Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supplementary Information

for

Transition metal-mediated reductive coupling of diazoesters

Amanda Grass, Sebastian A. Stoian, Richard L. Lord, and Stanislav Groysman

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1. Synthesis and Characterization of Complexes

General Methods and Characterization. All reactions involving air-sensitive materials were executed in a nitrogen-filled glovebox or by standard Schlenk line procedures. Iron chloride and thallium hexaflurophosphate was purchased from Strem; other reagents were purchased from Sigma Aldrich. The synthesis of the complex **1** was reported previously.[1] The diazoesters were synthesized according to a reported literature procedure.[2] All solvents were purchased from Fisher Scientific and were of HPLC grade. The solvents were purified using an MBRAUN solvent purification system and stored over 3-Å molecular sieves. Deuterated benzene was purchased from Cambridge Laboratories, degassed under argon, and stored over 3-Å molecular sieves. The complexes were characterized using IR, UV/Vis spectroscopies, X-ray crystallography, elemental analysis, and solution magnetometry by the Evans method. NMR and GC-MS spectra were recorded at the Lumigen Instrument Center (Wayne State University). NMR was performed on a Varian Mercury or Agilent 400 MHz Spectrometer in C_6D_6 at room temperature. Chemical shifts and coupling constants (J) were reported in parts per million (δ) and hertz (Hz), respectively. IR spectra of powdered samples were recorded on a Shimadzu IR Affinity-1 FT-IR Spectrometer outfitted with a MIRacle10 attenuated total reflectance accessory with a monolithic diamond crystal stage and pressure clamp. UV-visible spectra were obtained on a Shimadzu UV-1800 spectrometer. Elemental analyses were performed by Midwest Microlab LLC. Formation of the organic by-products was confirmed by GC-MS using Agilent 6890N spectrometer, Thermo TG5MS 30m × 0.32mm × 0.25μm column, 7683 series injector and Agilent 5973 detector. The ^{57}Fe Mössbauer spectrum was recorded using a spectrometer equipped with a LN_2-cooled cryostat. The spectrometer was operated in constant acceleration

mode. The isomer shift is quoted against the center of a zero-field spectrum recorded at room temperature for an iron metal-foil.

Synthesis of $(Fe(OR)_2)_2[\mu\text{-}\kappa2\text{:}\kappa2\text{-}(OC(OMe)C(Ph)NN)_2]$ (2). A yellow solution of diazoester in hexane (0.11 mL, 0.066 mmol) was added to the pale-yellow hexane solution of $Fe(OR)_2(THF)_2$ (43 mg, 0.067 mmol). There was an immediate color change to dark brown, which transitions to burgundy within 10 minutes. The reaction was stirred for 1 h at room temperature, during which solid crashed out. The volatiles were removed in vacuo, the resulting brown residue was washed with ether, dissolved in THF, filtered, and dried in vacuo. Subsequent recrystallization from diethyl ether at 35˚C yields X-ray quality crystals of **2** (37 mg, 81% yield). IR (cm^{-1}): 2970 (w), 2878 (w), 1559 (m), 1489 (w), 1443 (w), 1265 (s), 1157 (s), 1011 (s), 710 (s). λ_{max} ($\varepsilon_{M\ (L^{-1}cm^{-1}\ mol^{-1})}$) 516 (16403). μ_{eff} = (7.5±0.8) μ_B (calcd 8.4). Anal. Calcd for $C_{78}H_{108}N_4O_8Fe_2$: C, 69.84; H, 8.12; N, 4.18. Found: C, 69.67; H, 8.37; N, 3.95.

Synthesis of $(Fe(OR)_2)_2[\mu\text{-}\kappa2\text{:}\kappa2\text{-}(OC(OEt)C(Ph)NN)_2]$ (3). A yellow solution of diazoester in hexane (0.50 mL, 0.086 mmol) was added to a pale-yellow hexane solution of $Fe(OR)_2(THF)_2$ (53 mg, 0.083 mmol). There was an immediate color change to dark brown, which transitions to burgundy within 10 minutes. The reaction was stirred for 1 h at room temperature, during which solid crashed out. The volatiles were removed in vacuo, the resulting brown residue was washed with ether, dissolved in THF, filtered, and dried in vacuo. Subsequent recrystallization from ether at 35˚C yields **3** as a purple solid after 4 days (46 mg, 81% yield). IR (cm^{-1}): 2970 (w), 2878 (w), 2338 (w), 1558 (m), 1258 (m), 1142 (s), 1042 (m), 1003 (s), 702 (s), 648 (s). λ_{max} ($\varepsilon_{M\ (L^{-1}cm^{-1}\ mol^{-1})}$) 516 (22727). μ_{eff} = 7.3 ± 0.7 μ_B (calcd 8.4). Anal. Calcd for $C_{80}H_{112}N_4O_8Fe_2$: C, 70.16; H, 8.24; N, 4.09. Found: C, 70.25; H, 8.31; N, 4.06.

Synthesis of $(Fe(OR)_2)_2[\mu\text{-}\kappa2\text{:}\kappa2\text{-}(OC(OEt)C(4\text{-}Br\text{-}Ph)NN)_2]$ (**4**). An orange solution of diazoester in hexane (0.50 mL, 0.086 mmol) was added to the pale-yellow hexane solution of $Fe(OR)_2(THF)_2$ (53 mg, 0.083 mmol) . There was an immediate color change to dark brown, which transitions to burgundy within 10 minutes. The reaction was stirred for 1 h at room temperature, during which solid crashed out. The volatiles were removed in vacuo, the resulting brown residue was washed with ether, dissolved in THF, filtered, and dried in vacuo. Subsequent recrystallization from ether at 35˚C yields **4** as a purple solid after 4 days- (43 mg, 67% yield). IR (cm^{-1}): 2978 (w), 2878 (w), 1551 (m), 1490 (w), 1312 (w), 1281 (m), 1258(m), 1142 (s), 1065 (m), 1042 (w), 818 (m), 741 (m), 702 (s), 671 (m), 602 (s). λ_{max} ($\varepsilon_{M\ (L^{-1}cm^{-1}\ mol^{-1})}$) 516 (17241). Anal. Calcd for $C_{80}H_{110}N_4O_8Fe_2Br_2$: C, 62.91; H, 7.26; N, 3.67. Found: C, 62.69; H, 7.32; N, 3.49.

Reaction of 10 mol% of 1 and Ph_2CN_2: A C_6D_6 solution of the Ph_2CN_2 (0.2051mL, 0.5M) and TMB (1 equiv) was added to a stirred solution of **1** (0.0205 mmol, 0.0410 M). A notable color change occurred to dark brown. NMR of the reaction mixture was taken after 24 hours and 100% yield to $Ph_2CNNCPh_2$ was calculated with reference to internal standard (TMB).

