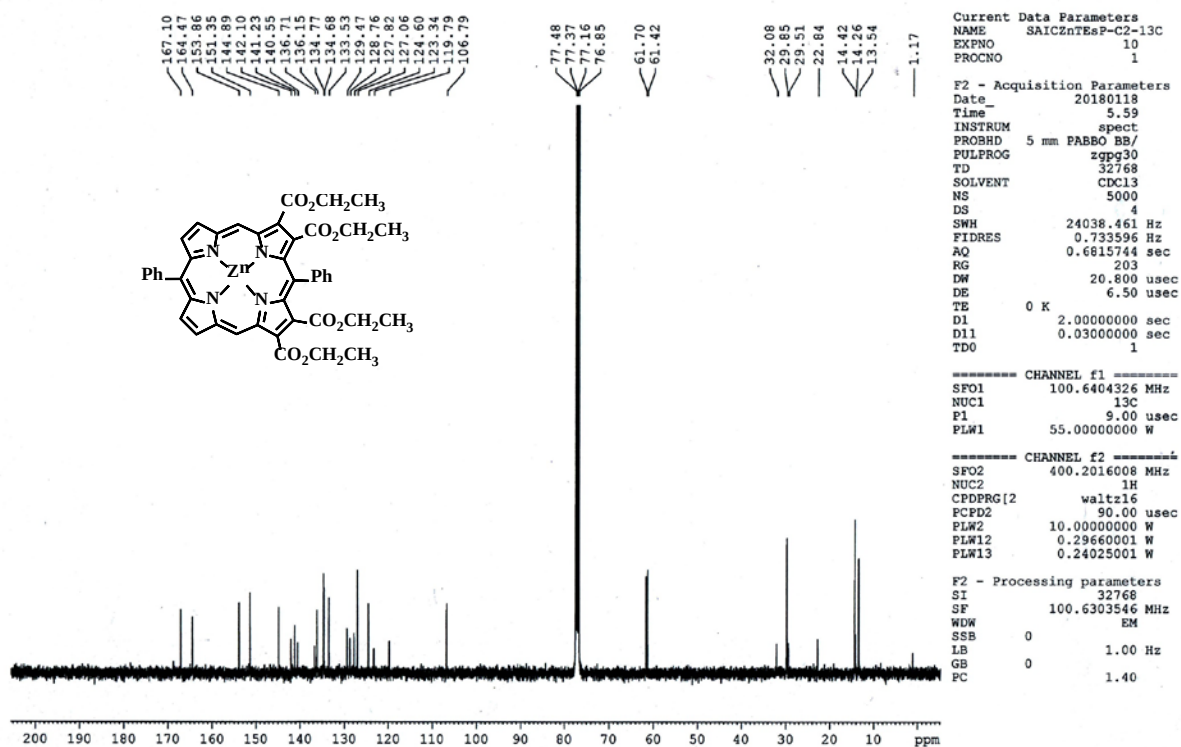


Figure S20. ¹³C NMR of ZnTEsP.

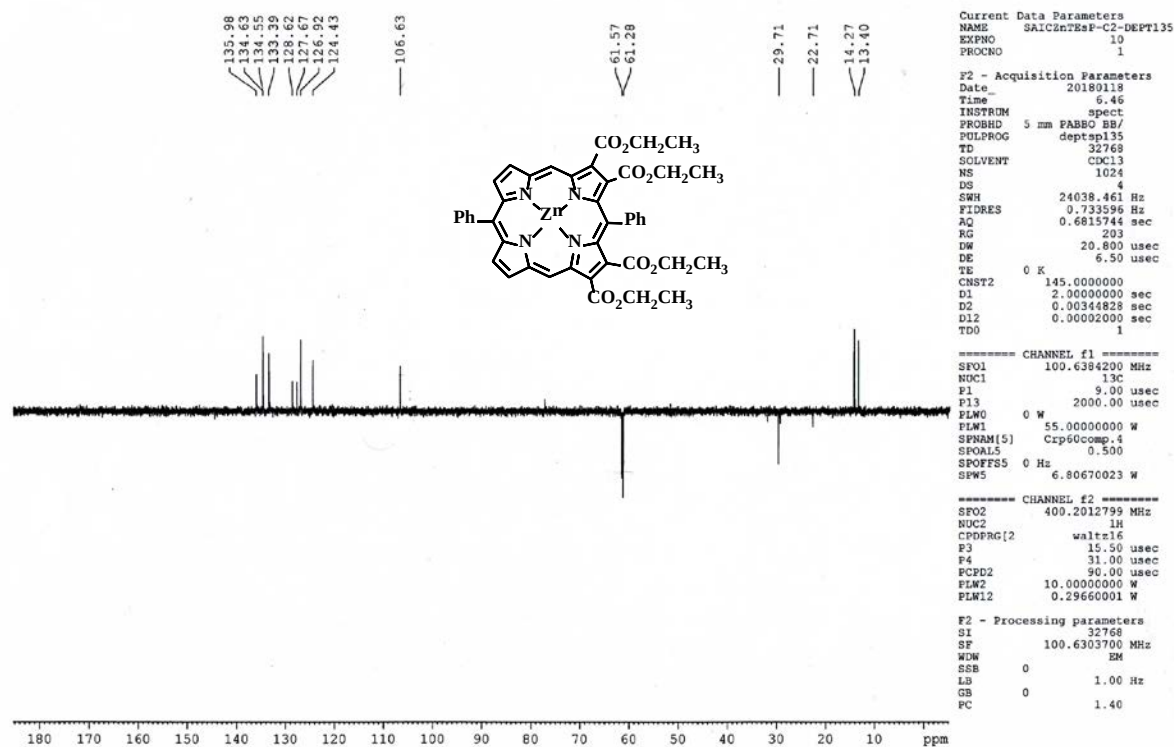


Figure S21. DEPT-135 NMR of ZnTEsP.

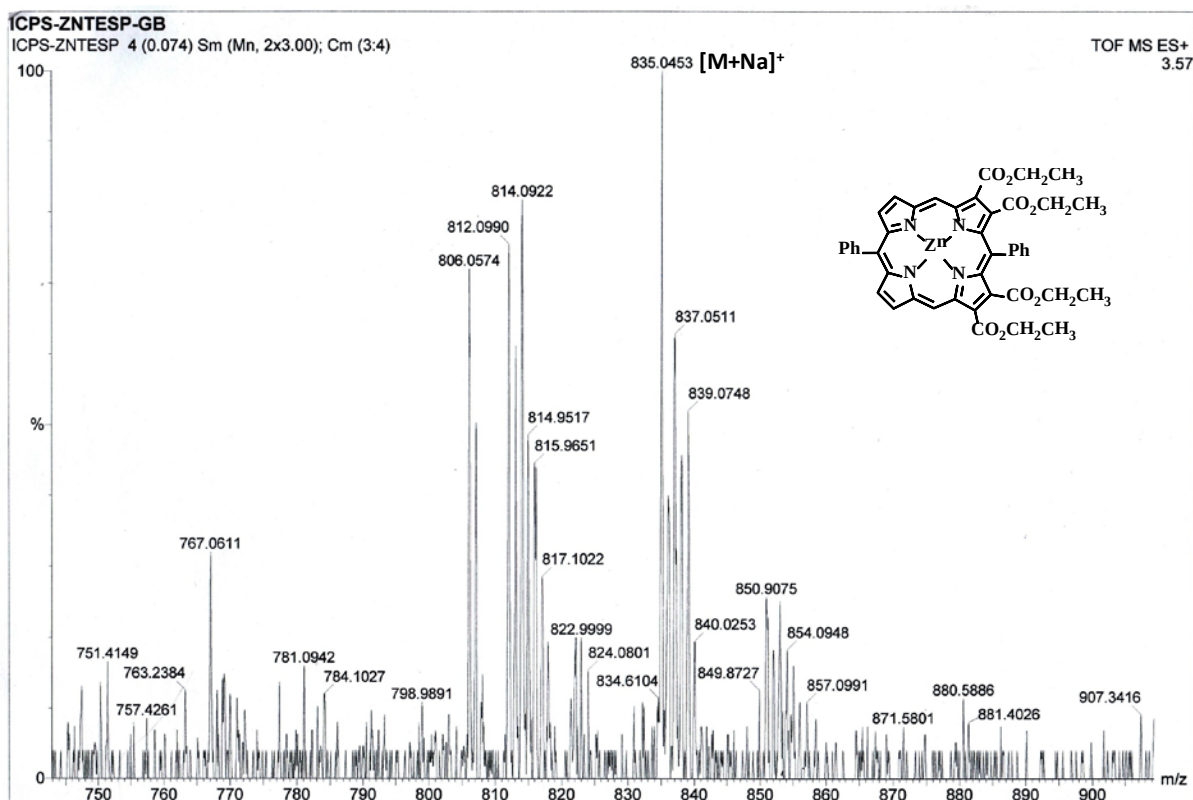


Figure S22. HRMS data of ZnTEsP.

2. Cyclic voltammetric data of FeTPP-NO, FeTPC-NO and FeDEsC-NO: scan rate dependence.

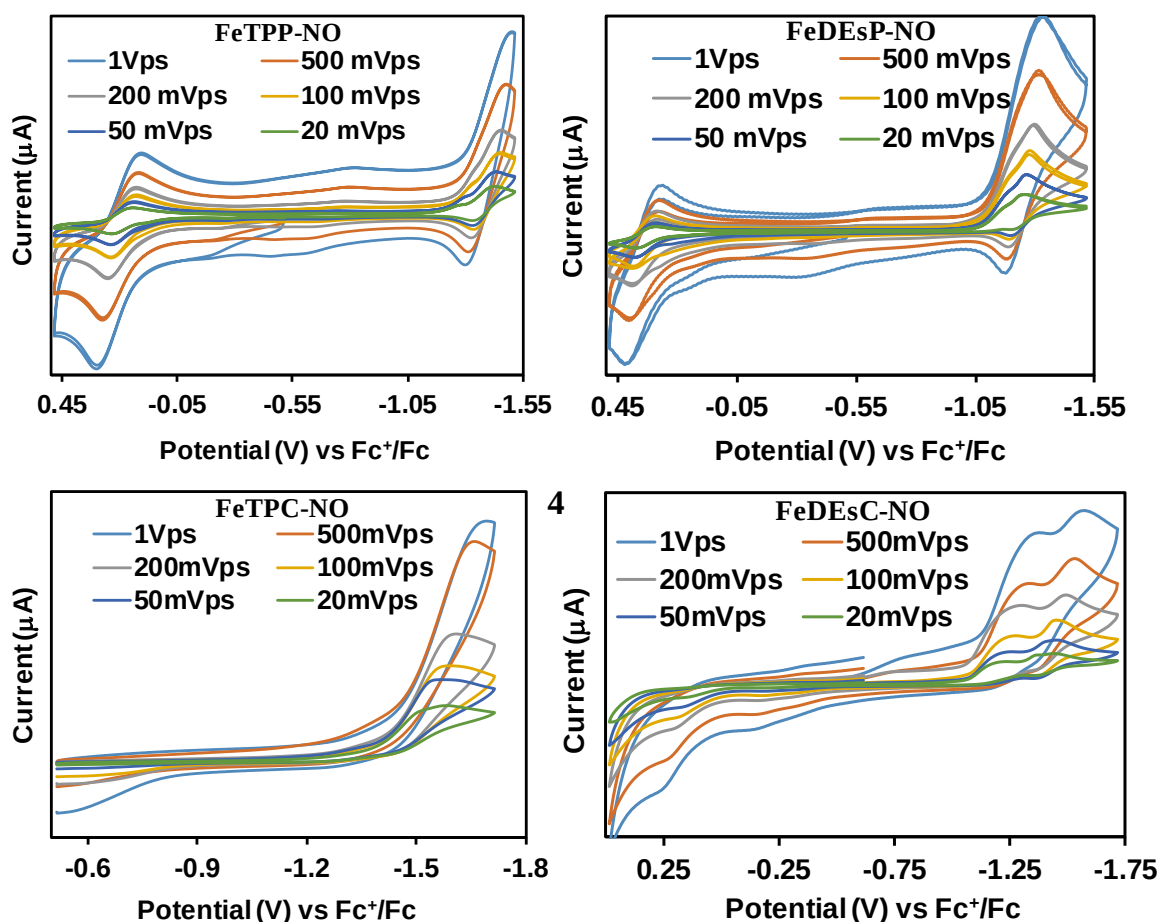


Figure S23A. Cyclic voltammogram of the complexes in dichloromethane at room temperature. Working electrode: glassy carbon; counter electrode: platinum; reference electrode: aqueous Ag/AgCl with 4M KCl; supporting electrolyte: tetrabutylammonium hexafluorophosphate (100 mM). Scan rate dependence of the corresponding {FeNO}^{6/7} redox process of 1) FeTPP-NO, 2) FeDEsP-NO, 3) FeTPC-NO and 4) FeDEsC-NO.

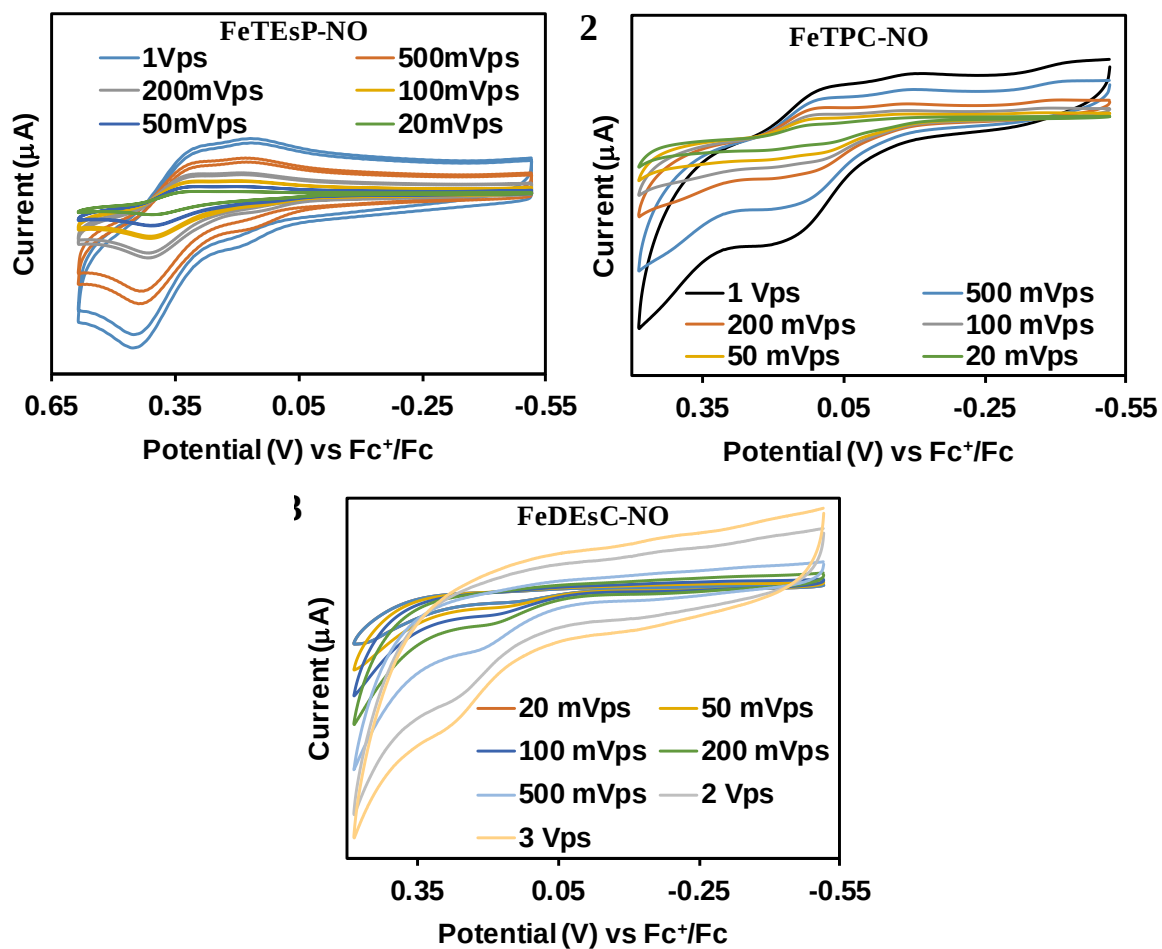


Figure S23B. Scan rate dependence of the oxidation wave of 1) FeTEsP-NO, 2) FeTPC-NO and 3) FeDEsC-NO.

3. resonance Raman and EPR spectra of the five-coordinate $\{\text{FeNO}\}^7$ species.

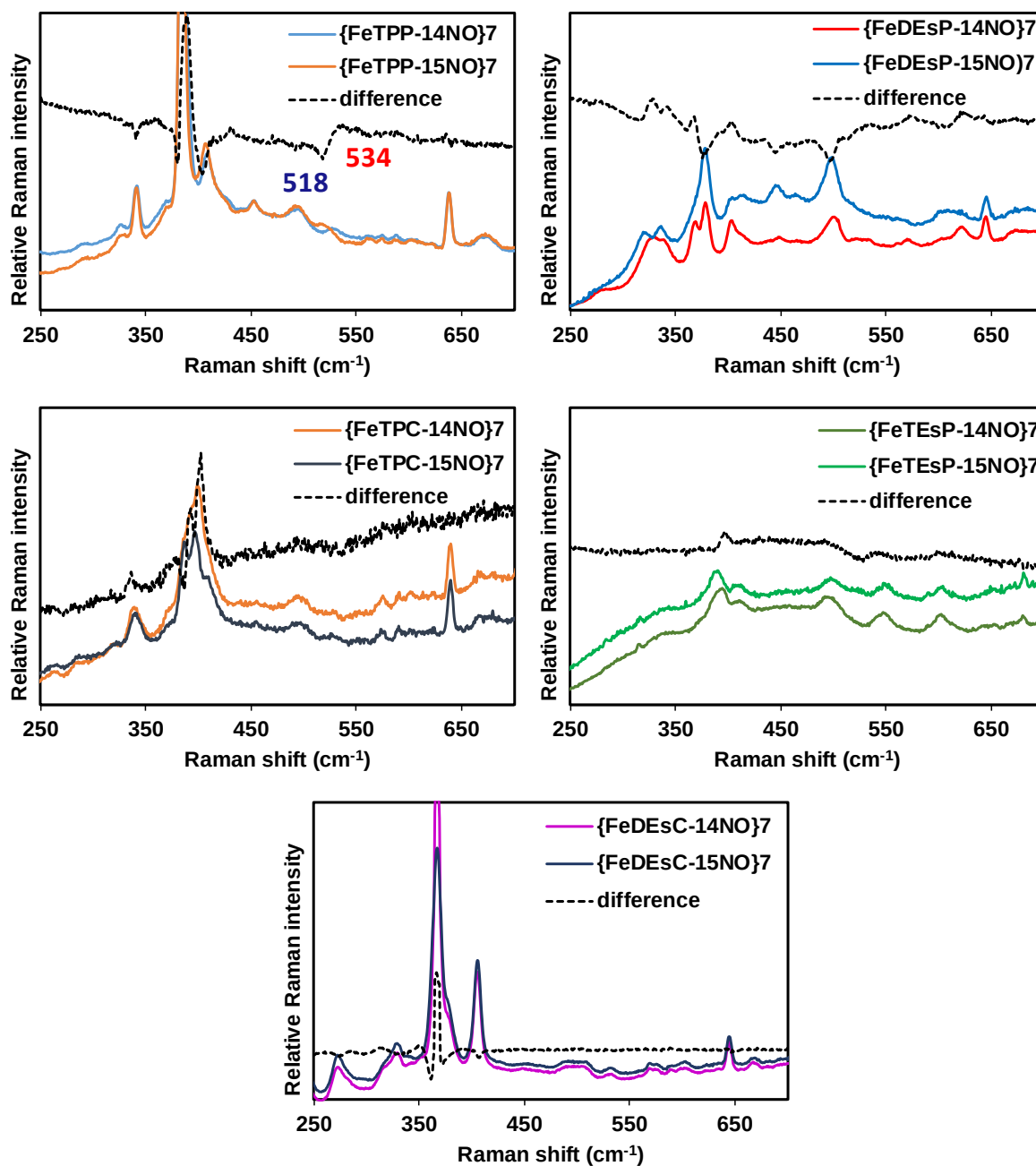


Figure S24A. Resonance Raman spectra of the 5C- $\{\text{FeNO}\}^7$ adducts in THF at 77K. Excitation wavelength: 413.1 nm.