Monitoring decomposition of 3 by UV-Vis: A THF solution of **2** (0.0036 M) was stirred at RT for 5 days. Every 24 hours, a 0.1 mL aliquot of the solution was diluted to 6 mL and the UV-Vis spectrum was recorded. The concentrations of the solutions were determined from a calibration curve of known concentrations of **2**. The color transitions from dark purple to brown over time and the characteristic peak at 518 nm decreases and a shoulder at 378 nm grows in on the third day.

2. X-ray crystallographic details

Crystals of compounds **2**-**4** were grown at -33 °C from concentrated ether solutions; in all cases, very dark purple-brown crystals were obtained. The structure of complex **2** was confirmed by X-ray diffraction analysis. The crystals of **3** and **4** were found to be highly unstable outside of their respective solutions. The decomposition of the crystals was indicated by the progressive transformation (within 1-2 minutes of exposure) of the single-crystal diffraction pattern into a powder-like diffraction pattern. The crystal of **2** was mounted on a Bruker APEXII/Kappa three circle goniometer platform diffractometer equipped with an APEX-2 detector. A graphic monochromator was employed for wavelength selection of the Mo Kα radiation (λ = 0.71073 Å). The data were processed and the structure was solved using the APEX-3 software supplied by Bruker-AXS. The structure was refined by standard difference Fourier techniques with SHELXL (6.10 v., Sheldrick G. M., and Siemens Industrial Automation, 2000). Hydrogen atoms were placed in calculated positions using a standard riding model and refined isotropically; all other atoms were refined anisotropically. Only half of a molecule of **2** (and one molecule of ether solvent) occupies an asymmetric unit, hence Z=2.

Table S1. Crystal data and structure refinement for **2**.

	2
formula	$C_{78}H_{108}Fe_2N_4O_8 \times 2C_4H_{10}O$
fw	1489.62
crystal system	monoclinic
space group	$P2_1/n$
a (Å)	14.9936(13)
b (Å)	16.3764(10)
c (Å)	17.6759(14)
α (deg)	90.00
β (deg)	110.103(3)
γ (deg)	90.00
V (Å^3)	4075.7(5)
D_c (g cm^{-3})	1.214
Z	2
μ (mm^{-1})	0.415
T (K)	100(2)
2θ, deg	55.08
R_1 (all data)	0.0557
wR_2 (all data)	0.1075
R_1 [(I>2σ)]	0.0390
wR_2 [(I>2σ)]	0.1018
GOF	1.088

3. Evans method formula and procedure

The Evans method was performed on all complexes using a Wilmad coaxial insert (purchased from Aldrich) and a standard NMR tube. The sample was carefully weighed (10 – 20 mg) and dissolved in 1 mL C_6D_6 to afford solutions with known concentrations to perform the calculations. The solutions were added to the insert, and the insert was placed inside the outer NMR tube, which contained C_6D_6. NMR spectra were taken. The molar susceptibility χ_m of the compound was first calculated using Equation 1[3]:

$$\chi_m=[\frac{3\Delta\nu}{4\pi m\nu_0}+\ \chi_0]M \quad (1)$$

where $\Delta\nu$ is the peak separation (Hz), m is the concentration of the solution (g/mL), $\nu 0$ is the spectrometer operating frequency in Hertz, $\chi 0$ is the molar susceptibility of the solvent (in cm^3/g), and M is the molar mass of the compound (g/mol). Diamagnetic corrections were calculated using Pascals constants. The solution state effective magnetic moment (μ_{eff}) was calculated using Equation 2:

$$\mu_{eff}=\sqrt{(2.383\times10^3)(\chi_m)} \quad (2)$$

Three measurements were taken, the average of the three and the corresponding standard deviation were calculated. The uncertainty was estimated to be at least 10%, based on weight measurement uncertainty.

Table S2. Magnetic moments for complexes **2** and **3** using the Evans method (μ_{obs} (μ_B)).

	2	**3**
1	7.71	7.32
2	7.32	7.10
3	7.39	7.37
average	7.47	7.26
standard deviation	0.21	0.14
μcalc (μB)	8.37	8.37

4. IR Spectra

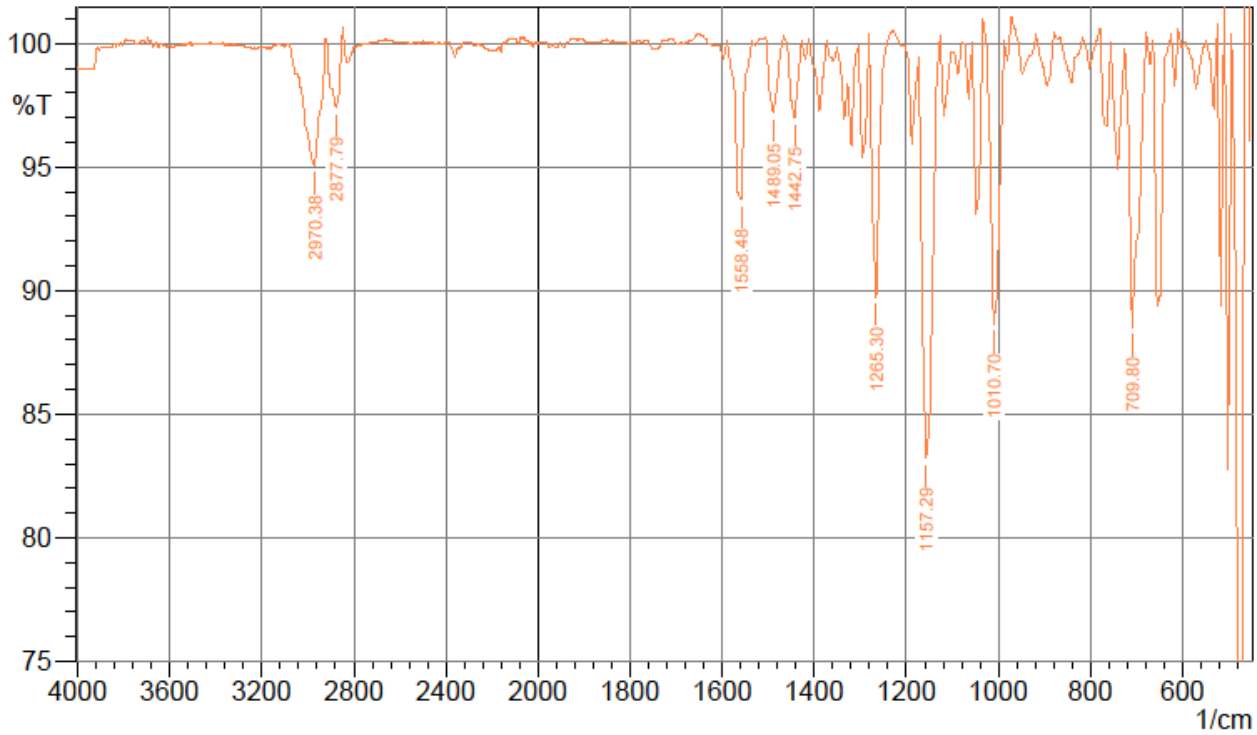


Figure S1. IR of $(Fe(OR)_2)_2[\mu\text{-}\kappa2\text{:}\kappa2\text{-}(OC(OMe)C(Ph)NN)_2]$ (**2**)

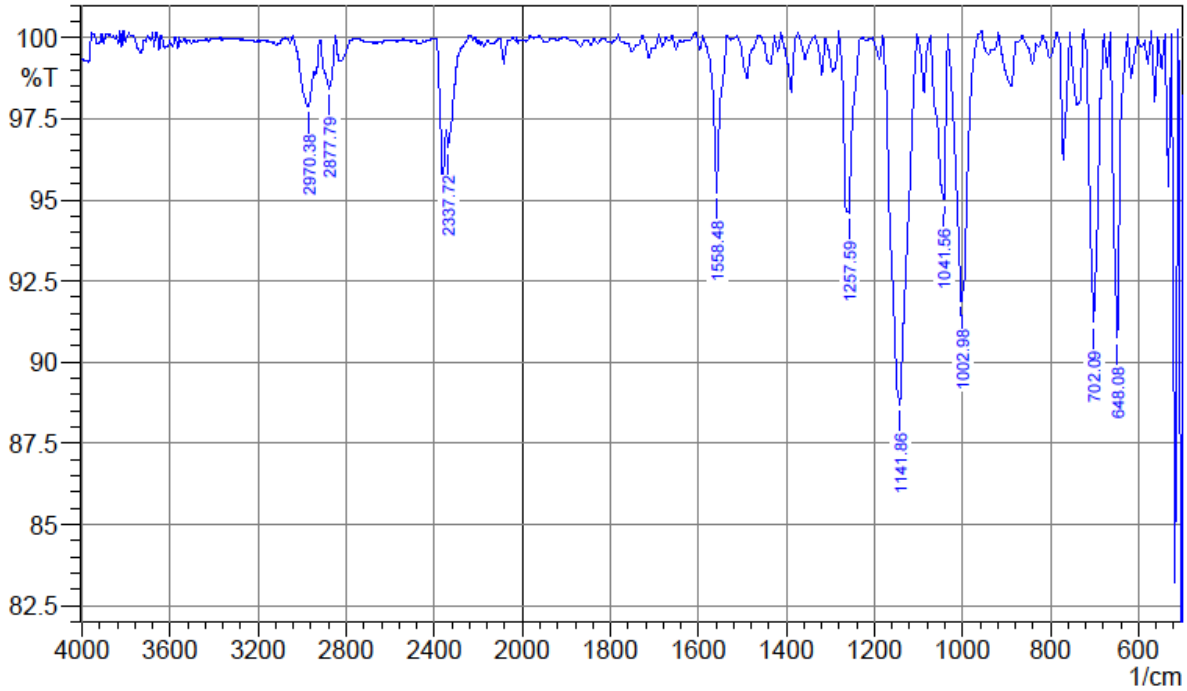


Figure S2. IR of $(Fe(OR)_2)_2[\mu\text{-}\kappa2\text{:}\kappa2\text{-}(OC(OEt)C(Ph)NN)_2]$ (**3**).

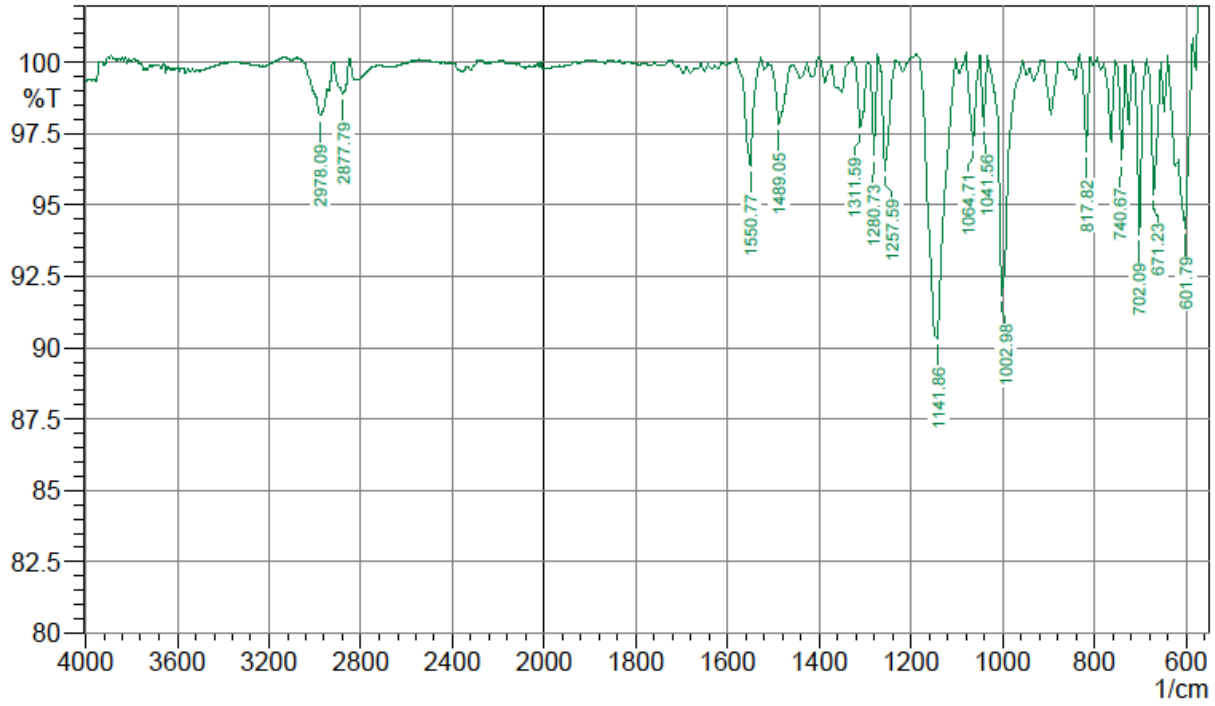


Figure S3. IR of $(Fe(OR)_2)_2[\mu\text{-}\kappa2{:}\kappa2\text{-}(OC(OEt)C(4\text{-}Br\text{-}Ph)NN)_2]$ (**4**).