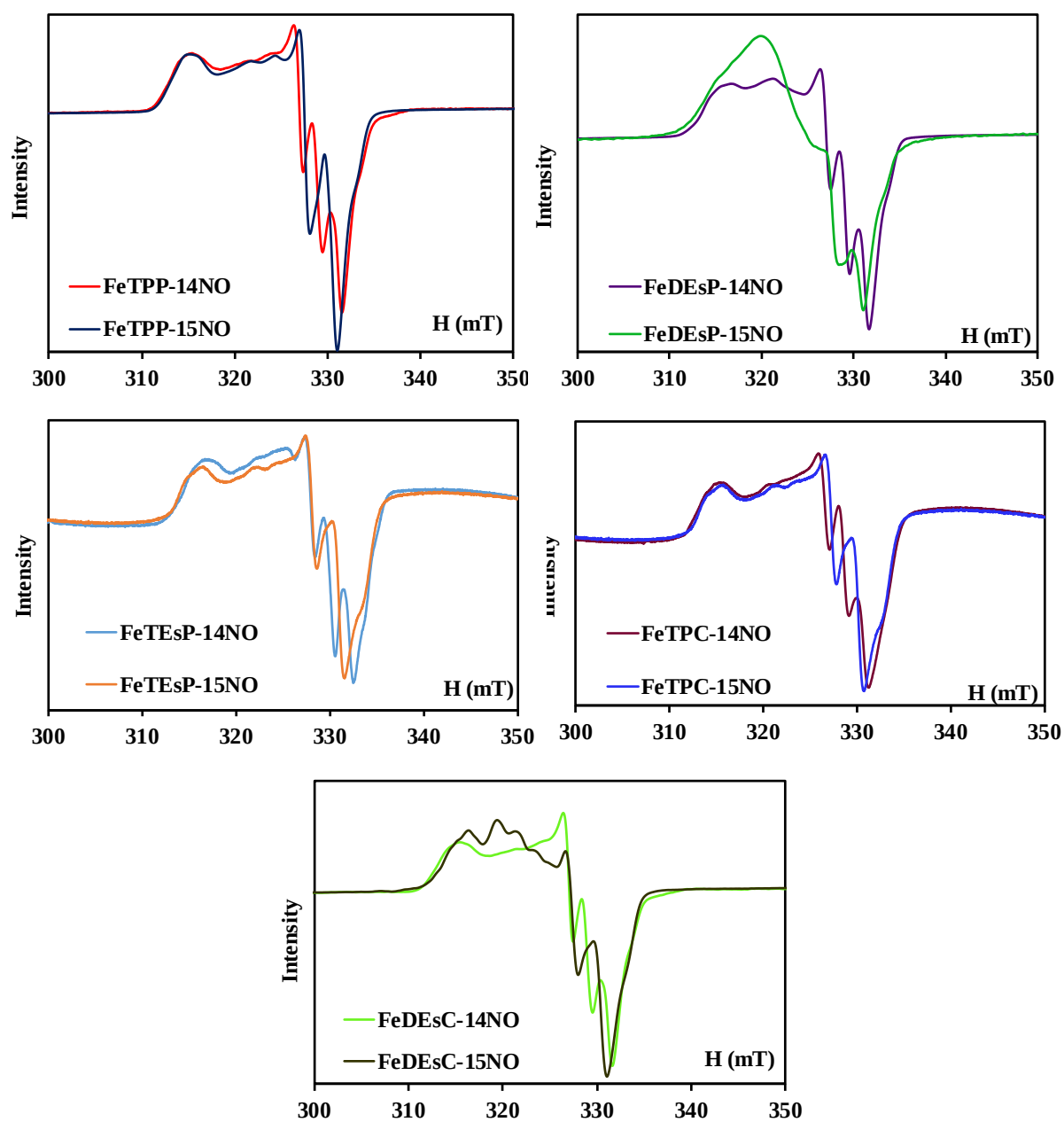


Figure S24B. EPR spectra of the 5C-{FeNO}⁷ adducts in THF at 77K. Power: 1 mW, Modulation amplitude: 0.25 mT.

4. FTIR and EPR data of the N-methylimidazole bound six-coordinate $\{\text{FeNO}\}^7$ species.

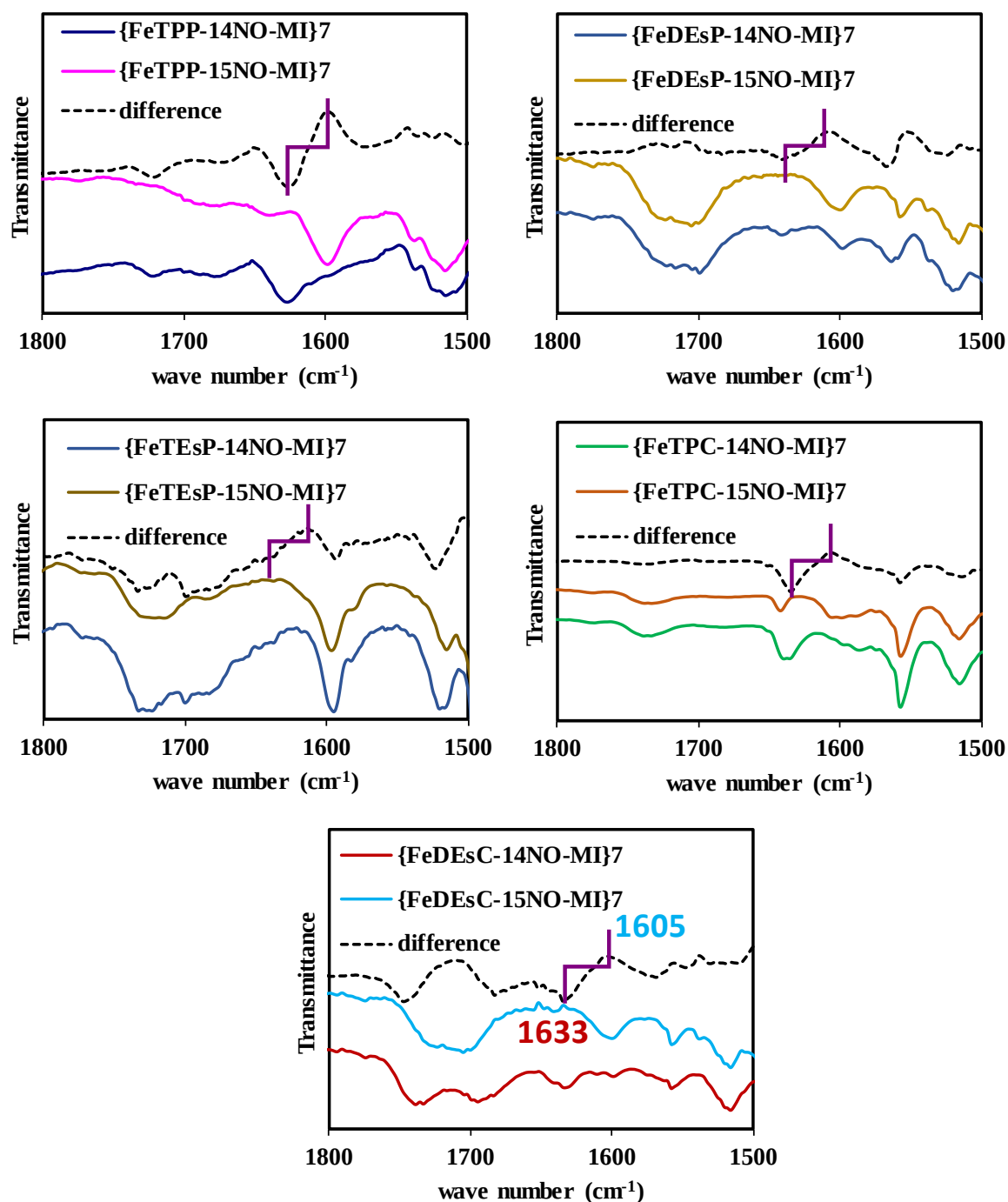


Figure S25A. FTIR data of the 6C- $\{\text{FeNO}\}^7$ adducts in dichloromethane at room temperature.

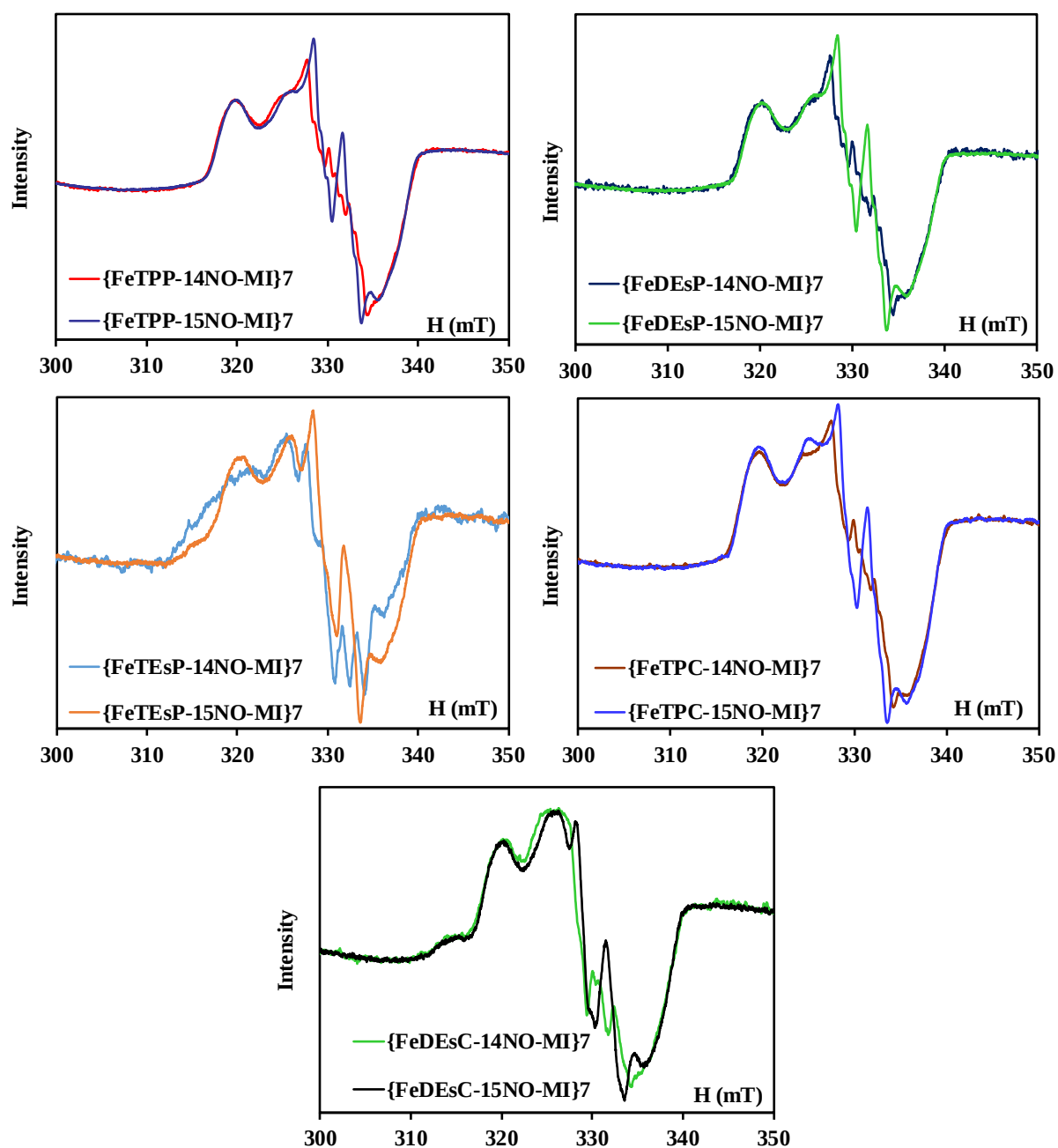


Figure S25B. EPR spectra of the N-methylimidazole bound 6C- $\{\text{FeNO}\}^7$ adducts in THF at 77K. Power: 1 mW, Modulation amplitude: 0.25 mT.

The super-hyperfine splitting constant A (mT) was determined from the double derivative of the EPR absorption data. The data for $\{\text{FeTPP-NO-MI}\}^7$ is shown below:

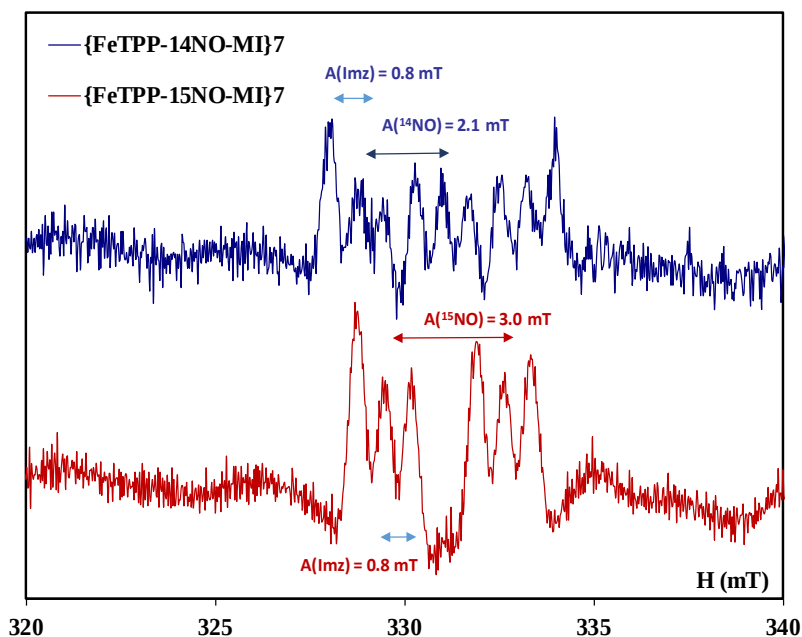


Figure S25C. Double derivative plot of the EPR absorption spectra of the N-methylimidazole bound 6C- $\{\text{FeTPP-NO}\}^7$ adduct in THF at 77K.

Table S1. Super-hyperfine splitting constant, A (mT) of the N-methylimidazole bound 6C- $\{\text{FeNO}\}^7$ adducts in THF at 77K				
	$A(^{14}\text{NO})$	$A(\text{Imz})$	$A(^{15}\text{NO})$	$A(\text{Imz})$
$\{\text{FeTPP-NO-MI}\}^7$	2.1	0.8	3.0	0.8
$\{\text{FeDEsP-NO-MI}\}^7$	2.2	0.7	3.1	0.7
$\{\text{FeTEsP-NO-MI}\}^7$	2.2	0.8	3.1	0.8
$\{\text{FeTPC-NO-MI}\}^7$	2.2	0.8	3.1	0.8
$\{\text{FeDEsC-NO-MI}\}^7$	2.2	0.7	3.0	0.7

5. N-O stretching frequency of the five-coordinate $\{\text{FeNO}\}^6$ species.

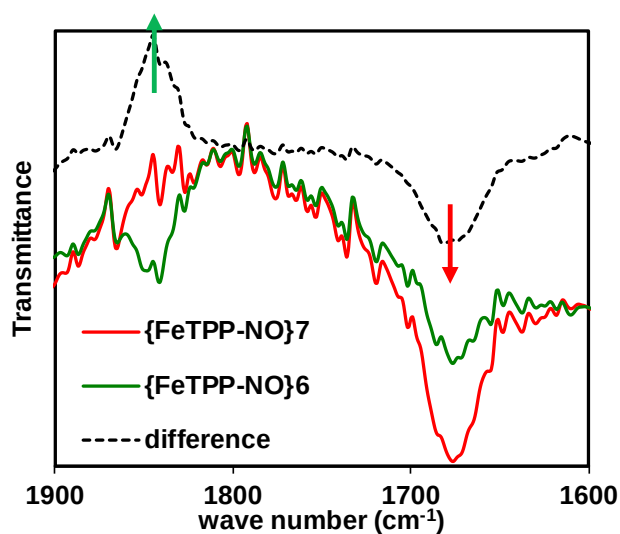


Figure S26. Spectroelectrochemistry data of the 5C- $\{\text{FeTPP-NO}\}^6$ adduct in dichloromethane at room temperature. Working electrode: Pt mesh; counter electrode: platinum; reference electrode: Ag wire; supporting electrolyte: tetrabutylammonium hexafluorophosphate (100 mM). Electrolysis potential was 0.20 V, versus Fc^+/Fc (reference).

6. N-O stretching frequency of the six-coordinate $\{\text{FeNO}\}^6$ species.

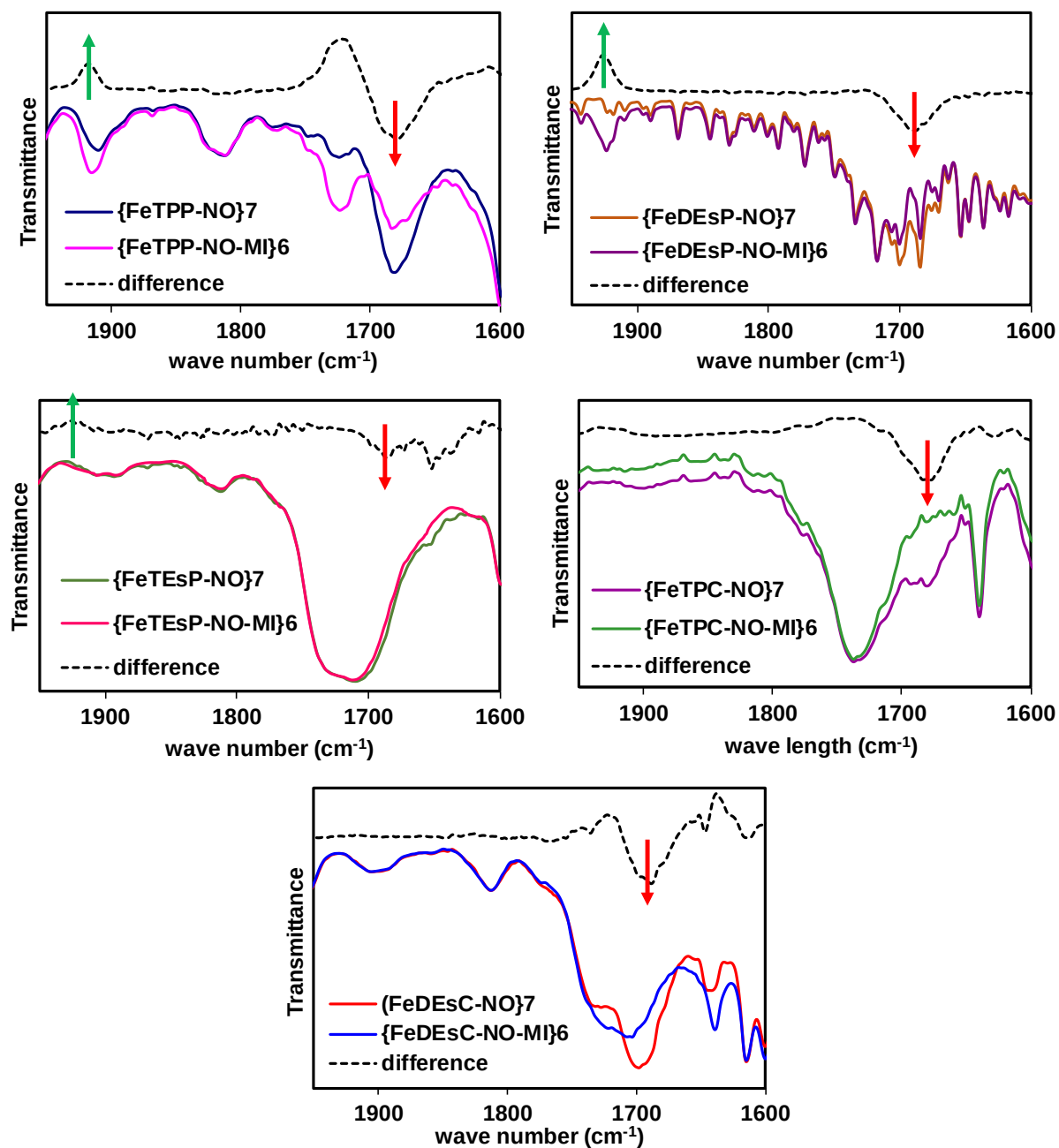


Figure S27. Spectroelectrochemistry data of the 6C- $\{\text{FeNO}\}^6$ adducts in dichloromethane at room temperature. Working electrode: Pt mesh; counter electrode: platinum; reference electrode: Ag wire; supporting electrolyte: tetrabutylammonium hexafluorophosphate (100 mM). Electrolysis potentials are 0.20, 0.34, 0.38, -0.04 and 0.10 V, respectively, vs Fc^+/Fc (reference) for the $\{\text{FeNO}\}^7$ species of FeTPP, FeDEsP, FeTEsP, FeTPC and FeDEsC, respectively.

7. N-O stretching frequency of the five-coordinate $\{\text{FeNO}\}^8$ species.

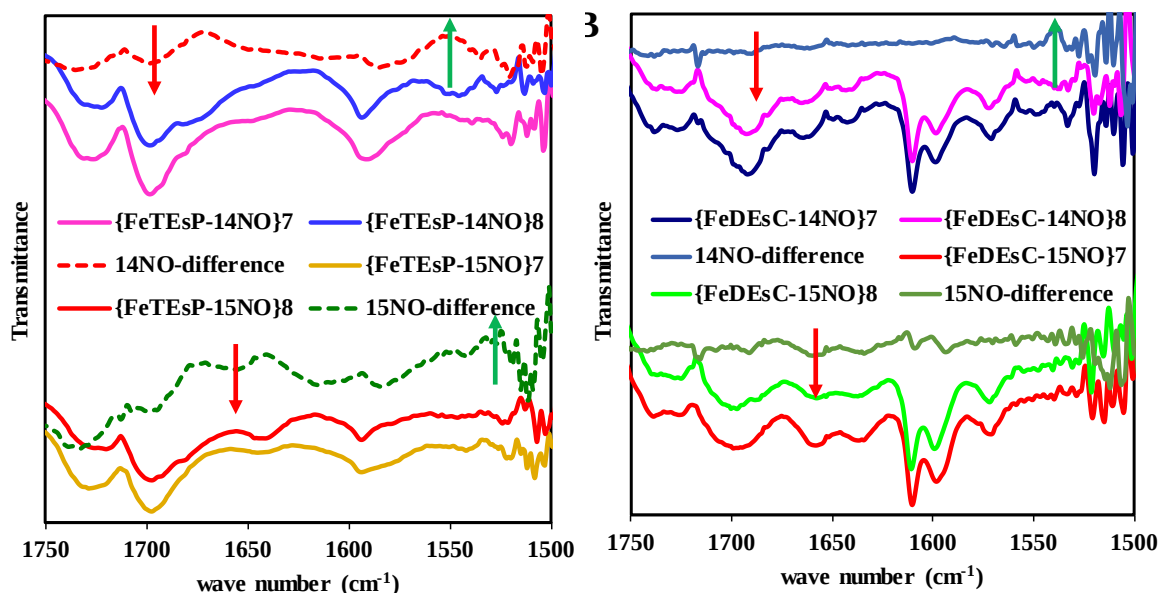


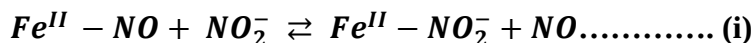
Figure S28. Spectroelectrochemistry data of the 5C- $\{\text{FeNO}\}^8$ adducts in THF at room temperature. Working electrode: Pt mesh; counter electrode: platinum; reference electrode: Ag wire; supporting electrolyte: tetrabutylammonium hexafluorophosphate (100 mM). Electrolysis potentials are -1.14 and -1.42 V, respectively, vs Fc^+/Fc (reference) for the species of FeTESP (A) and FeDEsC (B), respectively.