5. UV-Vis Spectra

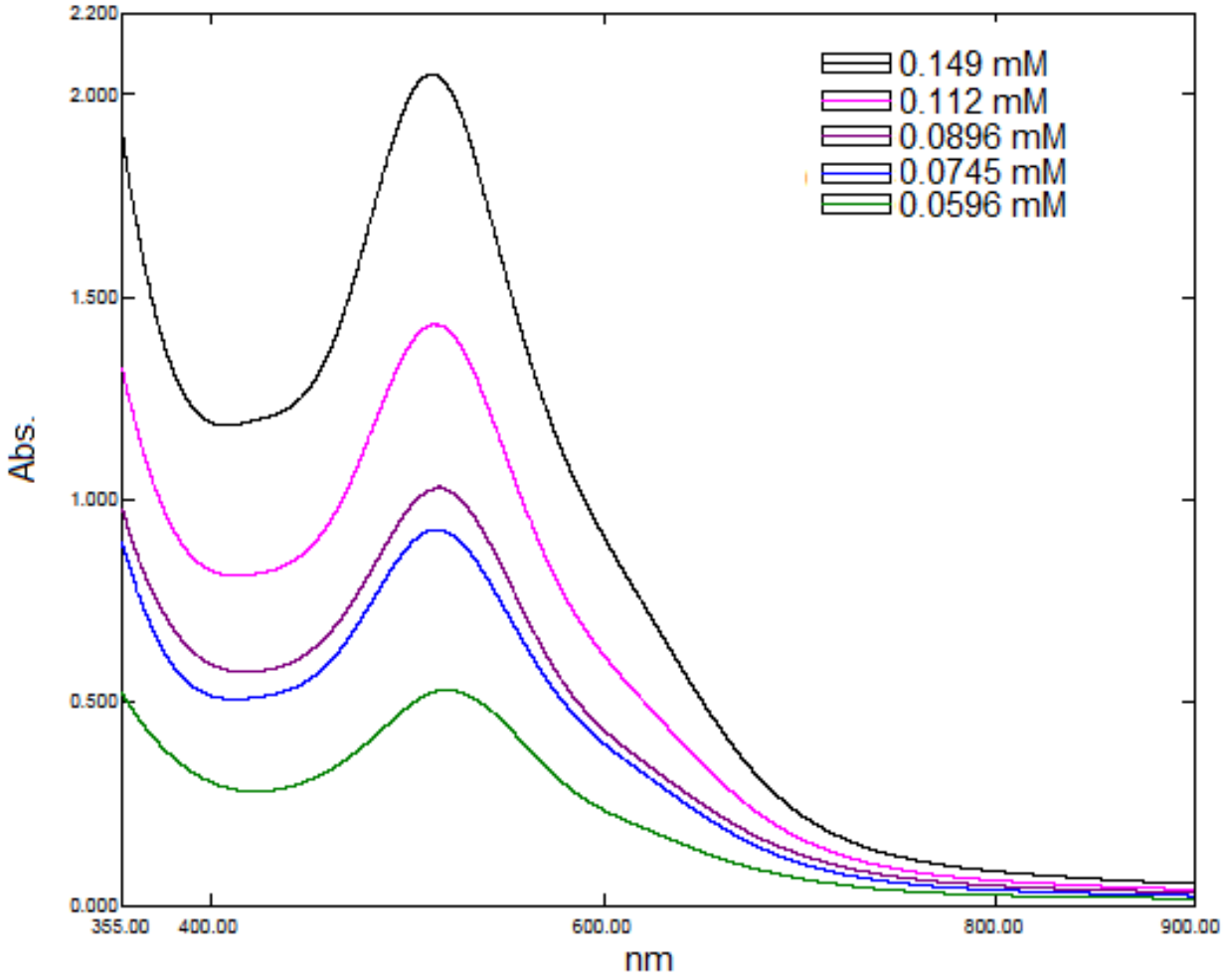


Figure S4. UV-Vis of $(Fe(OR)_2)_2[\mu\text{-}\kappa2{:}\kappa2\text{-}(OC(OMe)C(Ph)NN)_2]$ (**2**).

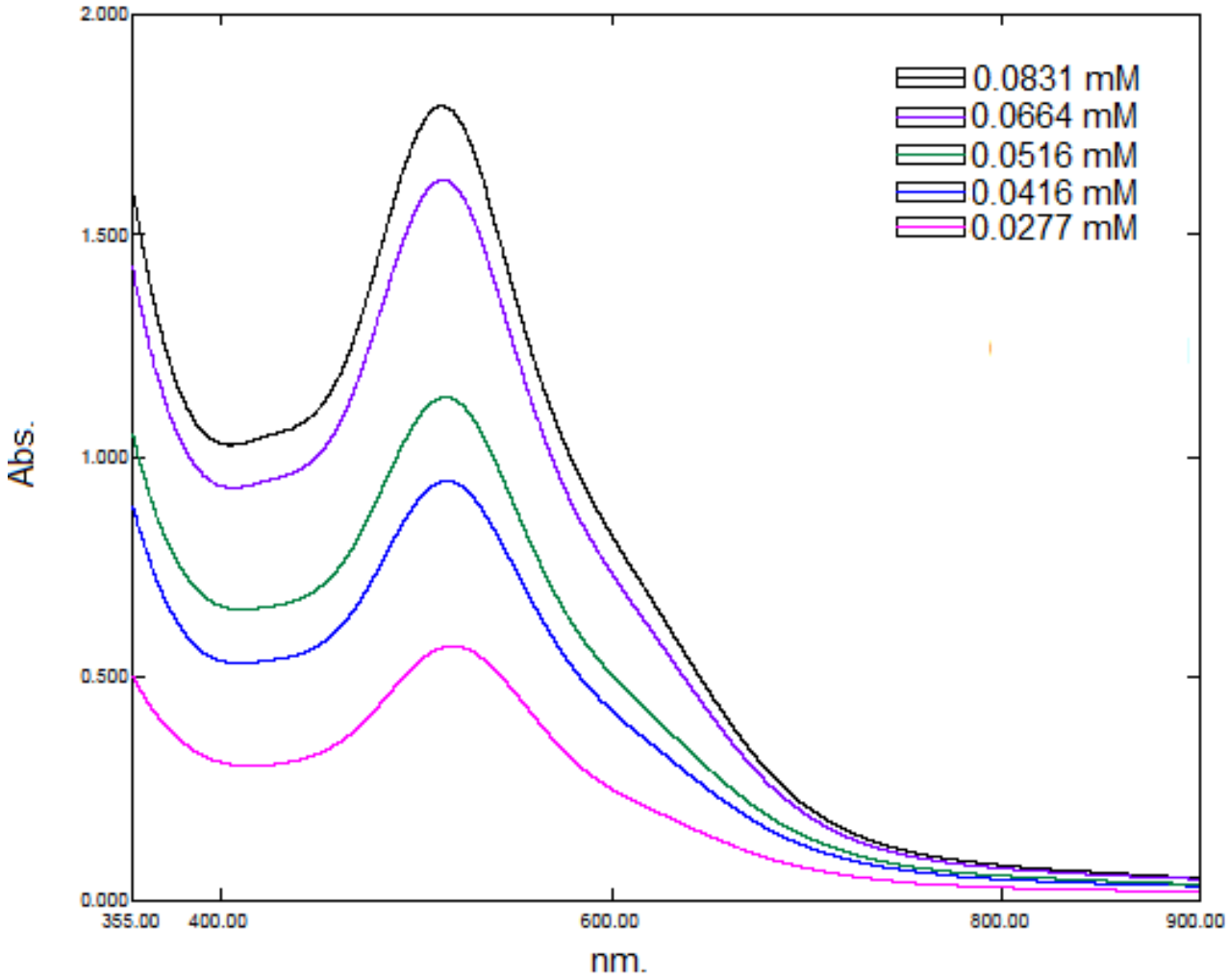


Figure S5.UV-Vis of $(Fe(OR)_2)_2[\mu\text{-}\kappa2\text{:}\kappa2\text{-}(OC(OEt)C(Ph)NN)_2]$ (**3**).