The $^{15}\text{N-O}$ vibration of FeDEsC-NO could not be observed because it is merged within the solvent vibrational peaks. Hence, the $^{14}\text{N-O}$ peak has been assigned considering the theoretically predicted value in the table below. The N-O frequency of the $\{\text{FeNO}\}^8$ species of other porphyrins could not be observed as they all might have merged into the intense solvent vibrational bands.

Table S2. Experimental and theoretical N-O stretching frequency (cm^{-1}) values				
	$\{\text{FeNO}\}^7$		$\{\text{FeNO}\}^8$	
	Experimental	Theoretical	Experimental	Theoretical
FeTESP	1688	1729	1550	1609
FeDEsC	1690	1713	1538	1586

8. Replacement of NO by NO₂⁻ from six-coordinate {FeNO}⁷ adducts: Estimation of NO dissociation constant

N-methylimidazole bound {FeNO}⁷ species were titrated against tetrabutylammonium nitrite. Replacement of NO by nitrite was considered:



The reaction was monitored by absorption spectra in UV-Vis region, which accompanied with distinct changes in absorption. From the absorbance data, the NO dissociation constant, K_d was calculated using the reported protocol.¹

$$K_d = \frac{[Fe^{II} - NO_2^-][NO]}{[Fe^{II} - NO][NO_2^-]} \dots \dots \dots (ii)$$

Where, [NO₂⁻] is the concentration of tetrabutylammonium nitrite in solution and r is defined as fraction of nitrite bound complex formed, then r is expressed as:

$$r = \frac{[NO_2^-]}{K_d + [NO_2^-]} \dots \dots \dots (iii)$$

The inverse of equation (iii) yields, a linear relationship between 1/r versus 1/[NO₂⁻], where the slope represents K_d of NO dissociation:

$$\frac{1}{r} = \frac{K_d}{[NO_2^-]} + 1 \dots \dots \dots (iv)$$

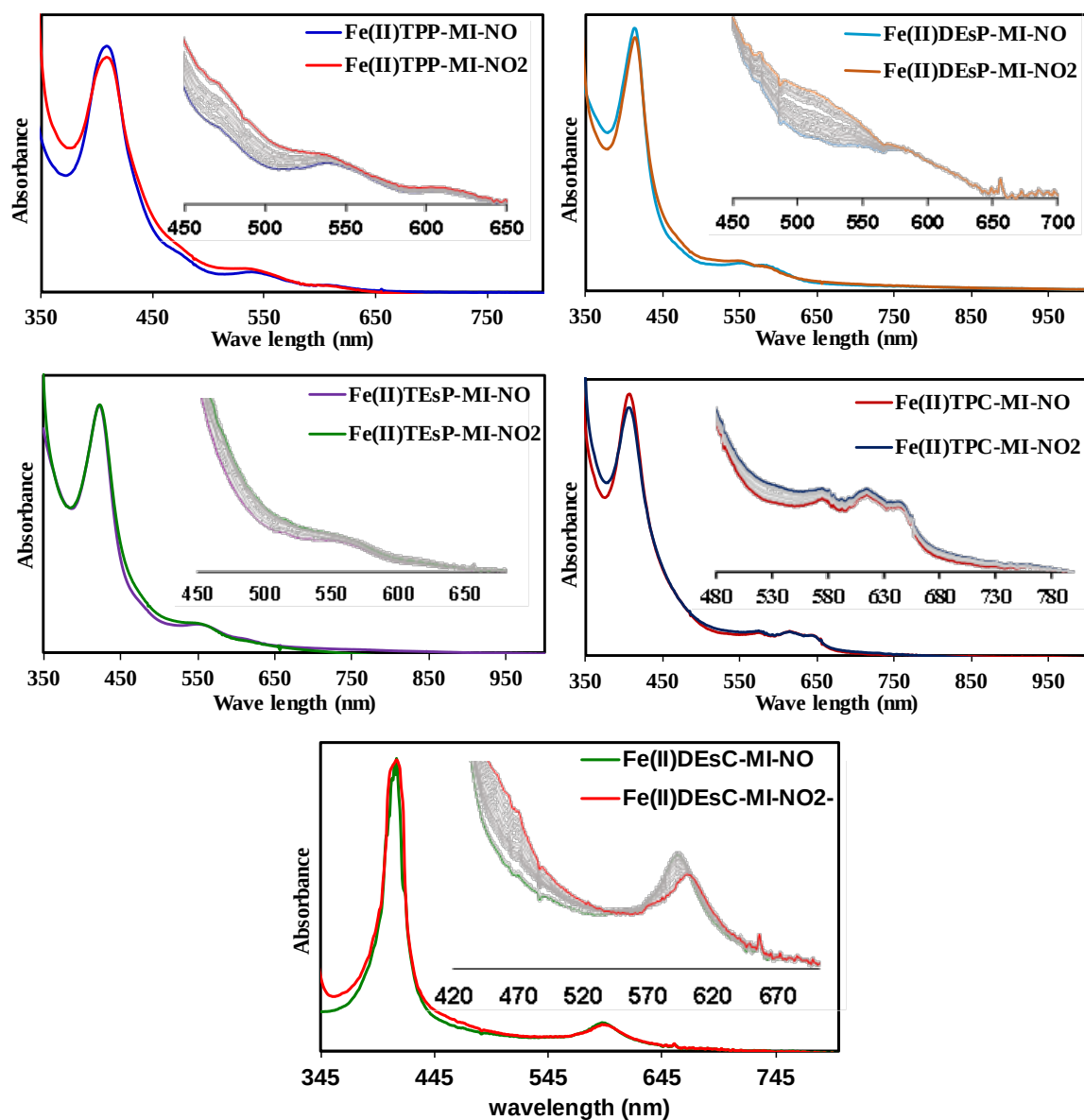


Figure S29. Titration of 6C- $\{\text{FeNO}\}^7$ species by tetrabutylammonium nitrite.

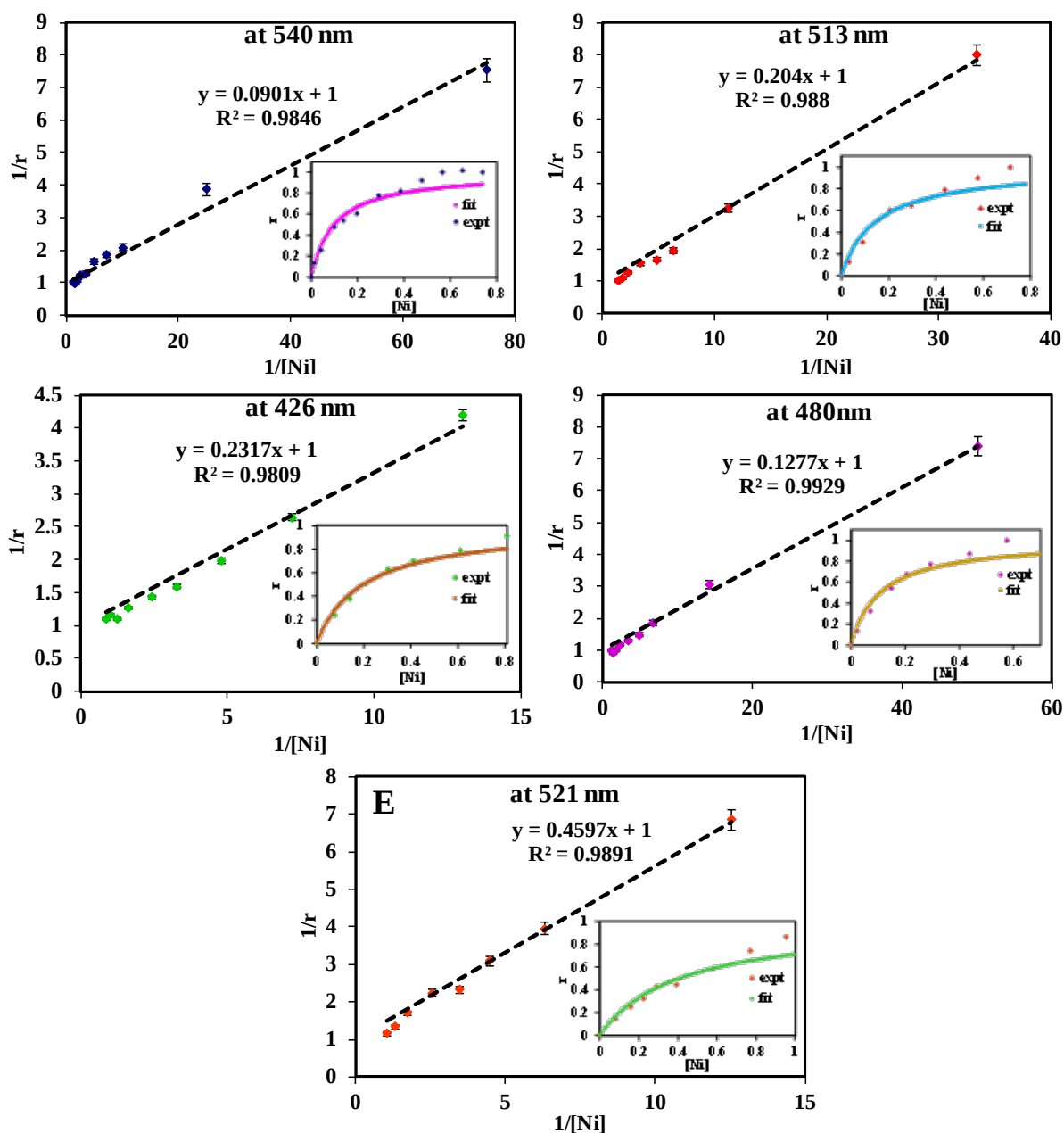


Figure S30. Determination of K_d from the titration of $6C-\{FeNO\}^7$ species by tetrabutylammonium nitrite. A, B, C, D, E represents $6C-\{FeTPP-NO\}^7$, $6C-\{FeDEsP-NO\}^7$, $6C-\{FeTEsP-NO\}^7$, $6C-\{FeTPC-NO\}^7$ and $6C-\{FeDEsC-NO\}^7$ respectively.

9. Ring ruffling

Ruffling parameters were obtained as per reported protocols.² Due to the lack of crystal structures of $\{\text{FeNO}\}^7$ complexes, we have calculated the ruffling parameters from the DFT optimized geometries. Actually, the ruffling parameters obtained from the DFT optimized structure of ZnDEsP, correlates with the crystal structure of ZnDEsP.

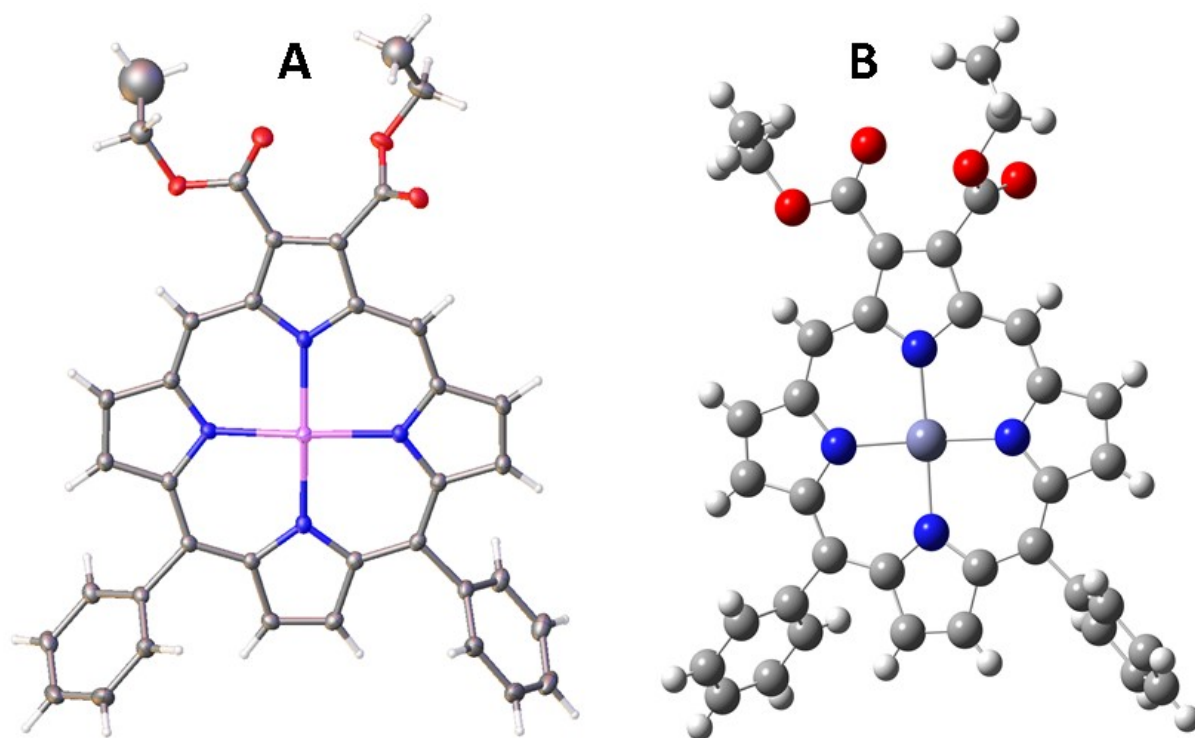


Figure S31. A) crystal structure of Zn DEsP; B) DFT optimized structure of ZnDEsP.

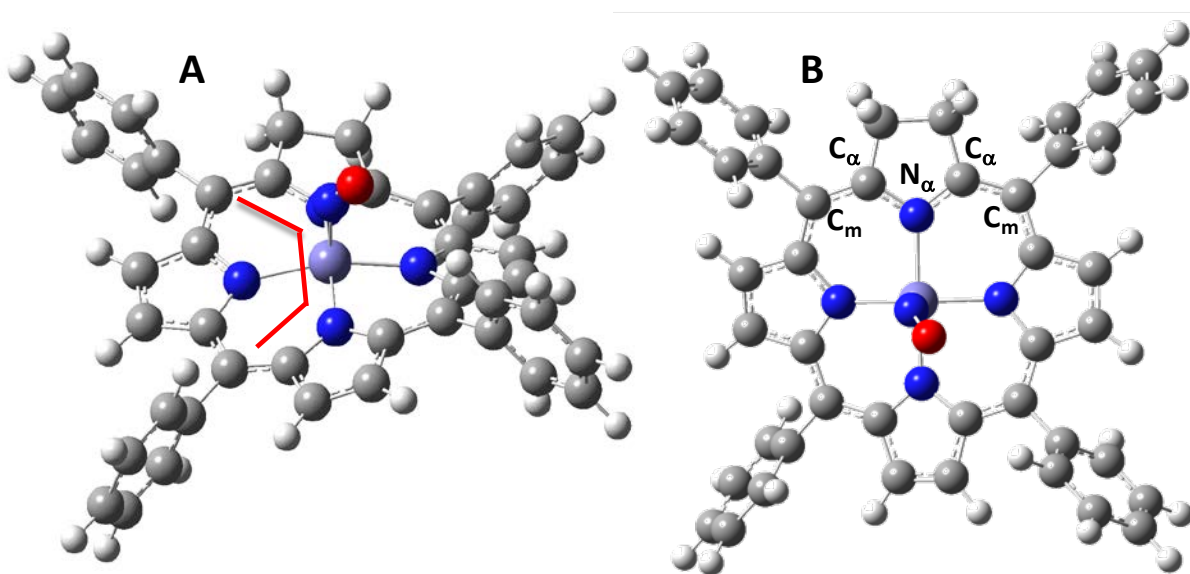


Figure S32. A) red line represents the C_{α} -N-N- C_{α} ruffling torsion angle of the $\{FeNO\}^7$ species; B) representation of the labelling of the atoms.

Table S3. Selected geometry parameters (Å, deg) between crystal structure and DFT optimized structure of ZnDEsP, averaged over the “symmetry unique” atoms

Complexes	ruffling	C_{α} -N- C_{α}^a	C_{α} -N- C_{α}^b	C_{α} - C_m - C_{α}^c	C_{α} - C_m - C_{α}^d	C_{β} - C_{β}^e	C_{β} - C_{β}^f	C_{α} - C_m	C_{α} - N^g	C_{α} - N^h	M- N^i	M- N^j
ZnDEsP (crystal)	3.22	107.3 4	106.4 5	126. 92	125. 35	1.3 7	1.3 5	1.4 0	1.3 7	1.3 7	2.0 6	2.0 4
ZnDEsP (DFT)	3.62	106.6 7	106.0 7	126. 45	124. 40	1.3 9	1.3 7	1.4 0	1.3 8	1.3 9	2.0 8	2.0 4

a. from unsymmetric pyrrole; b. rest symmetric pyrroles; c. from unsymmetric pyrrole; d. rest symmetric pyrroles; e. from unsymmetric pyrrole; f. rest symmetric pyrroles; g. from unsymmetric pyrrole; h. rest symmetric pyrroles; i. from unsymmetric pyrrole; j. rest symmetric pyrroles

Table S4. Selected geometry parameters (Å, deg) of the DFT optimized structures of $\{FeNO\}^7$ complexes, averaged over the “symmetry unique” atoms

Complexes	ruffling	C_{α} -N- C_{α}^a	C_{α} -N- C_{α}^b	C_{α} - C_m - C_{α}^c	C_{α} - C_m - C_{α}^d	C_{β} - C_{β}^e	C_{β} - C_{β}^f	C_{α} - C_m	C_{α} - N^g	C_{α} - N^h	M- N^i	M- N^j
$\{FeTPP-NO\}^7$	24.87	105.0 5	-	122.3 2	-	1.3 7	-	1.4 0	1.3 9	-	1.9 9	-
$\{FeDEsP-NO\}^7$	8.46	105.2 5	104.7 6	124.4 5	122.5 5	1.3 9	1.3 7	1.3 9	1.3 9	1.3 9	2.0 0	2.0 1
$\{FeTEsP-NO\}^7$	17.66	105.9 2	104.7 9	124.8 3	121.2 4	1.3 9	1.3 7	1.3 9	1.3 9	1.3 9	2.0 1	1.9 9

{FeTPC- NO} ⁷	27.10	108.4 1	105.2 1	122.9 9	122.1 1	1.5 5	1.3 7	1.3 9	1.3 8	1.3 8	2.0 4	1.9 8
{FeDEsC -NO} ⁷	25.48	108.6 0	105.0 1	124.5 7	122.3 0	1.5 7	1.3 7	1.3 8	1.3 7	1.3 9	2.0 4	1.9 9
a. from unsymmetric pyrrole; b. rest symmetric pyrroles; c. from unsymmetric pyrrole; d. rest symmetric pyrroles; e. from unsymmetric pyrrole; f. rest symmetric pyrroles; g. from unsymmetric pyrrole; h. rest symmetric pyrroles; i. from unsymmetric pyrrole; j. rest symmetric pyrroles												

10. Chemical identification of the {FeHNO}⁸ intermediate species from {FeDEsP-NO}⁷.

500 μ L of methanol and an excess amount of PPh₃ (5 equivalent) was added to 1 mM solution (d₆-DMSO) of {FeDEsP-NO}⁷ keeping in a NMR tube. It was then reduced by using 1 equivalent of cobaltocene. The colour changed immediately from bright red to reddish black. The sample was analysed by ³¹P-NMR and HRMS. The similar experiment was performed in 50 μ M scale with ¹⁵NO isotope and analysed by HRMS. The values obtained are clearly correlates with the previously reported values of Ph₃P=O and Ph₃P=NH, suggesting the reaction proceeds through the formation of {FeHNO}⁸ species.³