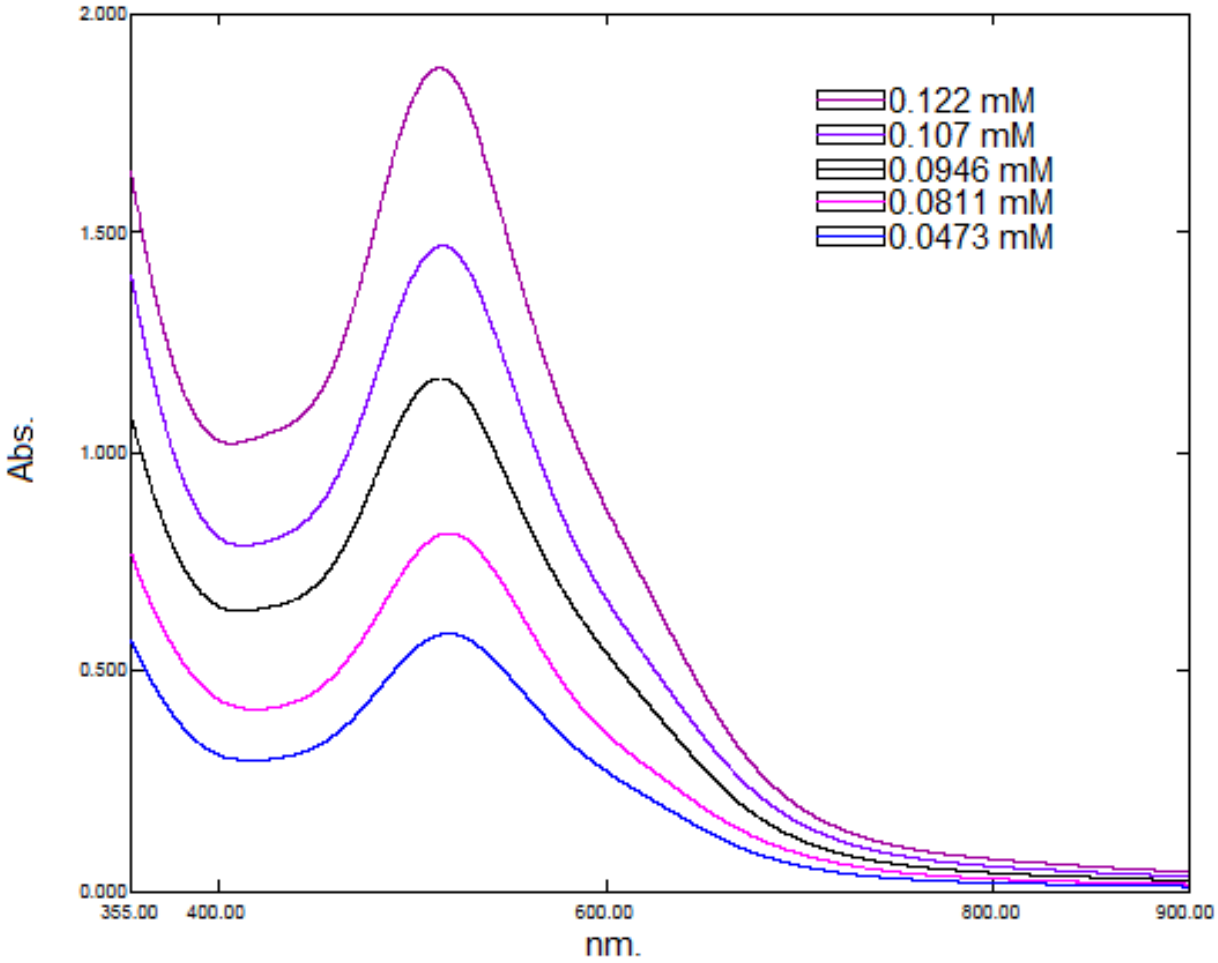


Figure S6. UV-Vis of $(Fe(OR)_2)_2[\mu\text{-}\kappa2\text{:}\kappa2\text{-}(OC(OEt)C(4\text{-}Br\text{-}Ph)NN)_2]$ (**4**).