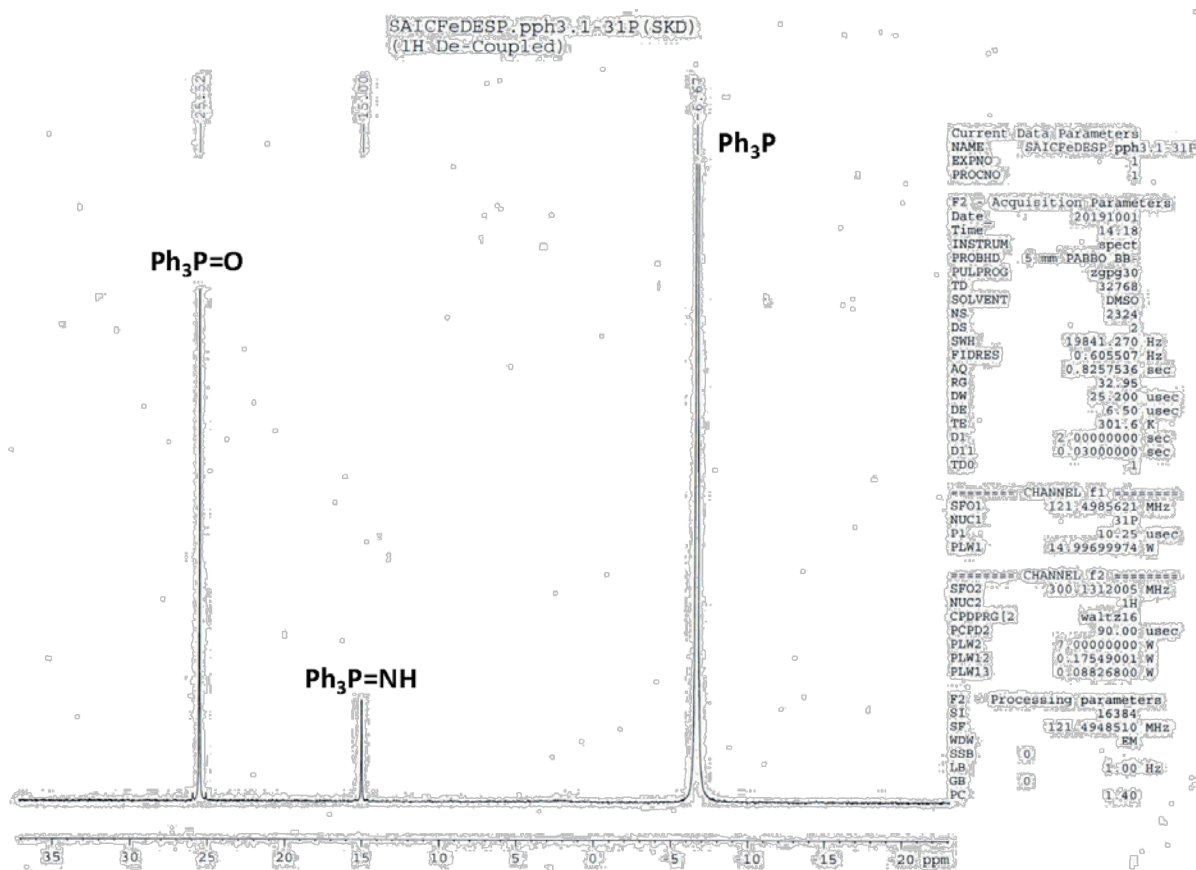


Figure S33. ³¹P-NMR spectrum

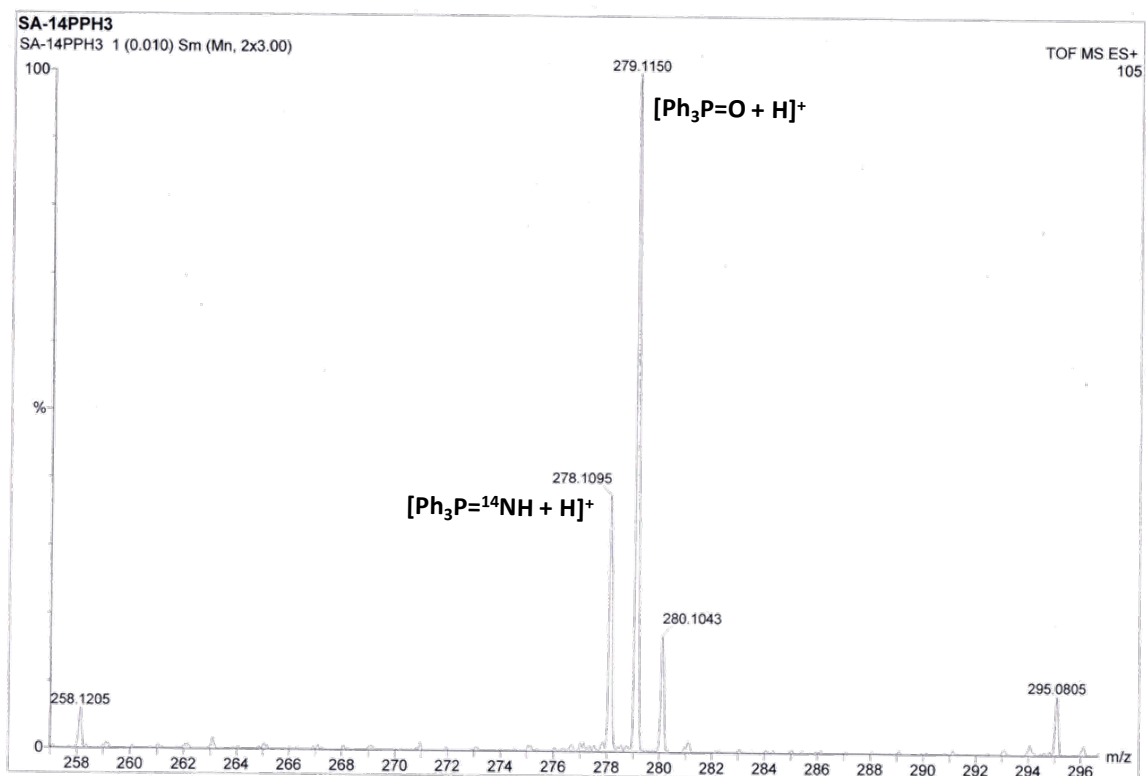


Figure S34. HRMS data of the sample containing {FeDESP-¹⁴NO}⁷ + cobaltocene + methanol

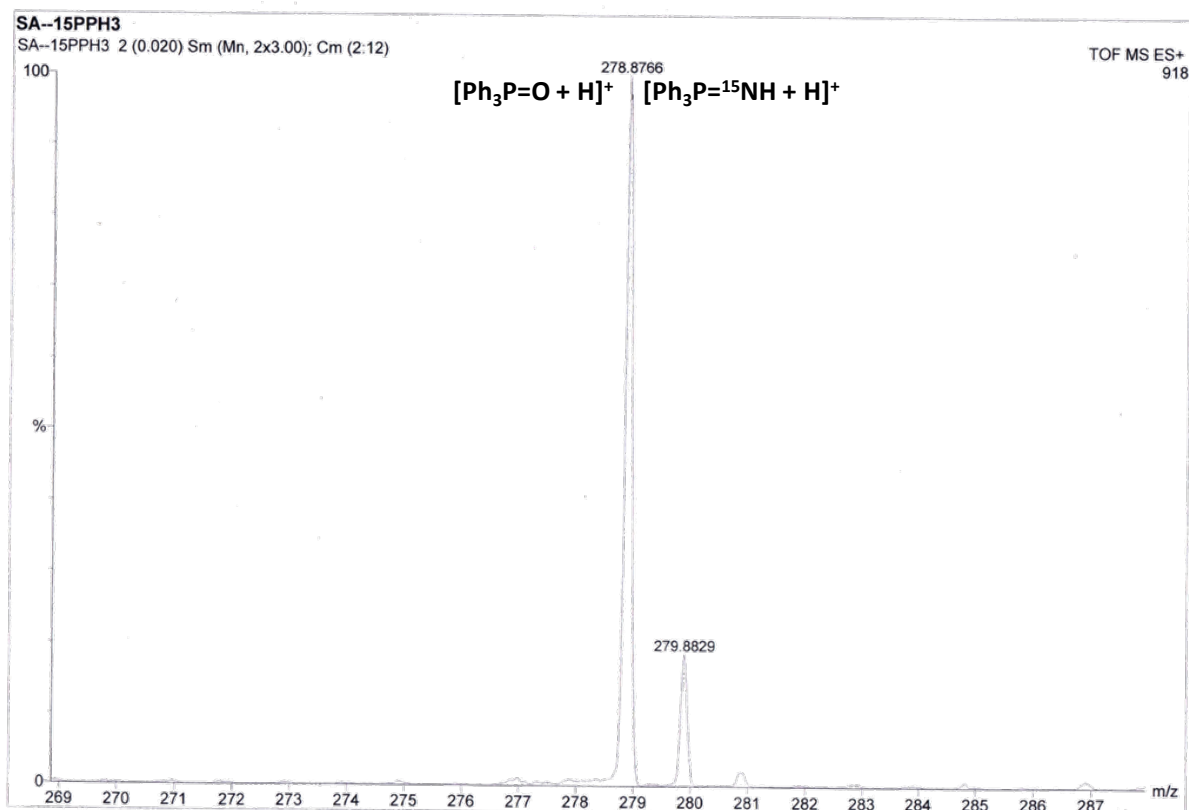


Figure S35. HRMS data of the sample containing $\{\text{FeDEsP-}^{15}\text{NO}\}^7$ + cobaltocene + methanol

11. References

1. Anne T. Marcoline; Timothy E. Elgren, Journal of Chemical Education, 1998, **75** (12), 1622-9278.
2. Vangberg, T.; Ghosh, A., Journal of the American Chemical Society, 1999, **121** (51), 12154-12160.
3. Rhine, M. A.; Rodrigues, A. V.; Urbauer, R. J. B.; Urbauer, J. L.; Stemmler, T. L.; Harrop, T. C., Journal of the American Chemical Society, 2014, **136** (36), 12560-12563.

12. Coordinates of the DFT optimized structures.

a. $\{\text{FeTPP-NO}\}^7$

Fe 3.89804100 12.94053100 3.37015500

N	3.37873600	14.87428400	3.43239000
N	2.34570400	12.59503500	2.19298300
N	4.07388100	10.98706800	3.67647700
N	5.10495900	13.26724700	4.94622100
N	5.00746600	12.94545700	2.09266700
C	1.32865600	14.86119800	2.02750500
C	2.73334400	10.17616800	1.75069400
C	5.60079300	10.93594300	5.64650900
C	5.22330100	15.74867100	4.85244800
C	4.13092200	15.90516400	3.98229200
C	2.32241900	15.50385000	2.78646300
C	1.37482200	13.48718200	1.73966000
C	2.06505300	11.39663600	1.54706900
C	3.64935800	9.99219700	2.79933500
C	4.87031600	10.32963600	4.61024500
C	5.71960900	12.33095500	5.76961100
C	5.60941000	14.49521500	5.35819600
C	3.54904000	17.18966800	3.65974800
H	3.94769200	18.15106000	3.98114000
C	2.41627800	16.93974300	2.93360600
H	1.70794700	17.65527300	2.51820100
C	0.44436000	12.81512700	0.86160100
H	-0.43529100	13.27772700	0.41631300

C	0.89293200	11.53008100	0.71348500
H	0.45020000	10.72230200	0.13224000
C	4.20912300	8.71345700	3.17201200
H	4.05027700	7.78149400	2.63150200
C	4.93665500	8.91667900	4.31357100
H	5.50304600	8.18740700	4.89110700
C	6.57988600	12.98436200	6.73139500
H	7.14594800	12.47556300	7.51025600
C	6.54701200	14.32233400	6.44567200
H	7.08288000	15.13061600	6.94134900
C	0.21836800	15.69021800	1.45826900
C	0.09240100	15.88494600	0.06455500
H	0.82652600	15.42546700	-0.60643400
C	-0.94821300	16.66831000	-0.45822700
H	-1.02650000	16.81310500	-1.54177000
C	-1.88023000	17.27062700	0.40285300
H	-2.69288100	17.88182400	-0.00559000
C	-1.76376100	17.08702100	1.79047100
H	-2.48829100	17.55092600	2.46945200
C	-0.72264000	16.30508700	2.31424100
H	-0.63543800	16.15705200	3.39638200
C	2.38049900	9.02084600	0.86621200
C	2.70233700	9.06476700	-0.50878700

H	3.22410700	9.94306200	-0.90427200
C	2.37511800	7.99402600	-1.35485400
H	2.63984000	8.04180900	-2.41728200
C	1.71607700	6.86434600	-0.84256900
H	1.45998800	6.02880600	-1.50370400
C	1.38451500	6.81236200	0.52138600
H	0.86133100	5.93911800	0.92753100
C	1.71318100	7.88159900	1.36922100
H	1.44104900	7.84666700	2.42997500
C	6.33472600	10.05150100	6.60778500
C	7.74692700	10.01725000	6.63735400
H	8.31032400	10.64571500	5.93886800
C	8.42456400	9.17839300	7.53561900
H	9.52037100	9.16065800	7.53985400
C	7.70251300	8.35876300	8.41873000
H	8.23180100	7.70389300	9.12001000
C	6.29832600	8.38107000	8.39624200
H	5.72712000	7.74660300	9.08354600
C	5.61986500	9.21866200	7.49742200
H	4.52445100	9.24021300	7.48385300
C	5.93545100	16.98115900	5.32388200
C	6.75499300	17.70774400	4.43225200
H	6.87030600	17.35039900	3.40296200

C	7.42248900	18.86731700	4.85660600
H	8.05883900	19.41530000	4.15239000
C	7.27918700	19.32152100	6.17784200
H	7.80017400	20.22696300	6.50880600
C	6.46172400	18.61067400	7.07192900
H	6.33689000	18.96296900	8.10224800
C	5.79384800	17.45088600	6.64848000
H	5.14557400	16.90439600	7.34259700
O	5.28433400	12.36044700	1.08937300

b. {FeTPP-NO}⁸

Fe	3.88489200	12.94634200	3.39884400
N	3.39472500	14.85445500	3.40180000
N	2.36029800	12.57816000	2.14608600
N	4.09936500	10.95888600	3.63868900
N	5.05726500	13.25381200	4.95420300
N	5.13354600	13.11100700	2.17462600
C	1.35136100	14.84087900	1.97462000
C	2.72784900	10.14750300	1.73233800
C	5.59319800	10.91454900	5.62648500
C	5.19904100	15.73271900	4.86474100
C	4.15171200	15.89249500	3.93961000
C	2.35668300	15.49000300	2.71816700

C	1.36438200	13.46178700	1.71714700
C	2.04433700	11.36782200	1.54607600
C	3.67074500	9.96573200	2.76755700
C	4.89657500	10.29729900	4.57301700
C	5.66849100	12.30842000	5.78624900
C	5.54700900	14.48179100	5.39988300
C	3.60814300	17.17744900	3.56150900
H	4.01391600	18.14193700	3.86582700
C	2.48318500	16.92378900	2.81871700
H	1.80363100	17.64305600	2.36138800
C	0.38976300	12.77440400	0.90124700
H	-0.51111300	13.22516300	0.48477800
C	0.82751600	11.48281800	0.76762300
H	0.34642400	10.66031900	0.23847000
C	4.26169100	8.69151400	3.11604200
H	4.12237300	7.76209600	2.56500500
C	4.99603000	8.89310300	4.25740300
H	5.58877000	8.16637300	4.81298300
C	6.48224800	12.96043900	6.78587700
H	7.02952100	12.44893800	7.57744000
C	6.44554200	14.30337500	6.51965300
H	6.95930800	15.10811100	7.04452000
C	0.24471000	15.67336600	1.40867800

C	0.04117400	15.78074600	0.01328000
H	0.72068200	15.24706100	-0.65992400
C	-1.00190500	16.56249300	-0.50800300
H	-1.13586000	16.63342000	-1.59446500
C	-1.86424400	17.25944500	0.35463200
H	-2.67886400	17.87080500	-0.05218800
C	-1.67165100	17.16835300	1.74353200
H	-2.34019300	17.70537500	2.42767100
C	-0.62923600	16.38529000	2.26303500
H	-0.48236600	16.30979200	3.34608800
C	2.34314300	8.99262000	0.86852600
C	2.48628000	9.07585500	-0.53809100
H	2.90009300	9.99480800	-0.96771700
C	2.12069600	8.00809200	-1.37136800
H	2.25028500	8.09861000	-2.45706000
C	1.60099100	6.82393000	-0.82088500
H	1.31785600	5.98737000	-1.47118300
C	1.44455500	6.72548800	0.57217500
H	1.02636800	5.81276700	1.01490400
C	1.80635800	7.79638100	1.40378800
H	1.66325600	7.72201000	2.48739300
C	6.33176000	10.03408700	6.58622300
C	7.74180700	10.07021600	6.68600900

H	8.29803900	10.75832500	6.04020600
C	8.42499300	9.23531100	7.58428800
H	9.51967900	9.27827300	7.63966700
C	7.71301700	8.34077500	8.40099600
H	8.24622500	7.68764200	9.10243300
C	6.31221600	8.28777500	8.30870400
H	5.74550900	7.59430700	8.94224300
C	5.63044200	9.12484900	7.41140900
H	4.53777500	9.08629700	7.34122600
C	5.91993800	16.95838600	5.33066900
C	6.74750000	17.67290300	4.43404100
H	6.85417500	17.29850800	3.41005900
C	7.42705400	18.83034900	4.84440100
H	8.06765600	19.36502300	4.13225500
C	7.29586900	19.29916700	6.16265200
H	7.82829000	20.20245600	6.48446700
C	6.47483100	18.60176100	7.06439000
H	6.35765400	18.96315000	8.09362900
C	5.79155300	17.44684000	6.65092900
H	5.14004800	16.91201500	7.35120200
O	6.01037600	13.95077600	2.16628600

c. {FeTPP-HNO}⁸

Fe	3.83913100	12.94152300	3.43586400
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N	3.34984200	14.85219800	3.45821600
N	2.33554400	12.57661900	2.18746800
N	4.07603600	10.97514600	3.65337100
N	5.04093600	13.25752000	4.97317200
N	5.04589400	13.08927100	2.21622300
C	1.32907700	14.84529300	2.00560200
C	2.71454500	10.15534700	1.74409900
C	5.59651100	10.92117400	5.62489700
C	5.18319800	15.73487000	4.88033800
C	4.10781400	15.88961800	3.99371700
C	2.31455800	15.48492200	2.77547100
C	1.36666100	13.46942900	1.72684600
C	2.03736600	11.37294200	1.55225300
C	3.65487700	9.97782300	2.77308100
C	4.89241000	10.31652900	4.57008100
C	5.67162100	12.31403300	5.78290000
C	5.55103400	14.48294700	5.39500100
C	3.54906700	17.17366000	3.63574900
H	3.95588300	18.13583000	3.94411800
C	2.42448000	16.92188100	2.89875200
H	1.73303200	17.63729200	2.45550300
C	0.42603700	12.79689200	0.86004500
H	-0.45231500	13.26239300	0.41507800

C	0.86024900	11.50616400	0.72496300
H	0.40575400	10.69561000	0.15690300
C	4.24980300	8.70630500	3.11730100
H	4.10108900	7.77781200	2.56799900
C	4.99003700	8.91080700	4.25021700
H	5.57954700	8.18626400	4.81051100
C	6.51690000	12.96467400	6.75958200
H	7.08320200	12.44988000	7.53435700
C	6.47970500	14.30468700	6.48770000
H	7.00682400	15.11197600	6.99424300
C	0.23090200	15.67865700	1.41950500
C	0.11328300	15.85732200	0.02292700
H	0.84602400	15.38231200	-0.63870900
C	-0.91709300	16.64402600	-0.51491700
H	-0.98845300	16.77632100	-1.60056100
C	-1.84783000	17.26556400	0.33378500
H	-2.65258000	17.87930600	-0.08635000
C	-1.73997600	17.09794000	1.72412600
H	-2.46349900	17.57690500	2.39367600
C	-0.70866400	16.31316500	2.26271800
H	-0.62794600	16.17796700	3.34701400
C	2.34045600	8.99211400	0.87795900
C	2.59960000	9.02687800	-0.51052000

H	3.08849900	9.90874400	-0.93949500
C	2.24738800	7.94673200	-1.33432100
H	2.46346100	7.98991100	-2.40790100
C	1.62427100	6.81405800	-0.78536900
H	1.34828000	5.97083100	-1.42842300
C	1.35354500	6.77002900	0.59222900
H	0.85777200	5.89493800	1.02766900
C	1.70769500	7.84913000	1.41672900
H	1.48276800	7.81945300	2.48851500
C	6.34706600	10.03570200	6.57321300
C	7.75944000	10.03151500	6.60888800
H	8.31218700	10.68589600	5.92580300
C	8.45124900	9.19152300	7.49540700
H	9.54716100	9.19793100	7.50511100
C	7.74327100	8.34108500	8.36054700
H	8.28353300	7.68576400	9.05301800
C	6.33906900	8.33328400	8.33159800
H	5.77877700	7.67444500	9.00484400
C	5.64661000	9.17166800	7.44421500
H	4.55108400	9.16918700	7.42511100
C	5.91464800	16.96162200	5.33501000
C	6.77277700	17.63691700	4.43966600
H	6.89982100	17.24131800	3.42604000

C	7.46183600	18.79077400	4.84456700
H	8.12818900	19.30024200	4.13913400
C	7.30229100	19.28834200	6.14839500
H	7.84043600	20.18932900	6.46390000
C	6.44764400	18.62669200	7.04543000
H	6.31165900	19.01277200	8.06217600
C	5.75755300	17.47257400	6.64190600
H	5.08152100	16.96318000	7.33788700
O	5.95290800	13.92483300	2.07285800
H	5.01794900	12.35501900	1.46031400

d. {FeDEsP-NO}⁷

C	2.78046000	-3.47529700	-0.13804500
C	3.91356300	-2.79623700	0.21459900
C	3.66333300	-1.40071700	-0.05917700
C	1.83384900	-2.48829500	-0.62052400
C	0.52131000	-2.79828000	-1.01339500
C	4.60490700	-0.40574900	0.16468300
C	4.42776400	0.93847800	-0.15884000
C	5.45733400	1.95189300	-0.04449200
C	4.91531200	3.11776100	-0.57201900
C	3.56824600	2.79320800	-0.98787400
C	2.69018700	3.70996300	-1.56263600
C	1.38341900	3.41929200	-1.92646700

C	0.49151100	4.39736100	-2.50409200
C	-0.71429100	3.77641600	-2.67567000
C	-0.55316600	2.41241700	-2.20943700
C	-1.57400300	1.44884600	-2.26374900
C	-1.35191200	0.09627600	-1.95423400
C	-2.36160500	-0.92990400	-2.10458600
C	-1.76425800	-2.12000700	-1.79642800
C	-0.40091800	-1.81782000	-1.41575700
H	4.84680000	-3.18888500	0.62174500
H	2.58125700	-4.54398600	-0.07319700
H	-2.19685900	-3.11912500	-1.81992900
H	-3.38687900	-0.75218500	-2.42557400
H	-1.63350400	4.18180900	-3.09619600
H	0.77428100	5.42361200	-2.74352500
N	3.27570700	1.46219800	-0.73196000
N	2.38755100	-1.21487900	-0.57938200
N	-0.15113900	-0.45374700	-1.51942700
N	0.74512900	2.19390500	-1.76673400
H	3.07442900	4.71554400	-1.74982400
H	5.55865500	-0.69643300	0.60865800
Fe	1.49612900	0.55020700	-0.90641100
C	-2.93533900	1.87943000	-2.72009900
C	-3.45250400	1.45393600	-3.96394600

C	-3.72211800	2.73349300	-1.91593600
C	-4.72406300	1.86864000	-4.38957500
H	-2.84387100	0.80266100	-4.60109400
C	-4.99433500	3.14617900	-2.34189100
H	-3.33032700	3.06541700	-0.94803700
C	-5.49909100	2.71477600	-3.57949900
H	-5.10729400	1.53370800	-5.36015500
H	-5.59356200	3.80405800	-1.70227100
H	-6.49186600	3.03783200	-3.91222200
C	0.08721300	-4.23339900	-0.98935800
C	0.62050600	-5.15945400	-1.91284400
C	-0.85715800	-4.68830400	-0.04271100
C	0.21882000	-6.50423100	-1.89105000
H	1.34813500	-4.81398700	-2.65577500
C	-1.25789800	-6.03340400	-0.02154600
H	-1.26911400	-3.97889900	0.68368100
C	-0.72147300	-6.94526500	-0.94550200
H	0.63899000	-7.20770800	-2.61881900
H	-1.98786900	-6.37008300	0.72334100
H	-1.03468000	-7.99514900	-0.92846700
C	6.87081300	1.75618700	0.38293800
C	5.51721800	4.47215400	-0.66719700
O	7.84273300	2.25928300	-0.16679900

O	6.96569500	0.92864400	1.47063600
C	8.32749300	0.68602800	1.93058700
H	8.90915500	0.24175700	1.10329500
H	8.79155700	1.65751600	2.17545200
C	8.24380900	-0.23219600	3.14101100
H	7.78695800	-1.20165200	2.87753800
H	9.25819800	-0.42517700	3.53224300
H	7.64358200	0.22671300	3.94486300
O	5.24868600	5.30441900	-1.53346300
O	6.38723300	4.70126000	0.35045400
C	7.09609300	5.97116900	0.28310600
H	6.35878000	6.79164300	0.34469200
H	7.59563300	6.04369800	-0.69874400
C	8.08704500	5.99286800	1.43726200
H	8.79666100	5.15256700	1.35448800
H	8.65881700	6.93741800	1.42180000
H	7.56733000	5.91850900	2.40796300
N	1.07591700	0.90691400	0.69133500
O	1.43099600	1.44903900	1.69048300

e. {FeDEsP-NO}⁸

C	2.80272500	-3.46742400	-0.07932100
C	3.87159700	-2.75793100	0.39358900
C	3.60556400	-1.35970900	0.11975000

C	1.86309300	-2.49840000	-0.61608700
C	0.57727700	-2.81873100	-1.06655000
C	4.51604600	-0.35490700	0.41516200
C	4.40568700	0.97727400	-0.01582100
C	5.45656300	1.97147300	0.05709400
C	4.97460600	3.09372900	-0.65439700
C	3.65569800	2.74564900	-1.10549200
C	2.79168600	3.61671400	-1.78652300
C	1.47418600	3.33556800	-2.09277700
C	0.58927300	4.30446700	-2.70246700
C	-0.64897400	3.73124900	-2.76230400
C	-0.52048000	2.38990000	-2.21767300
C	-1.56427300	1.45650100	-2.19583400
C	-1.35197900	0.09217500	-1.89915000
C	-2.35587700	-0.92983500	-2.03980200
C	-1.73261100	-2.13185500	-1.79633400
C	-0.36912700	-1.83725900	-1.44521400
H	4.78063800	-3.12989300	0.87157500
H	2.63744400	-4.54442300	-0.04993500
H	-2.16408200	-3.13141900	-1.84341100
H	-3.39568800	-0.75593200	-2.31375500
H	-1.57146000	4.14967500	-3.16466700
H	0.90025500	5.29990600	-3.02614500

N	3.30714700	1.46363700	-0.71104800
N	2.37154000	-1.20666000	-0.49765400
N	-0.13072400	-0.46522400	-1.51976700
N	0.79104800	2.14313700	-1.81911100
H	3.19665000	4.59234500	-2.06738100
H	5.42754400	-0.63602200	0.94435200
Fe	1.49231200	0.54046400	-0.93800900
C	-2.93615400	1.91860000	-2.57303100
C	-3.58245500	1.45196800	-3.74098900
C	-3.61686800	2.86002200	-1.76686500
C	-4.86514600	1.90468500	-4.08730600
H	-3.05981700	0.73391700	-4.38249600
C	-4.89834300	3.31609500	-2.11390300
H	-3.12596900	3.22359700	-0.85748400
C	-5.52958200	2.83888200	-3.27465000
H	-5.34378500	1.53275700	-5.00158100
H	-5.40822600	4.04342100	-1.47035900
H	-6.53141800	3.19353700	-3.54532700
C	0.17301800	-4.25962900	-1.10002400
C	0.79236400	-5.16379700	-1.99319200
C	-0.82570100	-4.76140400	-0.23349200
C	0.42896400	-6.51986700	-2.01885200
H	1.56410000	-4.78613600	-2.67324400

C	-1.19382600	-6.11545800	-0.26129700
H	-1.30472500	-4.07373100	0.47213500
C	-0.56767300	-7.00171600	-1.15423700
H	0.92278600	-7.20110100	-2.72267200
H	-1.96724200	-6.48185700	0.42485100
H	-0.85371900	-8.06022200	-1.17489900
C	6.83142800	1.79763400	0.54671900
C	5.56879900	4.42801300	-0.81096400
O	7.84268500	2.34172800	0.10045800
O	6.90692900	0.91510000	1.61859400
C	8.24734700	0.67668500	2.09773900
H	8.86607400	0.26415300	1.27850800
H	8.70543400	1.63901600	2.39218000
C	8.14673500	-0.28566600	3.27564800
H	7.70454900	-1.24860500	2.96606300
H	9.15147600	-0.48347800	3.69167900
H	7.51543200	0.13851100	4.07545800
O	5.36368500	5.21877400	-1.73964900
O	6.38745400	4.74885500	0.24492700
C	7.13067500	5.97524400	0.09158300
H	6.43314300	6.83471300	0.10150800
H	7.63477400	5.97591500	-0.89205800
C	8.12897100	6.03417500	1.24185000

H	8.78486300	5.14771200	1.21762600
H	8.75205700	6.94390700	1.16399900
H	7.60823500	6.05132100	2.21541200
N	0.87718100	0.90802600	0.63864700
O	-0.08771300	1.54411100	0.98836600

f.{FeDEsP-HNO}⁸

C	2.76901600	-3.48217800	-0.07696400
C	3.85498300	-2.78946900	0.38319400
C	3.62110200	-1.39815900	0.07540800
C	1.85595500	-2.50695600	-0.63816700
C	0.57553100	-2.82269000	-1.11985400
C	4.54459000	-0.39534700	0.33951900
C	4.41896100	0.92430200	-0.09692300
C	5.46546100	1.92403600	-0.01493600
C	4.98421800	3.04288300	-0.68660000
C	3.64929900	2.71179300	-1.13454800
C	2.79879300	3.60349900	-1.78783000
C	1.47420000	3.33474400	-2.09871500
C	0.57837200	4.32507100	-2.65048800
C	-0.66168300	3.75166700	-2.70118000
C	-0.51260200	2.39390600	-2.21450800
C	-1.55317400	1.45216700	-2.20365700
C	-1.32222200	0.09251200	-1.94768400

C	-2.32771300	-0.93371900	-2.11391900
C	-1.70968100	-2.13232400	-1.89185300
C	-0.34193400	-1.83956600	-1.52240900
H	4.75331400	-3.17242000	0.87029200
H	2.57855900	-4.55370500	-0.03251900
H	-2.13576900	-3.13279300	-1.95169800
H	-3.36365400	-0.74932200	-2.39410300
H	-1.59620300	4.18105800	-3.05991100
H	0.87906800	5.33284700	-2.94151500
N	3.31048200	1.41489000	-0.77605200
N	2.38996900	-1.22466000	-0.55531600
N	-0.09869700	-0.46778200	-1.58277300
N	0.80499600	2.13542700	-1.86067100
H	3.20798300	4.58411400	-2.04304800
H	5.45693700	-0.66712900	0.87388200
Fe	1.52977900	0.50413000	-1.02403000
C	-2.93831400	1.91635400	-2.53680500
C	-3.56064700	1.55848000	-3.75296100
C	-3.64115400	2.74052700	-1.63057100
C	-4.85653600	2.00784700	-4.05184900
H	-3.01577600	0.93286500	-4.46881800
C	-4.93738700	3.18770200	-1.93029600
H	-3.16463500	3.01759000	-0.68384500

C	-5.54912100	2.82223100	-3.14078000
H	-5.32311100	1.72487600	-5.00229600
H	-5.47187800	3.82105600	-1.21318200
H	-6.56088400	3.17234100	-3.37424200
C	0.16254200	-4.26418800	-1.15280500
C	0.74163400	-5.15106600	-2.08669900
C	-0.79894600	-4.76572500	-0.24785900
C	0.36501400	-6.50302400	-2.11823800
H	1.48584300	-4.76962000	-2.79475500
C	-1.17400000	-6.11800000	-0.27943900
H	-1.24528800	-4.08705700	0.48755900
C	-0.59391500	-6.99032700	-1.21504200
H	0.82041500	-7.17602000	-2.85360400
H	-1.91843400	-6.49129200	0.43300600
H	-0.88724200	-8.04581700	-1.23955200
C	6.84306300	1.73655300	0.51632900
C	5.62419200	4.36833700	-0.88113800
O	7.86531400	2.15251500	-0.01444800
O	6.84158200	1.02112100	1.68697200
C	8.16320700	0.78379800	2.25321400
H	8.77515600	0.23698800	1.51383400
H	8.65007100	1.75944300	2.42707800
C	7.97299900	-0.00134200	3.54287800

H	7.49029100	-0.97506900	3.35083100
H	8.95453000	-0.19072000	4.01192200
H	7.34932400	0.55964900	4.25953300
O	5.40881200	5.12263500	-1.82979500
O	6.46391700	4.67122500	0.14336600
C	7.21483300	5.90793500	-0.01694000
H	6.50494900	6.75459300	-0.02906500
H	7.72515900	5.88589000	-0.99555800
C	8.19584700	5.98922500	1.14328100
H	8.87384200	5.11939500	1.13694800
H	8.80207100	6.90817800	1.05746600
H	7.66567900	6.01356000	2.11095300
N	0.98978200	0.85746700	0.57457200
O	-0.10671400	1.27226000	0.97956700
H	1.69772100	0.70103500	1.33983400

g. {FeTEsP-NO}⁷

O	7.08212000	4.02967500	8.51845200
O	8.28656000	2.58595200	9.82701500
N	11.06051300	8.32557400	8.94167600
O	7.87719000	9.31310200	12.08470900
N	11.13084600	5.72190300	7.95544800
N	12.95604300	9.13351200	6.96957800
O	9.17912700	1.51400000	7.30444200

O	9.26923900	7.74854400	13.01032300
N	13.20132400	6.52572400	6.15089700
O	11.45664600	1.47862900	7.16893700
C	11.41981100	4.47837900	7.43399500
C	9.47545100	4.20111000	8.57966000
C	10.10102600	7.77782800	9.79780800
C	14.11766700	7.05623900	5.25395600
C	9.48474300	6.51855000	9.62867900
C	14.35597200	8.42669900	5.04652200
C	13.32306000	5.14911000	6.01060800
C	9.97651500	5.55923700	8.71897900
C	12.49692200	4.19732300	6.59064700
H	12.66415800	3.15116000	6.32961400
C	10.40875000	3.51134400	7.82008100
C	9.79957800	8.71619800	10.86627300
C	10.54438300	9.85943800	10.61784700
C	8.14525600	3.63169000	8.97349800
C	15.28324200	8.83949500	3.94737300
C	8.29586400	6.17906400	10.47055800
C	8.97009400	8.50553400	12.09785400
C	13.79184000	9.39947300	5.88753000
C	11.28422900	9.61108000	9.39841600
C	12.77547400	10.36396700	7.58858600

C	14.36180900	4.81595700	5.06205500
H	14.65955000	3.79861700	4.80293900
C	14.84695000	5.99971400	4.57911700
H	15.63850100	6.16348700	3.84906700
C	12.05215800	10.57895500	8.75124600
H	12.04145600	11.58080400	9.18724300
C	10.25592900	2.09370800	7.40862800
C	16.51185300	9.47880600	4.22882900
H	16.79100000	9.66455100	5.27190800
O	10.29972500	10.88375700	12.72702600
C	13.47921800	11.40817400	6.88253700
H	13.48632600	12.45765400	7.18076100
C	14.09039600	10.81613700	5.81143600
H	14.70611700	11.27919700	5.04167200
O	11.01855900	12.19456300	11.00597400
C	8.37962100	5.20159700	11.48501800
H	9.33735400	4.70971700	11.67967300
C	14.94794600	8.58230000	2.59886200
H	13.99490900	8.09256200	2.37025600
C	17.02910200	9.60103000	1.85326200
H	17.70428100	9.89729300	1.04273200
C	17.37658000	9.85636800	3.19007800
H	18.32818200	10.34539300	3.42738100

C	10.64457300	11.09848000	11.42509700
C	7.06615600	6.83540000	10.24902700
H	6.99544000	7.58856600	9.45767300
C	15.81280200	8.96227000	1.56108200
H	15.53214000	8.76245300	0.52079700
C	7.05522600	1.85861700	10.10273100
H	6.59858700	1.57479200	9.13936300
H	6.35981100	2.53823400	10.62680700
C	11.35300900	0.08332500	6.76084500
H	10.80486900	-0.46996500	7.54331700
H	10.75379700	0.02719700	5.83476200
C	7.25450200	4.88628600	12.26012500
H	7.33871500	4.14183600	13.05965200
C	7.04687500	9.23234500	13.27844900
H	7.66748900	9.49278400	14.15437100
H	6.71146300	8.18796900	13.40025400
C	6.02785200	5.52746500	12.01825000
H	5.14560500	5.27014000	12.61573700
C	12.76782800	-0.44287500	6.56883600
H	13.35180500	-0.35687300	7.50092700
H	12.73208900	-1.50780500	6.27936000
H	13.29657800	0.11062300	5.77368300
C	5.93617700	6.50174000	11.01000100

H	4.98014700	6.99747400	10.80786000
C	7.42673900	0.64662900	10.94423200
H	7.89684500	0.95029300	11.89559500
H	6.52027200	0.06056400	11.17747400
H	8.13106300	-0.00452400	10.39947800
C	5.88354600	10.19396000	13.08654300
H	5.22682200	10.16979600	13.97409000
H	6.24088600	11.22857300	12.94705800
H	5.28308400	9.91412200	12.20425400
C	10.39417800	12.05418900	13.58900600
H	9.61748100	12.77906300	13.28479000
H	11.37537400	12.53196800	13.42482200
C	10.21488600	11.58394600	15.02475300
H	10.29367400	12.44635000	15.70997900
H	9.22729500	11.11488800	15.17355700
H	10.99054600	10.84915900	15.29858000
Fe	11.90593300	7.49274400	7.33475700
O	10.16445200	8.85712400	5.71130000
N	10.69902900	7.93087400	6.23347400

h. {FeTEsP-NO}⁸

O	7.06830600	4.07351000	8.47240700
O	8.24356900	2.59771500	9.76535200
N	11.04439600	8.35819800	8.95114900

O	7.90875000	9.34928800	12.14244700
N	11.14627100	5.73607400	7.98745300
N	12.95409800	9.14889200	6.98845800
O	9.27338200	1.48592700	7.33944400
O	9.22547600	7.69185100	13.00518400
N	13.22306800	6.54136300	6.21872300
O	11.55429700	1.48030300	7.30096000
C	11.47429200	4.47284700	7.52265400
C	9.47240300	4.22775300	8.57437100
C	10.08662000	7.80647500	9.80282200
C	14.10541000	7.07113500	5.28288200
C	9.44590200	6.55879400	9.60048000
C	14.30983900	8.44153300	5.04203900
C	13.38358300	5.15694600	6.11208200
C	9.96364300	5.58519400	8.71056200
C	12.57988000	4.20012900	6.71022100
H	12.78064000	3.15315100	6.47654600
C	10.45876800	3.51124600	7.88669800
C	9.80638700	8.72392300	10.89334100
C	10.56465900	9.87369700	10.65887000
C	8.13534600	3.67193300	8.92143400
C	15.18825400	8.84672100	3.90385400
C	8.23733500	6.23301300	10.41765200

C	8.98180900	8.49601300	12.11379200
C	13.76020600	9.42153500	5.88936400
C	11.29714000	9.63201700	9.43797400
C	12.78588700	10.38112400	7.62014700
C	14.41685200	4.83167200	5.15795200
H	14.73958600	3.81552700	4.92062100
C	14.85305200	6.01457100	4.62527200
H	15.62664000	6.17812100	3.87537100
C	12.08020400	10.59215300	8.79484500
H	12.09062200	11.59081400	9.23845100
C	10.33011700	2.10057000	7.48688700
C	16.39568300	9.55368700	4.11189200
H	16.69390400	9.80036900	5.13688500
O	10.34032100	10.84057300	12.80265200
C	13.46525700	11.42677800	6.89698800
H	13.47266900	12.47733100	7.19502500
C	14.04551700	10.84147100	5.80215000
H	14.63065300	11.31281900	5.01317300
O	11.10985300	12.18408600	11.12937900
C	8.27022500	5.23377200	11.41624700
H	9.20911300	4.70616300	11.60909400
C	14.83279400	8.51624500	2.57494600
H	13.89636100	7.97498000	2.40131000

C	16.84290900	9.59219500	1.71803100
H	17.48063600	9.88186900	0.87427200
C	17.21188400	9.92511300	3.03216800
H	18.14562000	10.46930100	3.21990700
C	10.69996300	11.07712600	11.49240500
C	7.02789100	6.93145200	10.20649200
H	6.99260200	7.70398500	9.43134300
C	15.65027300	8.88363400	1.49507800
H	15.34919200	8.62184000	0.47340700
C	7.00310100	1.88786600	9.98914800
H	6.53627900	1.67034400	9.01264200
H	6.31594000	2.54392400	10.55526000
C	11.46540800	0.09988700	6.87924500
H	10.88747000	-0.47045800	7.62922000
H	10.90598200	0.04202600	5.92718800
C	7.12754000	4.93658400	12.17264600
H	7.17987200	4.17067100	12.95583100
C	7.08323600	9.23274100	13.32545600
H	7.69645500	9.46569200	14.21607200
H	6.73941500	8.18758100	13.41971800
C	5.92558600	5.62771600	11.94154300
H	5.02933000	5.38899900	12.52739100
C	12.88860800	-0.42633200	6.73848700

H	13.43357900	-0.34551900	7.69482000
H	12.87084700	-1.48900000	6.43597300
H	13.44845100	0.14105800	5.97483500
C	5.88090000	6.62755800	10.95519600
H	4.94561600	7.16561000	10.75840300
C	7.34554500	0.61516200	10.75333300
H	7.82387200	0.84953200	11.72059600
H	6.42853600	0.03083200	10.95158000
H	8.03975800	-0.00928500	10.16547000
C	5.92101900	10.20379200	13.16142300
H	5.25920500	10.15887000	14.04545600
H	6.28303600	11.24053400	13.04852400
H	5.32530700	9.94882100	12.26813300
C	10.46064000	11.98436100	13.67813300
H	9.70389500	12.74083100	13.39549100
H	11.45266400	12.44777500	13.53191000
C	10.26558200	11.49229300	15.10679800
H	10.35943100	12.33707500	15.81318800
H	9.26855000	11.03796700	15.23958500
H	11.02311000	10.73301300	15.36559600
Fe	11.95691800	7.48873000	7.37761600
O	10.89338300	8.13946000	5.01297600
N	10.74273300	7.80683900	6.16392000

i. {FeTEsP-HNO}⁸

O	7.11118500	4.11906100	8.40211200
O	8.21381100	2.61132900	9.72742600
N	11.08277000	8.32909400	8.97142800
O	7.90322700	9.32884600	12.12786400
N	11.18625000	5.74063700	8.01098700
N	12.96881800	9.14242500	7.00414200
O	9.25660500	1.53966000	7.26521400
O	9.25960100	7.71258600	13.01609400
N	13.27019700	6.53952300	6.25180100
O	11.53823200	1.48532500	7.28281200
C	11.49635500	4.48664400	7.51288100
C	9.50041400	4.22291400	8.57243000
C	10.11434500	7.78621000	9.82294100
C	14.14265800	7.07501000	5.31082400
C	9.48601400	6.53644600	9.63118000
C	14.32592600	8.44482400	5.05777000
C	13.42544100	5.16126200	6.13347300
C	9.99867800	5.57866800	8.73143000
C	12.60584100	4.20447900	6.71431000
H	12.79324600	3.15681700	6.47310900
C	10.46803100	3.52615900	7.86315200
C	9.81288200	8.71861100	10.89529200