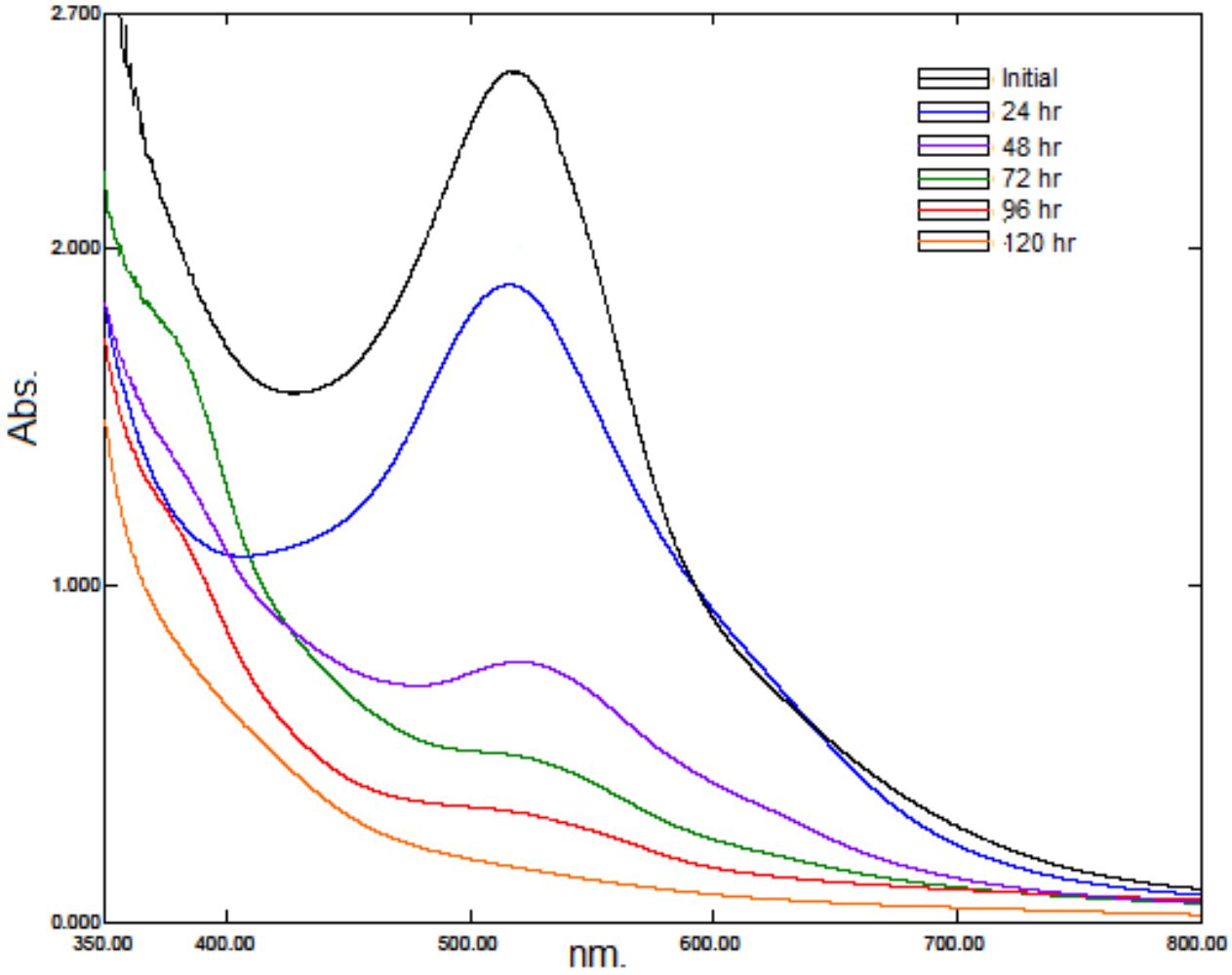


Figure S7. Changes in the UV-Vis spectrum of **2** at RT over 5 days (sampled once a day).

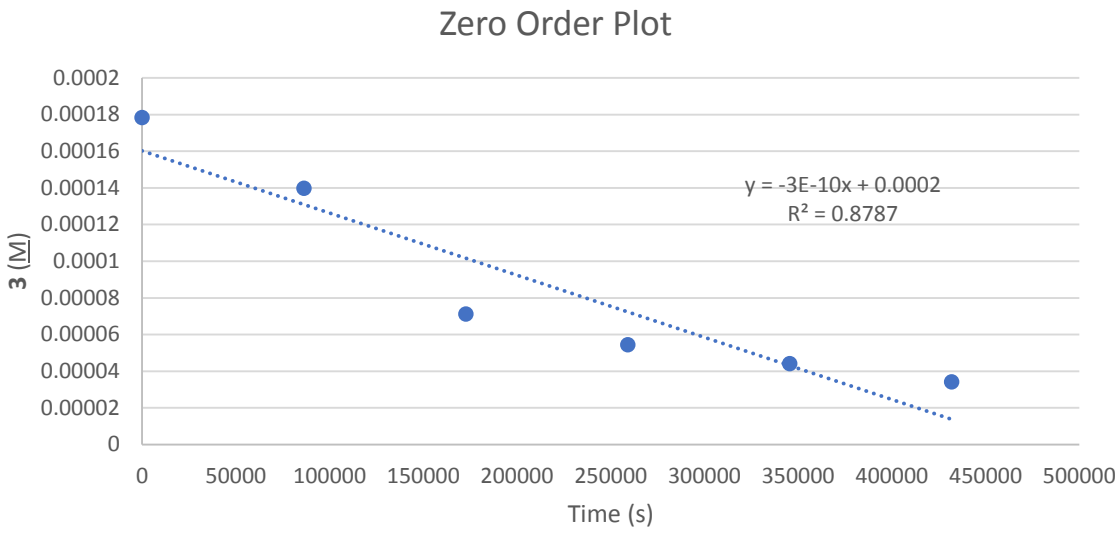


Figure S8. Zero-order plot for the decomposition of **2** monitored by UV-Vis (**Figure S7**).

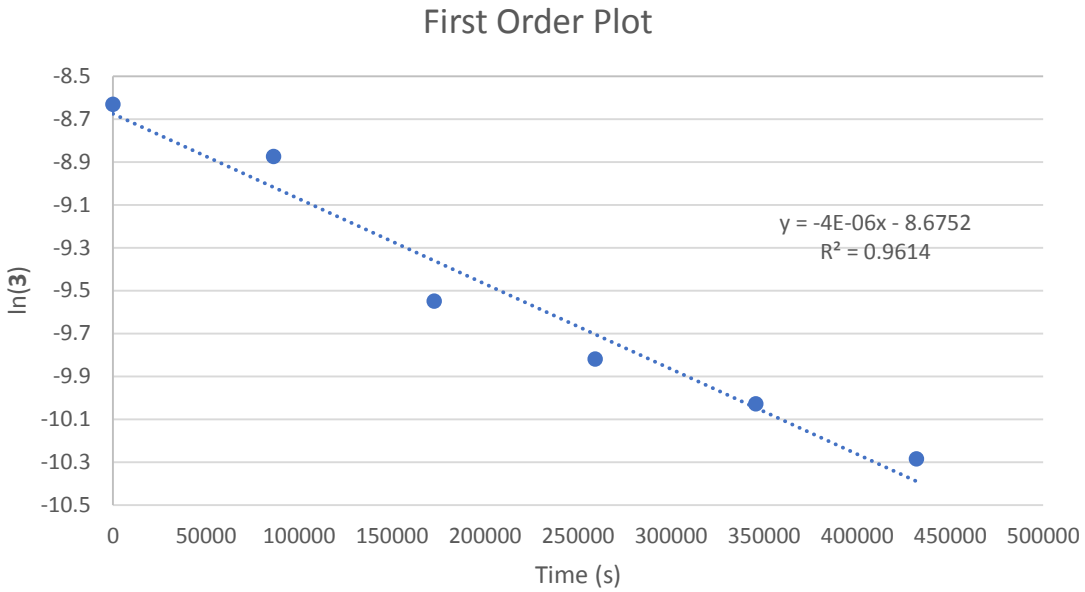


Figure S9. First order plot for the decomposition of **2** monitored by UV-Vis (**Figure S7**).