C	10.56762100	9.85761800	10.65655900
C	8.14206600	3.67889000	8.89366500
C	15.19354700	8.85661000	3.91096800
C	8.27873300	6.20143100	10.44778200
C	8.98013400	8.49829000	12.12162700
C	13.76103000	9.41824700	5.89523800
C	11.30870600	9.61469000	9.43742300
C	12.78196300	10.37466800	7.61787000
C	14.46010100	4.83929000	5.17781400
H	14.78406100	3.82572800	4.93560600
C	14.89066300	6.02470500	4.64867700
H	15.65792600	6.19451200	3.89448700
C	12.07273600	10.58533200	8.78984200
H	12.06007800	11.58704900	9.22640500
C	10.32909400	2.10958900	7.44213300
C	16.41565700	9.53338400	4.12276200
H	16.73665300	9.74983700	5.14776200
O	10.34746900	10.85885600	12.77896000
C	13.44377700	11.42805100	6.88210400
H	13.43753800	12.48013000	7.17150900
C	14.02606700	10.84139300	5.79318800
H	14.60510300	11.30952800	4.99849000
O	11.03950500	12.19038300	11.06222200

C	8.33020200	5.19932100	11.44052900
H	9.27486100	4.68220800	11.63345600
C	14.80298400	8.56125700	2.58549900
H	13.85280300	8.04399800	2.41345300
C	16.82034300	9.61689500	1.72389100
H	17.44949500	9.91285000	0.87697000
C	17.22175500	9.91038900	3.03754800
H	18.16948300	10.42946700	3.22039500
C	10.67450600	11.08888800	11.47470300
C	7.06597100	6.89036100	10.23212300
H	7.01916600	7.66575500	9.46050200
C	15.60935600	8.94091500	1.50152500
H	15.28688500	8.71173000	0.47954500
C	6.95000600	1.91868500	9.93766100
H	6.50805400	1.69522700	8.95190000
H	6.26664300	2.60078800	10.47453700
C	11.45131100	0.09172100	6.86513500
H	10.85168100	-0.45975800	7.61026300
H	10.91067800	0.04186800	5.90334000
C	7.19098400	4.89209700	12.19801300
H	7.25114000	4.12796400	12.98093500
C	7.07251800	9.23708300	13.32010500
H	7.69424500	9.48288300	14.19959300

H	6.73102200	8.19324400	13.42927900
C	5.98160900	5.56736000	11.96158300
H	5.08861900	5.31744800	12.54604900
C	12.87176100	-0.44371000	6.76017800
H	13.39695400	-0.36520800	7.72725800
H	12.84690100	-1.50732400	6.46475800
H	13.45312000	0.10892500	6.00204500
C	5.92153000	6.56616700	10.97529000
H	4.97957600	7.08991700	10.77768000
C	7.25426900	0.65740600	10.73239600
H	7.71133800	0.90030400	11.70724200
H	6.32085600	0.09698900	10.91744700
H	7.94716300	0.00493700	10.17479900
C	5.91471600	10.20795500	13.14107600
H	5.25810600	10.17661000	14.02848500
H	6.27796500	11.24216400	13.01436400
H	5.31235300	9.94251600	12.25560100
C	10.44811500	12.01990800	13.65240500
H	9.66370600	12.74431300	13.36731500
H	11.42456400	12.50464100	13.48035600
C	10.29084400	11.53250300	15.08509500
H	10.37309300	12.38755600	15.77907200
H	9.30843000	11.05502000	15.24147500

H	11.07479600	10.79980700	15.34035700
Fe	11.99945800	7.47342300	7.42432000
O	10.82987000	8.16693000	5.09222100
N	10.75859100	7.73234200	6.25081900
H	9.78127500	7.47681100	6.55156500

j. {FeTPC-NO}⁷

N	-0.26923100	11.64870000	6.64103700
C	2.36788400	11.21013200	9.85367300
C	-0.61780500	10.80555200	4.33106300
N	1.95080200	8.79349300	8.13789800
C	-0.36708000	13.16958100	8.61448400
C	0.72762800	12.61788000	9.27874200
C	-0.15178800	8.43289000	3.66501000
H	-0.58885700	8.48582400	2.66865300
C	-1.14487600	11.08840500	2.95747900
N	0.53528500	9.14019900	5.77391500
C	-2.53074500	11.12293100	2.68811400
H	-3.23854300	10.93220500	3.50248100
C	-0.79051200	12.72715200	7.33643000
C	0.76315000	7.77299300	5.62553300
C	-0.81197500	11.73992600	5.35519000
C	-1.72743300	13.45234600	6.51032600
H	-2.30972000	14.31382800	6.83292300

C	-0.71254500	11.56548200	0.59772700
H	0.00244500	11.73917900	-0.21459700
C	-0.03357800	9.54574600	4.57133300
C	2.78605500	8.85663900	9.23420400
C	-0.24135100	11.30689800	1.89426300
H	0.83469500	11.28095000	2.09818200
C	0.30519600	7.32525700	4.33529400
H	0.32999100	6.29271300	3.98977400
C	3.30194900	7.54920800	9.56361600
H	3.97755800	7.33640300	10.39120800
C	1.94892700	7.44837500	7.75630200
C	-1.69011900	12.87846600	5.26489100
H	-2.23772200	13.17490500	4.37124300
C	-3.00060200	11.38152000	1.39062500
H	-4.07944100	11.40068600	1.19805600
C	2.76437600	6.67088100	8.65782300
H	2.92727200	5.59667200	8.58048400
C	3.06998400	10.01931800	9.99269400
C	1.46790700	5.46957500	6.32067000
C	-2.09317300	11.60522900	0.34222900
H	-2.46054200	11.80657000	-0.67040800
C	1.37299500	6.94104200	6.58518100
C	0.76858300	4.55420600	7.13825900

H	0.14868300	4.93732500	7.95639600
C	1.64470900	2.68276600	5.85160500
H	1.71279300	1.60432800	5.66943500
C	2.26154100	4.96436400	5.26683100
H	2.82116500	5.66507300	4.63746600
C	2.34810300	3.58296400	5.03427100
H	2.97336300	3.20918800	4.21534800
N	1.36559100	11.44833400	8.93353700
C	0.85569100	3.17286400	6.90498600
H	0.30164200	2.47827700	7.54675500
C	2.56085400	12.36785600	10.81711500
C	1.37588600	13.30732900	10.47566600
C	2.05812400	14.65699000	10.12842500
H	1.50781000	15.25577500	9.38505800
H	2.15025300	15.27169300	11.06169900
C	3.82975600	13.22580900	10.54828400
H	4.17921100	13.67373100	11.51424900
H	4.66765900	12.64810200	10.12241900
N	3.36249500	14.24542900	9.60725800
C	4.29903000	15.34183900	9.40868600
H	4.53120000	15.89590100	10.35321800
H	5.24756000	14.95218000	8.99834200
H	3.88289500	16.06168400	8.68172900

Fe	1.09252300	10.34859400	7.23385700
N	2.35884200	11.01066700	6.33000800
H	0.66006300	13.43279100	11.30421600
H	2.55754700	12.01661100	11.86022500
C	4.11203600	9.89340400	11.07049300
C	5.48468800	9.94168800	10.74351700
C	3.74868600	9.68810700	12.41954900
C	6.46602800	9.80562700	11.73890100
H	5.77725000	10.08286400	9.69671000
C	4.72853400	9.55265600	13.41600300
H	2.68629100	9.62017300	12.68222400
C	6.09062000	9.61411400	13.07853800
H	7.52662400	9.84729200	11.46562200
H	4.42664700	9.39058100	14.45717400
H	6.85592700	9.50750900	13.85556900
C	-1.09159200	14.32688300	9.24288700
C	-1.03970300	15.63020600	8.69822900
C	-1.86562100	14.11993400	10.40639300
C	-1.73650800	16.69076600	9.29889800
H	-0.44403300	15.80682900	7.79534000
C	-2.56092800	15.17966100	11.00983700
H	-1.93087200	13.11006700	10.82836200
C	-2.49839700	16.46946500	10.45782800

H	-1.68065500	17.69384800	8.86067200
H	-3.16024900	14.99444400	11.90865000
H	-3.04223900	17.29723400	10.92663200
O	2.63018400	11.40579600	5.23715200

k. {FeTPC-NO}⁸

N	-0.26665500	11.68014300	6.61008600
C	2.33834800	11.19899300	9.86715300
C	-0.65327900	10.79425900	4.32084100
N	1.96441200	8.79056800	8.12819700
C	-0.34095700	13.20590900	8.58820300
C	0.71768900	12.62520600	9.27194700
C	-0.15282100	8.43732900	3.64785900
H	-0.61853000	8.48058700	2.66336900
C	-1.21948900	11.04940000	2.95932800
N	0.57461200	9.16608000	5.75128700
C	-2.61196100	11.14311900	2.73362400
H	-3.29376000	11.02121900	3.58241500
C	-0.77156100	12.77044700	7.29542600
C	0.81660500	7.79484800	5.58953300
C	-0.83954400	11.75389700	5.33473200
C	-1.70348400	13.49661400	6.47687800
H	-2.27484300	14.36919800	6.79164200
C	-0.86351500	11.41221800	0.56000000

H	-0.17243000	11.51779500	-0.28540500
C	-0.03932000	9.55604900	4.55654300
C	2.77922600	8.84544500	9.24098500
C	-0.35510500	11.18430100	1.84846800
H	0.72542800	11.11221100	2.01425300
C	0.34158000	7.34151600	4.30132500
H	0.37386600	6.30954100	3.95266000
C	3.28355300	7.54278400	9.57578400
H	3.93490400	7.32054900	10.42130800
C	1.97011900	7.44639500	7.74185600
C	-1.70491300	12.89292800	5.23581800
H	-2.26435700	13.18718600	4.34838700
C	-3.12165200	11.37488700	1.44608600
H	-4.20644500	11.43903500	1.29504500
C	2.76465800	6.66393000	8.64714800
H	2.94523600	5.59266700	8.55990700
C	3.04369100	10.01640600	10.01098800
C	1.53062000	5.49397900	6.26080000
C	-2.24960600	11.51173600	0.35300600
H	-2.64772800	11.69142000	-0.65311000
C	1.41897200	6.95939100	6.54102600
C	0.86752200	4.55429200	7.08364600
H	0.26471600	4.92289800	7.92094500

C	1.73909600	2.70433800	5.76097700
H	1.81875600	1.62775700	5.56715000
C	2.30693700	5.00265100	5.18595600
H	2.83956900	5.71916500	4.55112500
C	2.40734400	3.62476200	4.93626800
H	3.01863200	3.26861000	4.09780600
N	1.36180800	11.45148100	8.91671400
C	0.97002800	3.17617800	6.83806900
H	0.44151500	2.46788400	7.48812100
C	2.52142700	12.35090100	10.84333100
C	1.33998100	13.29052000	10.50130000
C	2.01829600	14.65538900	10.21876100
H	1.48124400	15.27352900	9.48133700
H	2.08329300	15.24216500	11.17513700
C	3.79437900	13.21371500	10.61282800
H	4.14947900	13.62083300	11.59725300
H	4.62732700	12.64773000	10.16107100
N	3.34102200	14.28034500	9.71905900
C	4.27127000	15.38597100	9.59496100
H	4.48279900	15.89795000	10.57166800
H	5.23246700	15.02328000	9.18705400
H	3.86692400	16.14062100	8.89587900
Fe	1.08897400	10.34526600	7.22893500

N	2.49641400	11.00835300	6.44865100
H	0.61481400	13.38713400	11.32671200
H	2.50194400	11.99732600	11.88583100
C	4.07938300	9.88409400	11.09043600
C	5.45336700	9.84892500	10.75963100
C	3.72537800	9.74591000	12.45184900
C	6.43645100	9.70567200	11.75206800
H	5.74042700	9.93468800	9.70542100
C	4.70529700	9.60669600	13.44849500
H	2.66285100	9.73462100	12.72270900
C	6.06646300	9.58880400	13.10261400
H	7.49615500	9.68699100	11.46910200
H	4.40331200	9.50143100	14.49800200
H	6.83317000	9.47910600	13.87915200
C	-1.04592200	14.38195500	9.19641100
C	-0.99953600	15.67153900	8.61393400
C	-1.80059500	14.22746000	10.38268100
C	-1.67270600	16.75797300	9.19444400
H	-0.42126100	15.81092200	7.69364800
C	-2.46958900	15.31292100	10.97084300
H	-1.86778800	13.23073300	10.83469400
C	-2.40966600	16.58500000	10.37859300
H	-1.61504600	17.74687000	8.72289500

H	-3.04982800	15.16103500	11.88953700
H	-2.93442000	17.43375000	10.83362400
O	2.92731400	10.81924000	5.33154200

I. {FeTPC-HNO}⁸

N	-0.51565800	11.59440300	6.87943400
C	2.10665300	11.14272600	10.07697700
C	-0.98287900	10.74057100	4.59400700
N	1.75737000	8.81660900	8.29297900
C	-0.35911300	13.29706300	8.68225100
C	0.75810500	12.73142100	9.28199300
C	0.17962700	8.75679400	3.58174900
H	-0.25867800	8.82993800	2.58723400
C	-1.74507000	10.94807600	3.32061300
N	0.64409400	9.31773300	5.80289100
C	-3.11802000	10.62869100	3.23484800
H	-3.62569600	10.21622000	4.11392300
C	-1.00903000	12.68840000	7.57995500
C	1.21691600	8.09140100	5.47473200
C	-1.26514100	11.55966500	5.69601000
C	-2.14674500	13.25521600	6.90550000
H	-2.73556200	14.09442700	7.27378600
C	-1.80319000	11.65163400	0.97812300
H	-1.28435900	12.05366000	0.10028800

C	-0.03579000	9.70454000	4.65082500
C	2.27838100	8.74567700	9.57848600
C	-1.09639200	11.46059300	2.17572400
H	-0.03177200	11.71267100	2.23544300
C	0.95426200	7.75216700	4.09523100
H	1.28021600	6.83466100	3.60697400
C	2.69361300	7.40355700	9.88817900
H	3.10142000	7.08188800	10.84583400
C	1.96271200	7.53999300	7.75235000
C	-2.28914500	12.57007500	5.72303200
H	-3.01392900	12.74220500	4.92824100
C	-3.82456400	10.82231000	2.03735100
H	-4.88884100	10.56482700	1.98767400
C	2.51314500	6.65874800	8.74774800
H	2.75284800	5.60869300	8.58493600
C	2.54225300	9.86682600	10.40423800
C	2.22403800	5.85037600	5.93190200
C	-3.16966900	11.33462000	0.90542800
H	-3.72125500	11.48415800	-0.02963500
C	1.79421200	7.20704500	6.40134500
C	1.52502900	4.69099000	6.33386800
H	0.65305500	4.79463500	6.98928500
C	3.03884100	3.29022700	5.04055500

H	3.35429300	2.29915200	4.69528200
C	3.33648300	5.70667300	5.07379700
H	3.88718100	6.60089000	4.76126200
C	3.73964100	4.43687900	4.63168200
H	4.60771600	4.34374100	3.96896800
N	1.17753100	11.42741200	9.09106900
C	1.93050800	3.42139200	5.89314100
H	1.37355700	2.53286600	6.21214000
C	2.62441100	12.39759100	10.75692900
C	1.68847400	13.50419000	10.20013500
C	2.63398700	14.40908400	9.35880900
H	2.13968300	14.86377400	8.48409100
H	3.04367900	15.23142000	9.99562800
C	4.02480400	12.76854200	10.19265100
H	4.56039800	13.43840500	10.90940700
H	4.66280800	11.89034200	9.99812200
N	3.69639300	13.47588100	8.94231900
C	4.84389100	14.12974600	8.31383000
H	5.32760800	14.87973200	8.98420300
H	5.59717100	13.37203500	8.03772000
H	4.51959300	14.64384700	7.39278100
Fe	0.93603100	10.38643900	7.43718400
N	2.34140400	11.22960800	6.83124700

H	1.15867200	14.08687400	10.96770200
H	2.64405500	12.32300600	11.85407700
C	3.37129900	9.66527700	11.63884600
C	4.72439100	9.26740000	11.55080800
C	2.81160500	9.85911300	12.92159400
C	5.49644200	9.08085400	12.70844800
H	5.16650000	9.10091200	10.56201000
C	3.58199800	9.67186500	14.07993500
H	1.75607700	10.14434600	13.00363200
C	4.92838700	9.28461700	13.97664500
H	6.54509500	8.77488700	12.61851400
H	3.12663600	9.82027900	15.06585400
H	5.53031400	9.13711100	14.88040200
C	-0.85148800	14.63029500	9.16371900
C	-0.79078200	15.77668600	8.33978600
C	-1.39475300	14.76579100	10.46109600
C	-1.24915600	17.02054400	8.80232400
H	-0.38173600	15.68335200	7.32741500
C	-1.85399800	16.00841500	10.92449000
H	-1.46793900	13.87898100	11.10175400
C	-1.78061300	17.14103100	10.09672400
H	-1.18996700	17.89822500	8.14843300
H	-2.27814000	16.09011400	11.93190100

H	-2.13983500	18.11149900	10.45721900
O	2.94192900	11.13258300	5.74685000
H	2.77094900	11.95079300	7.48615600

m. {FeDEsC-NO}⁷

N	1.04005500	11.69519200	8.69398100
O	1.05627100	6.73483500	11.34629600
O	2.21247100	8.01368000	12.84640500
C	2.42584800	7.73971900	8.25049800
C	0.18461600	13.61411100	7.38053700
N	0.68283000	8.78241800	6.05403000
C	1.98383600	10.40613600	10.57741500
H	2.26919100	10.45435700	11.63235000
C	2.24150600	9.23932600	9.89490000
C	-1.16517100	13.33152200	5.28771600
H	-1.49328200	14.36707300	5.20807100
C	-0.03276200	15.09421300	7.31288800
N	-0.09410600	11.45391300	6.15575900
C	-0.92663300	15.74875300	8.18958200
H	-1.47935000	15.15651900	8.92717700
C	1.48250800	11.57962700	9.99338100
C	-0.85035600	11.10819200	5.03850900
C	0.75794200	13.05282800	8.52766100
C	1.46781500	12.85418800	10.66563200

H	1.77077200	13.01515900	11.70186600
C	0.45881200	17.25272300	6.26904700
H	1.00490500	17.83524200	5.51826800
C	-0.28183700	12.82450200	6.30768400
C	1.33164100	7.56303600	6.05573400
C	0.65250000	15.86509300	6.34728500
H	1.34745300	15.36571800	5.66323900
C	-1.54356500	12.25997000	4.51936500
H	-2.23397800	12.24602900	3.67726600
C	0.92108900	6.75665200	4.93594100
H	1.28945900	5.75032500	4.73053300
C	-0.14237600	8.75375000	4.92401300
C	1.05561400	13.78056100	9.74101400
H	0.94145400	14.85647900	9.86678800
C	-1.12166000	17.13653300	8.10888400
H	-1.82399300	17.62628500	8.79314400
C	-0.01155200	7.48624400	4.24334700
H	-0.55037000	7.21105600	3.33759500
C	2.20953500	7.10403600	7.04872000
H	2.63759700	6.10961900	6.91532200
C	-1.78683800	9.60585300	3.26130000
C	-0.42786300	17.89319200	7.15031000
H	-0.58021100	18.97661900	7.08808100

C	-0.91011300	9.82537700	4.45547000
C	-2.88594600	8.72171900	3.34008700
H	-3.09326000	8.21404800	4.28858400
C	-3.44792900	9.15813400	1.01241800
H	-4.09079700	8.98557500	0.14189600
C	-1.53166700	10.25881200	2.03464800
H	-0.67224900	10.93388500	1.95826600
C	-2.35549300	10.03636700	0.92042200
H	-2.13805300	10.54636100	-0.02505000
C	1.97885700	7.49446500	11.60875500
C	3.02456700	5.62762600	9.61929900
O	2.50780400	4.83411700	8.84817600
O	3.59244000	5.26883000	10.81045700
C	3.50675900	3.85129000	11.15344800
H	4.40253500	3.67054900	11.77006600
H	3.57309000	3.26626000	10.22163400
C	1.25289300	7.61674000	13.87309400
H	1.29980700	6.51947900	13.98805100
H	0.23819500	7.87212700	13.52172100
C	2.22120700	3.54024000	11.91209700
H	2.14939500	4.14285500	12.83303900
H	2.20667500	2.47144000	12.19261500
H	1.33984700	3.75302300	11.28688000

N	1.92814900	8.98001600	8.58421700
C	-3.71016100	8.50107400	2.22567200
H	-4.56181200	7.81615800	2.30793600
C	1.62713700	8.34701700	15.15374100
H	2.64956400	8.08607000	15.47634600
H	0.92748600	8.06536100	15.96008400
H	1.57294900	9.44058000	15.01720700
C	3.26443400	7.12873600	9.36799900
C	2.95962200	8.06773800	10.58447800
C	4.35150100	8.47082100	11.11969000
H	4.34569200	9.43804300	11.64981000
H	4.72691400	7.68795200	11.82186200
C	4.80786600	7.35182300	9.12578200
H	5.37685900	6.46499100	9.49428700
H	5.03281400	7.48828500	8.05334000
N	5.13006500	8.56418400	9.88502300
C	6.55899900	8.76873600	10.07943200
H	7.05116600	7.93620900	10.64144200
H	7.05572000	8.86138200	9.09751800
H	6.72587900	9.70794000	10.63536400
Fe	1.10468100	10.28744800	7.25722700
N	2.60660500	10.59330900	6.53859100
O	3.54302700	10.04832300	6.03964000

n. {FeDEsC-NO}⁸

N	1.12400400	11.68180100	8.67691300
O	1.08035700	6.93381800	11.52821700
O	2.43922600	8.19926900	12.85992100
C	2.39699700	7.66257500	8.25391200
C	0.05956100	13.54998700	7.44763300
N	0.75531400	8.74160100	5.99001200
C	2.25034000	10.42580300	10.49397400
H	2.61028300	10.49556500	11.52559100
C	2.39395800	9.22885800	9.84020100
C	-1.32450300	13.23068100	5.38840000
H	-1.74731500	14.23483400	5.36344600
C	-0.27797300	15.00713000	7.43518100
N	-0.08745300	11.40086500	6.17719400
C	-1.11075400	15.58184500	8.42295800
H	-1.51924900	14.93566500	9.20767700
C	1.70520800	11.59619000	9.92744600
C	-0.80907600	11.05832500	5.02248000
C	0.76722300	13.02641000	8.54435200
C	1.71884500	12.86977400	10.58520800
H	2.12807600	13.05051900	11.58240700
C	-0.08244300	17.22078300	6.39656000
H	0.32776700	17.85652000	5.60213400