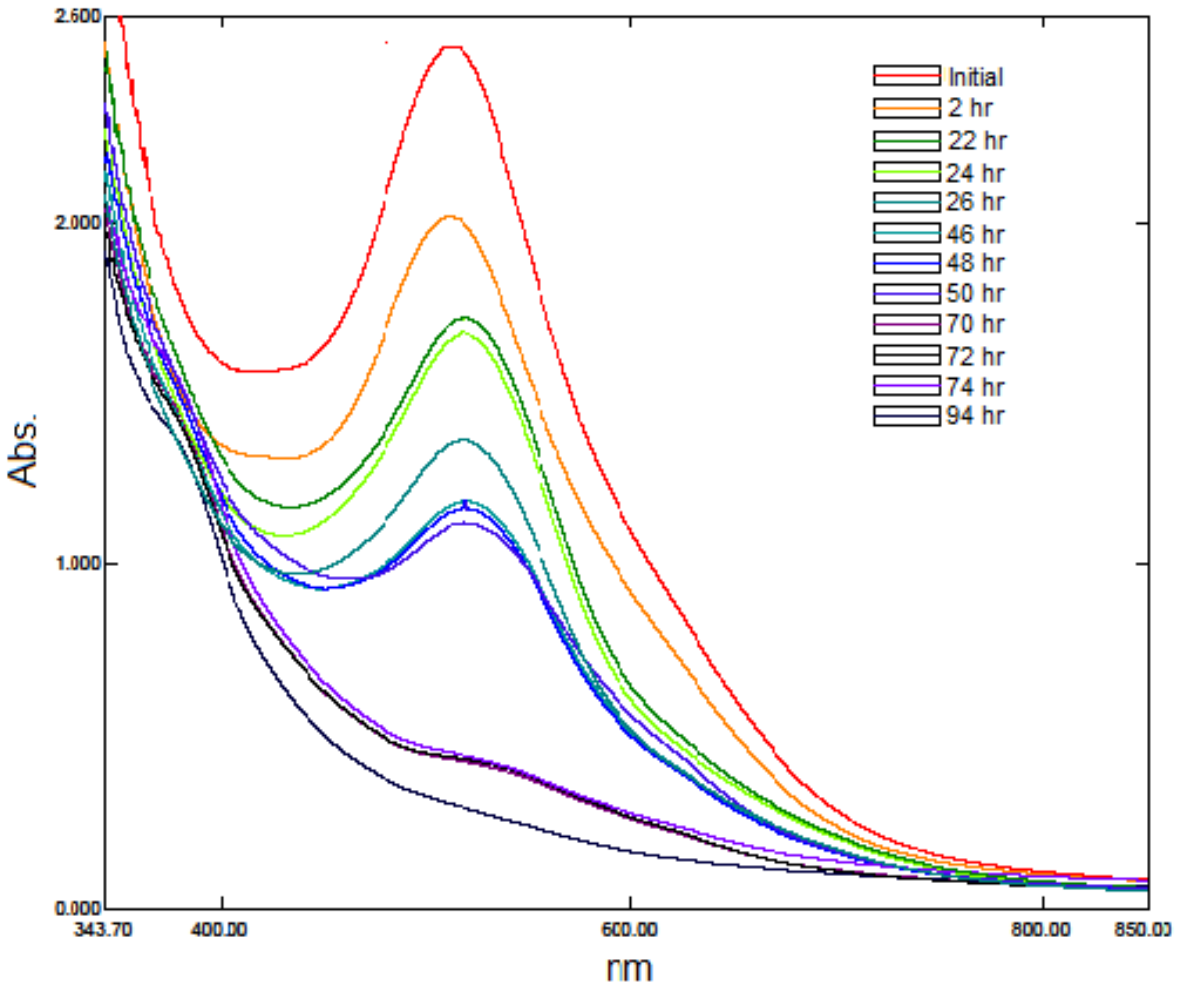


Figure S10. Changes in the UV-Vis spectrum of **2** at RT over 5 days (sampled several times a day).

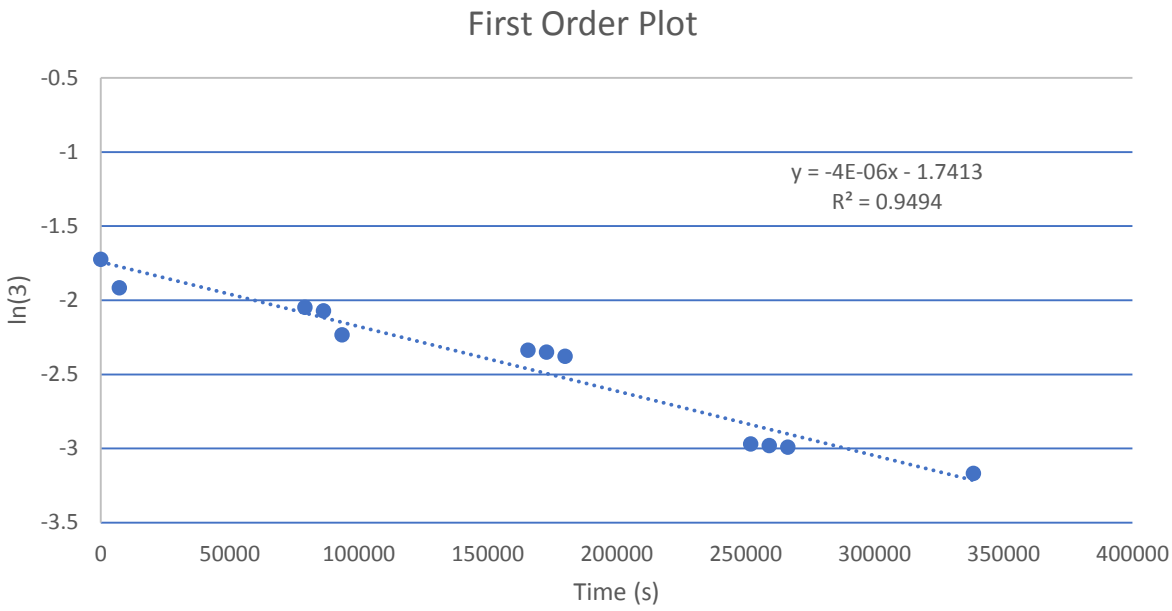


Figure S11. First order plot for the decomposition of **2** monitored by UV-Vis (**Figure S10**).