C	-0.39153200	12.75338200	6.38414400
C	1.37092300	7.50699400	6.01797900
C	0.22881600	15.85236400	6.42081000
H	0.87840100	15.41776700	5.65323500
C	-1.59861300	12.17722800	4.56053600
H	-2.28459300	12.14893900	3.71425400
C	1.01848200	6.72139400	4.86769400
H	1.37532700	5.70683800	4.67597900
C	-0.00864100	8.73160900	4.82183100
C	1.15568800	13.77608100	9.71104400
H	1.01108200	14.84749100	9.84720700
C	-1.42164200	16.95066000	8.40119600
H	-2.07509100	17.37145800	9.17563400
C	0.14800900	7.48291900	4.11956000
H	-0.32626700	7.23304000	3.17050100
C	2.17786500	7.01539900	7.06313100
H	2.54472700	5.99147700	6.96073400
C	-1.58639600	9.63360300	3.12198600
C	-0.90842900	17.77746200	7.38766400
H	-1.15160600	18.84688100	7.36957100
C	-0.77974800	9.81593000	4.36940200
C	-2.62985300	8.68067300	3.06872600
H	-2.84427100	8.08640200	3.96372100

C	-3.11250200	9.26365100	0.75365600
H	-3.70180100	9.12132000	-0.16041800
C	-1.32329200	10.39462200	1.95944900
H	-0.50996300	11.12802600	1.98425700
C	-2.07801000	10.21379100	0.78977100
H	-1.85090900	10.81312800	-0.10061700
C	2.08643600	7.62111600	11.66438400
C	2.76054000	5.56586900	9.72689500
O	2.06249000	4.82003100	9.05944700
O	3.38510100	5.16302000	10.89013600
C	3.11450700	3.79762900	11.30332600
H	4.02835700	3.48469300	11.83759200
H	2.98397200	3.17850500	10.39964300
C	1.48429400	8.00138100	13.93366300
H	1.38422400	6.91837700	14.13100100
H	0.49586400	8.36858300	13.60462600
C	1.88229300	3.71561800	12.20101800
H	2.00328300	4.34826600	13.09664200
H	1.72635100	2.67040300	12.52773200
H	0.98739000	4.05612200	11.65710800
N	2.00470700	8.95233100	8.54750400
C	-3.38428900	8.49696200	1.89926400
H	-4.19223700	7.75493400	1.88539900

C	2.00325700	8.75895300	15.14847500
H	2.99592000	8.38473300	15.45409000
H	1.30766100	8.63294100	15.99753400
H	2.09236400	9.83697000	14.93036300
C	3.18928100	7.00292500	9.38396300
C	3.04784700	8.02971900	10.55798000
C	4.49740700	8.31804100	11.00690000
H	4.61254600	9.32411700	11.44519000
H	4.82089300	7.56238300	11.76600200
C	4.73834000	7.00497900	9.09415700
H	5.20881400	6.08210400	9.51422500
H	4.93666400	7.03721100	8.00831500
N	5.23882200	8.21529400	9.75136100
C	6.68246500	8.25009400	9.89562400
H	7.08998400	7.40311900	10.50820500
H	7.15750800	8.20815400	8.89854500
H	6.98535100	9.19782600	10.37632200
Fe	1.11734500	10.27415300	7.24593400
N	2.63211300	10.77028300	6.52856500
O	2.83111400	11.75560900	5.84871000

o. {FeDEsC-HNO}⁸

N	0.68276600	11.53770600	8.81630100
O	1.36055300	7.01867400	12.14990200

O	3.06510500	8.33245000	12.91592100
C	1.75392800	7.47778700	8.50347700
C	-0.21393200	13.47274300	7.54214300
N	0.23036600	8.64929600	6.20787000
C	1.89416700	10.33665600	10.60835200
H	2.34218600	10.44031400	11.60118300
C	2.06413700	9.14462600	9.94481300
C	-0.88215200	13.37096500	5.13095900
H	-1.17727500	14.41473800	5.03422500
C	-0.56487600	14.92941700	7.57659200
N	-0.11481200	11.40882600	6.14985800
C	-1.68455000	15.38714800	8.30545700
H	-2.30640300	14.66061300	8.84030100
C	1.20118500	11.44176200	10.09749800
C	-0.51622700	11.16350200	4.83784000
C	0.24708100	12.86489200	8.71496300
C	1.03583000	12.66976300	10.82422200
H	1.35460000	12.82838700	11.85601100
C	-0.10201400	17.23881800	6.91399700
H	0.52269500	17.95797000	6.37189200
C	-0.35363900	12.77140400	6.33292400
C	0.47909300	7.30074400	6.40944200
C	0.22208000	15.87366400	6.88080200

H	1.09602700	15.52690500	6.31838400
C	-0.97534400	12.37389000	4.19960500
H	-1.36445400	12.43222500	3.18414500
C	0.01620700	6.51302600	5.29967700
H	0.08748700	5.42559000	5.24158900
C	-0.31986500	8.71553900	4.92101500
C	0.44421800	13.55969000	9.96291900
H	0.18326300	14.60222000	10.13991400
C	-2.00788700	16.75287800	8.33803700
H	-2.88383000	17.08967800	8.90432400
C	-0.46450800	7.39338100	4.36360000
H	-0.87024500	7.17773300	3.37604400
C	1.22548200	6.75380900	7.46176200
H	1.41301800	5.67881300	7.43922400
C	-1.10342100	9.81295100	2.82051800
C	-1.21776000	17.68288000	7.64272200
H	-1.47084800	18.74883000	7.66803300
C	-0.62224700	9.89724100	4.23714900
C	-2.36435100	9.25681500	2.51173700
H	-3.00030400	8.89141800	3.32580600
C	-1.99810400	9.66338500	0.13942800
H	-2.34445700	9.60535200	-0.89865500
C	-0.29935300	10.29603000	1.76464600

H	0.68183400	10.72487900	1.99633500
C	-0.74320700	10.22095100	0.43529700
H	-0.10376300	10.59604800	-0.37200500
C	2.35594100	7.69769400	11.93960500
C	2.40014500	5.48857400	10.02699800
O	1.50273200	4.76651800	9.62203200
O	3.31217300	5.11451300	10.97451000
C	3.13228200	3.77530500	11.53179100
H	4.15176300	3.46465800	11.81382700
H	2.75235200	3.11829400	10.73232000
C	2.54107700	8.16221500	14.26902700
H	2.55150300	7.08555900	14.51318700
H	1.48915900	8.49644900	14.28131600
C	2.18929500	3.78819800	12.72968700
H	2.56532500	4.45411200	13.52442000
H	2.10487600	2.76653600	13.14249300
H	1.18691400	4.13273000	12.43127100
N	1.49715500	8.81353900	8.73741800
C	-2.80738600	9.18237500	1.18169300
H	-3.79107700	8.75233800	0.96082200
C	3.42248700	8.97483100	15.20501000
H	4.46966200	8.62954000	15.16478400
H	3.06186800	8.86554900	16.24279200

H	3.39883700	10.04654500	14.94350200
C	2.75910200	6.88485400	9.48442900
C	2.91603400	8.02353900	10.55545000
C	4.41786600	8.40425600	10.49898200
H	4.60176900	9.45311300	10.78523600
H	5.00701200	7.74196500	11.17717300
C	4.18350200	6.84358100	8.81641000
H	4.79683800	6.04366500	9.29192800
H	4.12106400	6.64757900	7.73220100
N	4.73607400	8.17911200	9.08310800
C	6.15895700	8.28950400	8.76981800
H	6.78715600	7.56639200	9.34443200
H	6.31575200	8.10444300	7.69295300
H	6.50903200	9.31125100	8.99715400
Fe	0.75806500	10.13695100	7.40531600
N	2.38131200	10.39256300	6.84863600
O	2.83081300	11.05668100	5.90010600
H	3.12756600	9.89541400	7.40631000

p. ZnDEsP

Zn	-6.43230300	2.32142100	15.63942900
O	-2.35476800	3.94257500	11.38112200
O	-3.23549100	2.50073400	9.83661900
O	-2.79363700	-0.23836000	10.69650900

O	-4.97347900	-0.94450900	10.75554300
N	-7.50408100	2.66023700	17.34929500
N	-7.09463800	0.40215700	15.60502100
N	-5.34374300	1.97729700	13.90278500
N	-5.80303200	4.25354900	15.65463700
C	-7.64753400	3.86935000	18.01354000
C	-8.62323800	3.73558200	19.07936000
H	-8.94987200	4.54040200	19.73678500
C	-9.05741500	2.43572200	19.06365600
H	-9.80664800	1.97418700	19.70574600
C	-8.35062300	1.76587600	17.98778100
C	-8.53653700	0.40783800	17.63439700
C	-7.92407000	-0.22131200	16.52295600
C	-8.06857700	-1.62784600	16.18590700
H	-8.64766400	-2.35191400	16.75767000
C	-7.33657500	-1.84192800	15.04648700
H	-7.20292200	-2.77406300	14.49440800
C	-6.73158300	-0.57604500	14.69054600
C	-5.90172200	-0.39662500	13.57981700
H	-5.74543900	-1.26601100	12.93713700
C	-5.26504200	0.79383800	13.19491200
C	-4.39691900	0.95610900	12.03814900
C	-3.94963100	2.27527600	12.06694100

C	-3.08568900	2.99339300	11.09656000
C	-4.54654200	2.88797200	13.24109900
C	-4.34463700	4.21591800	13.64731700
H	-3.64887000	4.80292700	13.04152800
C	-4.90936100	4.83425600	14.76578000
C	-4.62602000	6.19807700	15.15990300
H	-3.94597300	6.86932700	14.63249000
C	-5.35369600	6.44400000	16.29519700
H	-5.38232500	7.35653100	16.88931000
C	-6.09551800	5.22939200	16.59343800
C	-6.97398200	5.07275300	17.69308700
C	-7.21035000	6.26178600	18.57408400
C	-6.82644400	6.24001600	19.93413200
H	-6.34066900	5.34416500	20.33652000
C	-7.04695200	7.35312000	20.75980300
H	-6.73548200	7.31951300	21.81004700
C	-7.65655300	8.50751100	20.24164000
H	-7.82885400	9.37646500	20.88653600
C	-8.04389000	8.54173200	18.89189900
H	-8.52629500	9.43566500	18.48053100
C	-7.82216300	7.42970400	18.06506700
H	-8.13494600	7.45370000	17.01528300
C	-9.45046100	-0.41698200	18.48887600

C	-10.64049800	-0.96340800	17.95691800
H	-10.89522300	-0.76786800	16.90934100
C	-11.49699800	-1.73328300	18.75867900
H	-12.41926200	-2.14199600	18.33026800
C	-11.17889900	-1.97257300	20.10574400
H	-11.84766900	-2.57439300	20.73120400
C	-9.99876700	-1.43593300	20.64640800
H	-9.73928600	-1.62259200	21.69469300
C	-9.14269900	-0.66431300	19.84575400
H	-8.21731900	-0.25431300	20.26534700
C	-2.35862200	3.07653000	8.82397700
H	-2.26021300	4.15792800	9.01589500
H	-2.90469700	2.91658700	7.88013500
C	-3.94319500	-0.10621600	11.09896600
C	-4.61924700	-2.03333800	9.85011700
H	-5.34264300	-2.82969400	10.08992300
H	-3.59798200	-2.37289200	10.08896700
C	-0.99970800	2.38182300	8.81848400
H	-0.39413600	2.74894100	7.97008200
H	-1.12128100	1.29026900	8.72419100
H	-0.45347300	2.59405000	9.75202700
C	-4.73074900	-1.59051700	8.39429500
H	-4.53222000	-2.44762600	7.72581200

H	-3.99373700	-0.80122100	8.17440200
H	-5.74142100	-1.20582900	8.17528800

q. ZnDEsC

Zn	12.26367700	16.03434800	7.95782800
O	11.93651800	17.24481200	13.25595700
O	13.75623300	18.52807800	13.80981700
N	12.41914400	18.04862400	7.91320000
N	11.51140300	16.03877800	6.04992100
N	13.01657400	16.02728700	9.96625600
N	15.93283000	15.92704600	11.52380900
C	12.95468800	18.86244500	8.89357800
C	12.98237700	20.23701500	8.44946800
H	13.36864700	21.07351200	9.03425900
C	12.44914900	20.25665000	7.18553100
H	12.32083500	21.11389600	6.52601900
C	12.08623500	18.89051700	6.85622200
C	11.49508900	18.49328500	5.63548600
C	11.20343000	17.15011800	5.28465500
C	10.51792900	16.74384600	4.07458600
H	10.13637500	17.41867000	3.30942500
C	13.40464700	18.44688700	10.15849600
H	13.80092500	19.21588300	10.82687700
C	13.38513300	17.14433400	10.65790100

C	13.92919400	16.82529700	12.05805200
C	11.15046900	19.56167000	4.64295100
C	11.77620900	19.59823500	3.37619300
H	12.52919700	18.84091400	3.13168900
C	11.45419300	20.59803000	2.44575300
H	11.95609900	20.61428100	1.47161000
C	10.49882700	21.57774000	2.76285300
H	10.24708800	22.35764900	2.03552000
C	9.86827700	21.55184500	4.01768700
H	9.11697900	22.30818300	4.27181000
C	10.19159300	20.55368200	4.94966900
H	9.69159000	20.52763400	5.92419800
C	17.32781600	15.84835000	11.04474700
C	15.37687200	17.17919700	11.77476800
C	13.24286100	17.63674800	13.15443000
C	10.55346200	19.21927200	13.76346900
H	9.90408700	19.66921000	14.53616300
H	9.94349100	19.03526100	12.86238000
H	11.34736000	19.94278700	13.51630000
C	11.15897900	17.92107400	14.28850000
H	11.81483100	18.10459100	15.15517100
H	10.38157400	17.18908800	14.56150200
N	12.15289600	14.01941800	8.01083100

C	12.57923500	13.19269500	9.03303100
C	12.43113600	11.80607700	8.65317400
H	12.70700400	10.95571000	9.27910900
C	11.89972000	11.79386400	7.38853200
H	11.66334800	10.92979900	6.76895400
C	11.71419800	13.17789600	6.99337500
C	11.17704500	13.58966300	5.75262600
C	11.06015500	14.94118500	5.33770000
C	10.42895100	15.37430300	4.10758800
H	9.96151200	14.71824900	3.37434500
C	13.07506300	13.60002100	10.28340800
H	13.34955600	12.81256500	10.98654300
C	10.69539400	12.52897000	4.81016600
C	11.30569800	12.35392200	3.54740800
H	12.14735100	12.99772400	3.26915600
C	10.85466400	11.36163000	2.66360400
H	11.34613500	11.23655600	1.69205300
C	9.78287400	10.52839900	3.02420400
H	9.42983400	9.75457600	2.33337900
C	9.16585000	10.69337500	4.27511800
H	8.32424100	10.05266100	4.56204900
C	9.61811900	11.68375100	5.16058400
H	9.12856900	11.81869900	6.13140200

O	12.43522500	13.63815800	13.18828400
O	13.66040200	15.07018200	14.48567800
C	13.22225000	14.91234100	10.73388100
C	13.83158700	15.26271400	12.09268600
C	13.29745000	14.66558800	13.38864100
C	12.91402800	11.89395900	14.86345000
H	12.48943200	11.36671200	15.73668900
H	13.09197000	11.15331500	14.06506300
H	13.87876200	12.33544600	15.16163500
C	11.94839500	12.97937500	14.39942700
H	11.80252200	13.74614500	15.17764500
H	10.97359400	12.56233800	14.09947100
C	15.24525500	14.74900300	11.79359200
H	17.73564300	14.86478400	11.31779300
H	17.34643300	15.96261800	9.94761400
H	17.90631500	16.66474100	11.50050500

r. {FeOEP-NO}⁸

Fe	3.26000900	2.65532900	6.54446100
O	4.49482300	1.08609600	4.82051100
N	4.82039300	2.10666100	7.63625200
N	2.37318100	0.92943100	6.94147400
N	1.53077900	3.34652100	5.76388400
N	3.99068000	4.53659300	6.47455100

N	3.94404100	2.15778900	4.98976500
C	5.94668300	2.85663700	7.96728200
C	6.93301800	2.05483200	8.66988200
C	6.40698600	0.78130700	8.76464000
C	5.10150500	0.83505900	8.12463300
C	4.23440300	-0.25049700	8.04168800
H	4.57550900	-1.20487100	8.45634500
C	2.95203500	-0.20392000	7.50336900
C	2.02616800	-1.32671300	7.52439400
C	0.84900000	-0.86324000	6.97115700
C	1.08279300	0.52400100	6.60684300
C	0.13937600	1.32671500	5.96793600
H	-0.84027300	0.88363700	5.75762400
C	0.34493100	2.64319700	5.56880600
C	-0.65384100	3.45772400	4.89730000
C	-0.06196900	4.68530500	4.67106800
C	1.28356200	4.59743300	5.22260300
C	2.18942900	5.65846100	5.22211500
H	1.87187900	6.59461600	4.75113700
C	3.43859800	5.63905300	5.84209700
C	4.30313500	6.80727600	5.95202000
C	5.40419700	6.40630700	6.68287700
C	5.19839900	5.00046500	6.98953300

C	6.11326600	4.20944400	7.67572000
H	7.04135600	4.68532900	8.01084600
C	8.28232700	2.53969400	9.13642600
H	8.65958800	1.87345100	9.93651500
H	8.18808500	3.54230100	9.59993100
C	9.33336300	2.60824900	8.00338400
H	9.48856500	1.61028400	7.55588000
H	10.30785400	2.97648800	8.37820200
H	8.99429800	3.28057300	7.19612900
C	6.99974000	-0.42741400	9.44211300
C	2.34369200	-2.71012200	8.02999600
H	1.40287300	-3.24352500	8.26855700
H	2.90208500	-2.64709100	8.98606800
C	3.16237400	-3.55829600	7.02823800
H	2.60431700	-3.69106800	6.08417800
H	3.39220300	-4.56009000	7.44003300
H	4.11411500	-3.05791600	6.77840800
C	-0.45439200	-1.60213400	6.80253900
C	-2.03014800	2.99678300	4.48900300
H	-2.69312600	3.87460900	4.36108800
H	-2.48508100	2.39185300	5.29897100
C	-2.03638400	2.16910300	3.18210600
H	-1.64035500	2.76631800	2.34132000

H	-3.05883500	1.83505700	2.91956200
H	-1.39382700	1.27711100	3.28265700
C	-0.67134400	5.91734100	4.05266900
C	4.02299200	8.16024000	5.35031100
H	4.61418300	8.93318000	5.87930100
H	2.96033400	8.43393700	5.50922400
C	4.33770100	8.23620800	3.83754400
H	5.40712000	8.03028800	3.65205200
H	4.09982800	9.23562600	3.42466000
H	3.75619600	7.48197700	3.27912800
C	6.58080600	7.23631800	7.12933200
H	-0.26369100	-2.69278700	6.78485000
H	-0.90408500	-1.36049200	5.81890100
H	0.06898000	6.41915700	3.39754600
H	-1.50894600	5.62500900	3.38957000
H	7.52008300	6.66024400	7.00795000
H	6.68364600	8.11978500	6.46959700
H	6.80721200	-1.33562600	8.83640200
H	8.10172200	-0.32561700	9.48566900
C	-1.48349600	-1.29059300	7.91426500
H	-1.70597100	-0.20966900	7.94818900
H	-2.43284700	-1.83629000	7.75131200
H	-1.08577000	-1.57663300	8.90459200

C	-1.18848000	6.93750900	5.09457100
H	-0.37121800	7.25548200	5.76549700
H	-1.60872900	7.83821000	4.60664800
H	-1.97593500	6.48602200	5.72451700
C	6.47449400	7.71431700	8.59651400
H	6.38487400	6.85293400	9.28141600
H	7.36192900	8.30518400	8.89502000
H	5.57700100	8.34305700	8.73792600
C	6.46191900	-0.65760200	10.87427600
H	6.90258500	-1.56443700	11.33195900
H	6.69718700	0.20587100	11.52233200
H	5.36387600	-0.77304700	10.86484700

s. {FeOEP-HNO}⁸

Fe	2.68439400	2.95916800	6.05054100
O	4.49829300	1.11318600	5.27235100
N	3.67905700	2.81737800	7.76802000
N	1.66665200	1.31622000	6.52356400
N	1.41571300	3.29860000	4.53289100
N	3.45128800	4.79041800	5.76502300
N	3.86567100	2.16461100	5.08201800
C	4.64777700	3.68337600	8.26059900
C	5.25154500	3.17061400	9.48095400
C	4.65159200	1.95353600	9.72799900

C	3.68930500	1.75021400	8.65667300
C	2.88142600	0.62455300	8.54709300
H	2.99332100	-0.15507600	9.30612800
C	1.93389800	0.42117800	7.55097700
C	1.06604800	-0.74446800	7.48711900
C	0.25296700	-0.55885100	6.38894400
C	0.64530200	0.71321700	5.80022600
C	0.06752700	1.24160300	4.65090000
H	-0.73151300	0.66271700	4.17847000
C	0.42204600	2.44936600	4.05882500
C	-0.22314200	2.99173800	2.87390600
C	0.40090000	4.19347700	2.60799100
C	1.41275400	4.36306100	3.63843000
C	2.27419100	5.45362800	3.70688800
H	2.18666200	6.21792300	2.92905800
C	3.21951800	5.66137500	4.70662600
C	4.06215200	6.84393300	4.79156500
C	4.82498900	6.69277600	5.93133800
C	4.44089300	5.41671100	6.51442500
C	4.99982200	4.89537100	7.67646700
H	5.77630300	5.48653400	8.17088800
C	6.35152200	3.84339000	10.26165200
H	6.33484400	3.47849200	11.30552700

H	6.16169100	4.93268400	10.32287100
C	7.75828100	3.60360200	9.66502900
H	7.99603100	2.52561200	9.64326000
H	8.53362100	4.11656100	10.26253800
H	7.81906900	3.97593300	8.62731900
C	4.87522700	1.01928600	10.88929800
C	1.10656900	-1.91634000	8.43420900
H	0.13087200	-2.43681500	8.41445200
H	1.23214800	-1.55790000	9.47462200
C	2.22785400	-2.92986400	8.10580400
H	2.09338300	-3.34827900	7.09289900
H	2.22792900	-3.76650700	8.82788600
H	3.22093600	-2.44834100	8.13408800
C	-0.85993500	-1.44515200	5.89151400
C	-1.32257200	2.32069900	2.09099900
H	-1.88879500	3.08485500	1.52653600
H	-2.05278300	1.85815500	2.78299000
C	-0.80360400	1.24711900	1.10600600
H	-0.12073800	1.69450800	0.36234100
H	-1.64031300	0.77143400	0.56303500
H	-0.24330800	0.45759000	1.63684500
C	0.08415800	5.18792200	1.52049100
C	4.08870200	7.97019300	3.78974600

H	4.50506300	8.87588400	4.26830500
H	3.05575100	8.23750600	3.49242800
C	4.91411900	7.64240500	2.52350400
H	5.96463500	7.42576700	2.78578400
H	4.90318400	8.48912600	1.81349500
H	4.51185400	6.75381200	2.00589800
C	5.82411100	7.65608700	6.52000100
H	4.09849100	2.64380200	4.17342300
H	-0.68906200	-2.47876100	6.24558100
H	-0.83447500	-1.50014200	4.78566200
H	-0.41604900	4.66610000	0.68345100
H	1.02097100	5.60040800	1.09728300
H	6.69794800	7.10206600	6.91469800
H	6.22124900	8.30732600	5.71905300
H	5.88272300	1.19456400	11.31053200
H	4.87872200	-0.03004700	10.53531900
C	3.82338500	1.17528400	12.01229900
H	2.80452800	0.98528600	11.63144000
H	4.01988400	0.46931500	12.83951600
H	3.83707700	2.20018200	12.42310200
C	-2.26307000	-0.97934100	6.34602400
H	-3.04888200	-1.64924200	5.95237000
H	-2.33630100	-0.97234700	7.44779800

H	-2.47460500	0.04550000	5.99377400
C	-0.81351200	6.35276900	1.99943800
H	-1.01419100	7.06253800	1.17648600
H	-1.78150800	5.97374600	2.37168400
H	-0.33585400	6.90781900	2.82573700
C	5.23168100	8.53921700	7.64295300
H	4.84069800	7.92044000	8.46955000
H	5.99676200	9.22234000	8.05428200
H	4.39407600	9.14913200	7.26127400

t. {FeOEPone-NO}⁸

Fe	3.23980700	2.77652800	6.58016200
O	5.00836500	2.36948000	4.67016900
N	4.81897000	2.14709600	7.60871700
N	2.33767500	0.99697300	6.94379500
N	1.50271300	3.47119100	5.87222400
N	3.99643200	4.62465500	6.58197800
N	3.82958300	2.35180100	4.96365800
C	6.01394200	2.83198700	7.82894300
C	6.98237800	2.01162700	8.53873800
C	6.36204600	0.80167600	8.77385500
C	5.03675100	0.89679200	8.18565100
C	4.12559000	-0.15595100	8.17607400
H	4.43130900	-1.09117300	8.65771200

C	2.86619800	-0.11876600	7.58951100
C	1.94169200	-1.23510100	7.56107300
C	0.82740700	-0.79359300	6.86791600
C	1.09703000	0.58647500	6.50571500
C	0.18775000	1.40593700	5.81867400
H	-0.76056100	0.95544400	5.50642400
C	0.36623500	2.75154500	5.57011800
C	-0.74390600	3.58572000	4.92440800
C	-0.09667800	4.97595800	4.94159300
C	1.23425100	4.80001400	5.52112700
C	2.10248700	5.86985400	5.62646400
H	1.70560400	6.83155100	5.28272200
C	3.40821800	5.79266700	6.10739600
C	4.32741600	6.91253200	6.15731800
C	5.51745500	6.41699200	6.65659900
C	5.28947000	5.00622400	6.91864400
C	6.24062600	4.15727000	7.47909200
H	7.22728400	4.57799500	7.69887600
C	8.38323700	2.42990200	8.90473100
H	8.74939100	1.80507400	9.74251900
H	8.38257100	3.47085000	9.28617700
C	9.38195800	2.32811600	7.72795000
H	9.45537600	1.28619100	7.36839800

H	10.39346200	2.66412500	8.02707400
H	9.04808000	2.94578100	6.87616600
C	6.89928800	-0.38861600	9.52732400
C	2.20664300	-2.60875900	8.12307900
H	1.24524300	-3.11422000	8.33934300
H	2.72779900	-2.52747200	9.09778300
C	3.04316500	-3.50563800	7.18047000
H	2.52388200	-3.64713600	6.21576600
H	3.22469700	-4.50252000	7.62652300
H	4.01977500	-3.03903300	6.96260900
C	-0.45414500	-1.53667300	6.58790900
C	-1.03387700	3.14071100	3.46221100
H	-1.75788700	3.85784900	3.03109400
H	-1.53552800	2.15154900	3.49029200
C	0.20680300	3.06854300	2.55690100
H	0.66470000	4.06563900	2.43225500
H	-0.06600300	2.69506900	1.55236400
H	0.97595500	2.39798600	2.97824100
C	4.02397900	8.31338400	5.68960900
H	4.70123300	9.02767000	6.19725200
H	2.99818000	8.59995400	5.99389100
C	4.15944600	8.49095000	4.15920500
H	5.18660400	8.25508900	3.82736400

H	3.92555600	9.52860300	3.85336200
H	3.47410400	7.81050100	3.62486100
C	6.79301900	7.16724900	6.94357200
H	-0.26406500	-2.62742300	6.61395900
H	-0.80284200	-1.31847100	5.55859000
H	7.66877400	6.54720900	6.66595200
H	6.84593700	8.06547700	6.29809700
H	6.63150700	-1.32600200	9.00002100
H	8.00588000	-0.35395100	9.53233600
C	-1.59061500	-1.20208900	7.58249400
H	-1.81859400	-0.12177100	7.56572000
H	-2.51759900	-1.75619400	7.33915700
H	-1.29392600	-1.46060900	8.61492000
C	6.93499100	7.60327900	8.42097500
H	6.89862900	6.72761700	9.09271900
H	7.89005500	8.13522900	8.59551000
H	6.10744400	8.27547300	8.71087500
C	6.39219100	-0.47125600	10.98599100
H	6.79472000	-1.36315700	11.50333900
H	6.69572200	0.42533800	11.55577400
H	5.28961700	-0.52210000	11.01422400
C	-2.03744500	3.56178900	5.79728100
H	-2.36691200	2.50848000	5.89943500

H	-1.76064000	3.89207500	6.81744000
C	-3.20524900	4.42286900	5.28376900
H	-4.02114700	4.44684800	6.03056300
H	-2.86882000	5.45471700	5.08902300
H	-3.62898000	4.02250800	4.34480200
O	-0.60155000	6.03035600	4.50928900

u. {FeOEPone-HNO}⁸

Fe	3.25456900	2.75987100	6.56308300
O	4.57342100	1.34595000	4.67775800
N	4.81952300	2.15648500	7.62810500
N	2.35887800	1.03373400	6.94940700
N	1.55299600	3.46316000	5.76312500
N	4.00246600	4.63238900	6.55433000
N	3.89645000	2.32639300	5.02188900
C	5.93428100	2.89737100	8.01316700
C	6.93365300	2.06142600	8.65614500
C	6.43056100	0.77649400	8.64163300
C	5.12218500	0.85957600	8.01545400
C	4.25515800	-0.22309600	7.88636600
H	4.61112900	-1.20105300	8.22307800
C	2.95243000	-0.13756200	7.42003000
C	2.00770600	-1.24067500	7.43220800
C	0.81244900	-0.73088900	6.96372700

C	1.06134000	0.66519800	6.64473500
C	0.11918300	1.50139100	6.03581200
H	-0.87547700	1.08638000	5.84585000
C	0.35957700	2.78821300	5.59879200
C	-0.71010700	3.60434200	4.87665500
C	0.09461000	4.84665600	4.49489800
C	1.41292800	4.70050200	5.14822700
C	2.31502400	5.74588900	5.16179400
H	2.00564000	6.64573200	4.62017800
C	3.51364200	5.74106900	5.87468700
C	4.37789900	6.89471900	6.03368900
C	5.42774400	6.48058100	6.83165000
C	5.19248500	5.07619400	7.11951800
C	6.08723300	4.26312700	7.80792900
H	7.00315100	4.72835000	8.18410000
C	8.27063400	2.53249200	9.16915300
H	8.63905600	1.82268500	9.93299000
H	8.15639700	3.50150600	9.69322000
C	9.33647600	2.67631400	8.05729800
H	9.50819100	1.71009400	7.55138600
H	10.29871000	3.02321000	8.47550600
H	9.01360200	3.39904100	7.28758600
C	7.05079900	-0.47330400	9.21181300

C	2.31940600	-2.65229200	7.85761900
H	1.38184000	-3.16308000	8.14542100
H	2.94597900	-2.64230500	8.77063400
C	3.03104100	-3.47835100	6.76051200
H	2.40313400	-3.55231200	5.85534000
H	3.24629200	-4.50232900	7.11577100
H	3.98451300	-3.00784600	6.46335500
C	-0.51249800	-1.43524200	6.82202400
C	-1.30345100	2.90520900	3.62458100
H	-1.96091300	3.63969000	3.12555000
H	-1.95197300	2.07013200	3.95586700
C	-0.26182400	2.39653600	2.61522400
H	0.35143900	3.22818300	2.22437300
H	-0.75947000	1.91893700	1.75284800
H	0.41509600	1.65202000	3.06986400
C	4.14524900	8.24992500	5.41594300
H	4.68504200	9.01614100	6.00294000
H	3.07325500	8.51666700	5.48757400
C	4.59201300	8.33716200	3.93790800
H	5.67118900	8.12440900	3.83892400
H	4.40022300	9.34518900	3.52841100
H	4.04939000	7.60589000	3.31346200
C	6.58343600	7.29753400	7.34999100

H	-0.34237300	-2.52651200	6.76769400
H	-0.98692700	-1.15960300	5.85995400
H	7.52420000	6.71858400	7.26836700
H	6.72158000	8.18358300	6.70317100
H	6.83650700	-1.33647900	8.55234900
H	8.15161400	-0.36569500	9.21234000
C	-1.49358700	-1.13254600	7.97853100
H	-1.70386300	-0.05087200	8.04965600
H	-2.45269000	-1.66117300	7.83144000
H	-1.06912300	-1.45151000	8.94668400
C	6.39749800	7.76125100	8.81355200
H	6.27829600	6.89815100	9.49181000
H	7.26796500	8.35033700	9.15446400
H	5.49515300	8.38946800	8.91481900
C	6.57455700	-0.79630900	10.64751100
H	7.04798700	-1.72184000	11.02219700
H	6.82913700	0.02538800	11.33990200
H	5.47912700	-0.93075000	10.68293700
C	-1.83293400	4.00665700	5.89825400
H	-2.27349100	3.06959000	6.29151800
H	-1.34766600	4.50195100	6.76140400
C	-2.94104300	4.91335400	5.33920400
H	-3.60935800	5.23602100	6.15751300

H	-2.51791300	5.81149900	4.85961300
H	-3.56214400	4.39021800	4.59144900
O	-0.27780100	5.79455200	3.79527000
H	3.68680600	2.99698200	4.23614400

v. {Fe(2,4-OEPdione)-NO}⁸

Fe	2.53096000	3.05356300	6.15725100
O	3.96595400	1.05723700	5.21265100
N	3.70926800	2.76034900	7.77016900
N	1.45104000	1.49148100	6.64835300
N	1.20447800	3.57485300	4.74015100
N	3.43692100	4.85992300	5.90281100
N	3.61126600	2.20282400	5.02778800
C	4.73075200	3.56540000	8.25709500
C	5.43115500	2.93322700	9.35899000
C	4.83643400	1.69744900	9.54072500
C	3.77419600	1.61853000	8.55984500
C	2.88008300	0.55626800	8.45490000
H	2.98378300	-0.31346200	9.11265600
C	1.79477400	0.53134400	7.60395100
C	0.83594100	-0.57847600	7.66619900
C	-0.28674100	-0.23354300	6.68733800
C	0.27204100	1.04311300	6.06609100
C	-0.35801600	1.66617300	5.01129500

H	-1.27479000	1.23236500	4.59546000
C	0.07937600	2.83337600	4.39151400
C	-0.63605900	3.39278300	3.25336500
C	0.10168600	4.68661800	2.87926700
C	1.25088700	4.65954400	3.88558400
C	2.22171000	5.64063700	3.90943700
H	2.17148800	6.41796600	3.14193800
C	3.22419600	5.76149100	4.88339900
C	4.11684700	6.90647700	4.97597500
C	4.89103800	6.70204200	6.10213500
C	4.46975300	5.42605300	6.65369300
C	5.06537400	4.82253100	7.75015000
H	5.88363100	5.36047200	8.24090600
C	6.61408000	3.51052300	10.09467700
H	6.68477600	3.04908900	11.09874300
H	6.46147000	4.59372100	10.27256300
C	7.95562900	3.30659500	9.35245800
H	8.16156400	2.23105600	9.20788500
H	8.79940000	3.74885500	9.91598100
H	7.92375200	3.77219500	8.35192200
C	5.15147500	0.64795900	10.57626500
C	-0.52135400	-1.38161700	5.67019200
H	-1.38145200	-1.11342100	5.02407300

H	-0.81946800	-2.27775200	6.24629000
C	0.69861900	-1.72549300	4.80077600
H	1.04264600	-0.84842700	4.22627200
H	0.45125900	-2.53086100	4.08475900
H	1.54270100	-2.07389200	5.42178900
C	0.57410900	4.64294700	1.40237700
H	1.11141600	5.58099200	1.16114200
H	-0.33648500	4.62029800	0.77097400
C	1.46905500	3.44086300	1.05835700
H	2.36328100	3.41055500	1.70567100
H	1.80787500	3.49345300	0.00707900
H	0.92290800	2.49055800	1.19018300
C	4.17482700	8.05244300	3.99829800
H	4.64894100	8.92867900	4.48145600
H	3.14903000	8.37630600	3.72998400
C	4.94790100	7.71209600	2.70275200
H	5.99386000	7.44196100	2.93348600
H	4.95672900	8.56851000	2.00173700
H	4.49096800	6.84821500	2.18931200
C	5.93826900	7.60926100	6.69600200
C	-0.92848800	5.83951300	3.12039900
H	-1.83514300	5.55117900	2.55218700
H	-1.21565600	5.82008000	4.18970700

C	-0.51654400	7.27085800	2.74176900
H	0.33183000	7.62689400	3.35127300
H	-0.23446900	7.35548300	1.67672400
H	-1.36225700	7.96310200	2.91340100
C	-1.59717000	0.10438100	7.47716800
H	-2.32247500	0.53026700	6.75610500
H	-1.35928300	0.91956400	8.18784300
C	-2.23816400	-1.06797200	8.23956100
H	-3.07187400	-0.70440900	8.86908300
H	-2.65053900	-1.82814600	7.55211600
H	-1.49738400	-1.56601000	8.88753300
O	-1.65150600	2.94830100	2.68490300
O	0.90845200	-1.59270100	8.38174000
H	6.33237600	8.28497700	5.91231400
C	5.41491000	8.46008000	7.87670800
H	6.21312500	9.10144500	8.29694300
H	4.58412100	9.11129100	7.55058200
H	5.02924100	7.81296200	8.68402400
H	6.80663500	7.01307800	7.04095700
H	6.20957900	0.74355800	10.88884300
H	5.05891300	-0.36167300	10.13046300
C	4.24840600	0.72651600	11.82948200
H	3.18619000	0.60434700	11.55481600

H	4.50836500	-0.06187300	12.56124600
H	4.35265200	1.70785900	12.32669600
w. {Fe(2,4-OEPdione)-HNO}⁸			
Fe	2.53453700	3.10905800	6.13754500
O	4.05284600	1.06969700	5.20824000
N	3.59336300	2.92039000	7.81672000
N	1.42835900	1.52006000	6.65362800
N	1.22113200	3.55855400	4.69043300
N	3.45479300	4.84816200	5.78592800
N	3.60286200	2.22163200	5.10994800
C	4.75834000	3.60555000	8.15042900
C	5.33033000	3.11043300	9.38663500
C	4.49553700	2.09653300	9.82375800
C	3.45220700	1.97671300	8.82869000
C	2.47923500	0.97828900	8.83043900
H	2.44227200	0.25543900	9.65198600
C	1.58229900	0.76281400	7.80833800
C	0.68824400	-0.41627900	7.82009900
C	-0.11163200	-0.36238600	6.51904700
C	0.46647700	0.90181300	5.88954100
C	-0.01276300	1.40720100	4.69304900
H	-0.77443100	0.85170100	4.13592600
C	0.29866000	2.66145800	4.18961000

C	-0.45501700	3.22650900	3.05131100
C	-0.05060300	4.70132000	2.96782300
C	1.11820600	4.72667200	3.94481800
C	2.01020300	5.77261000	4.01702200
H	1.85382600	6.61878900	3.34262500
C	3.14556900	5.80888500	4.84290800
C	4.13997800	6.86440500	4.80403400
C	5.10199400	6.52566800	5.73852300
C	4.65676900	5.28901800	6.35033400
C	5.27676400	4.68216200	7.43246700
H	6.20965400	5.12603500	7.79295800
C	6.60333300	3.60459400	10.02478800
H	6.58679800	3.36492300	11.10408300
H	6.65462400	4.70912900	9.96551400
C	7.87792500	2.99892700	9.39186900
H	7.87882900	1.89910400	9.48820300
H	8.78659700	3.38949500	9.88444600
H	7.94009100	3.23603900	8.31518600
C	4.59802600	1.27629000	11.08385500
C	0.13053900	-1.63138300	5.65292800
H	-0.48539300	-1.54703300	4.73566100
H	-0.26000300	-2.49439600	6.22191700
C	1.59925300	-1.89166900	5.28229500

H	2.04781900	-1.03799000	4.74522000
H	1.67835600	-2.78120600	4.63272300
H	2.21134000	-2.08069600	6.18164300
C	0.27874200	5.12368300	1.51546100
H	0.53424300	6.19945900	1.49182400
H	-0.65574900	5.00856600	0.93410200
C	1.39775700	4.30872400	0.84758700
H	2.34412700	4.38388100	1.41295600
H	1.58708100	4.67619100	-0.17632100
H	1.12393500	3.24177200	0.77324300
C	4.11416500	8.05968200	3.88536100
H	4.71803100	8.87328000	4.32850800
H	3.08374800	8.45946000	3.81332600
C	4.64294600	7.75751300	2.46370600
H	5.68948400	7.40681900	2.49951700
H	4.60456700	8.66039000	1.82788200
H	4.04503900	6.96835500	1.97469800
C	6.32933400	7.30769500	6.13160800
H	3.96011700	2.74670700	4.27091100
C	-1.28757500	5.49314500	3.53319200
H	-2.14885900	5.21083900	2.89766600
H	-1.50893100	5.10897900	4.54757400
C	-1.15302300	7.02168400	3.59295000

H	-0.32075900	7.33269700	4.24786100
H	-0.99384100	7.46631600	2.59483400
H	-2.08060100	7.46025400	4.00244300
C	-1.63511900	-0.15359000	6.82669500
H	-2.14730600	0.05445400	5.86765300
H	-1.73673000	0.76769800	7.43266500
C	-2.33066900	-1.31991200	7.54748900
H	-1.78745400	-1.60286200	8.46392100
H	-3.35890300	-1.02644400	7.82508600
H	-2.40529500	-2.21477300	6.90551800
O	-1.28349800	2.64631100	2.34494800
O	0.62338800	-1.27237900	8.70816500
H	5.64247100	1.29518100	11.44651900
H	4.37666000	0.21450600	10.86256800
H	6.68424100	7.89023800	5.26089400
H	7.15541600	6.61566400	6.38448200
C	6.08702800	8.26960300	7.31850300
H	7.00990500	8.82033600	7.57505400
H	5.30274900	9.00681700	7.07257300
H	5.75321300	7.71797400	8.21475700
C	3.65909400	1.76595700	12.21069100
H	2.60276100	1.72900000	11.89170100
H	3.76691300	1.13758700	13.11291400

H	3.88732000	2.81023600	12.48810600
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