6. NMR spectra

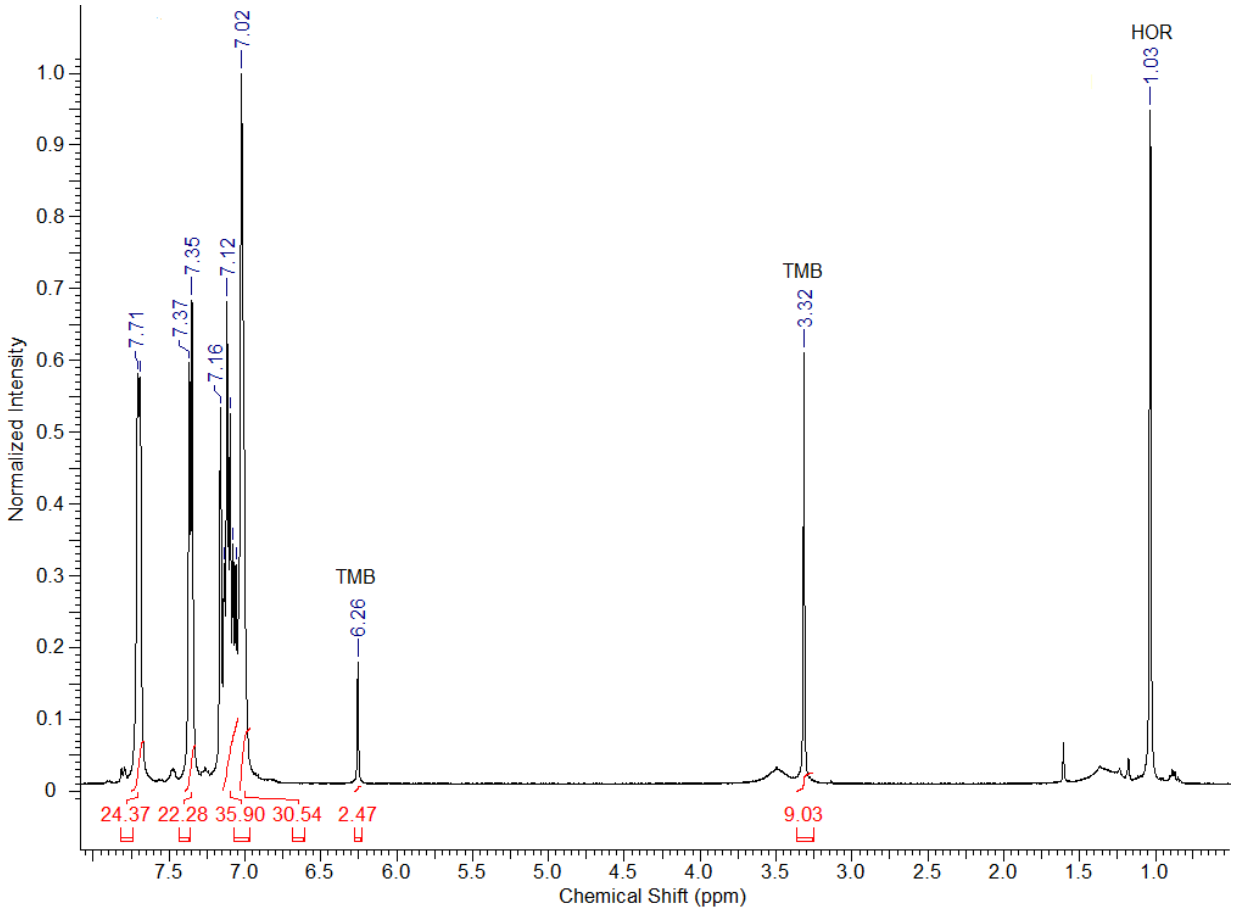


Figure S12. ^{1}H NMR spectrum demonstrating catalytic formation of $Ph_2CNNCPh_2$ from **1**. The peaks at 6.26 and 3.32 ppm correspond to trimethoxybenzene (TMB) used as an internal standard.

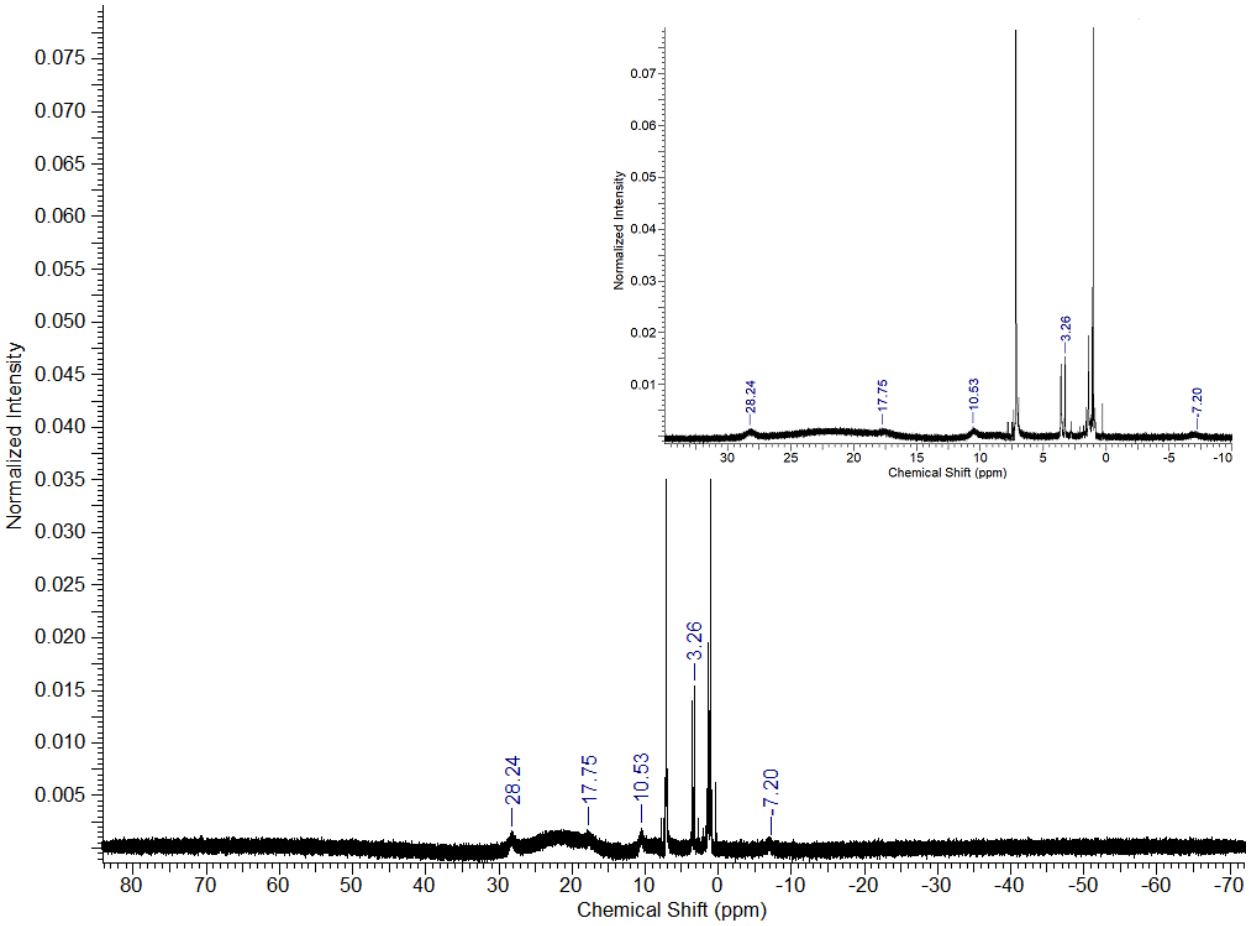


Figure S13: ^{1}H NMR spectrum of **2**.

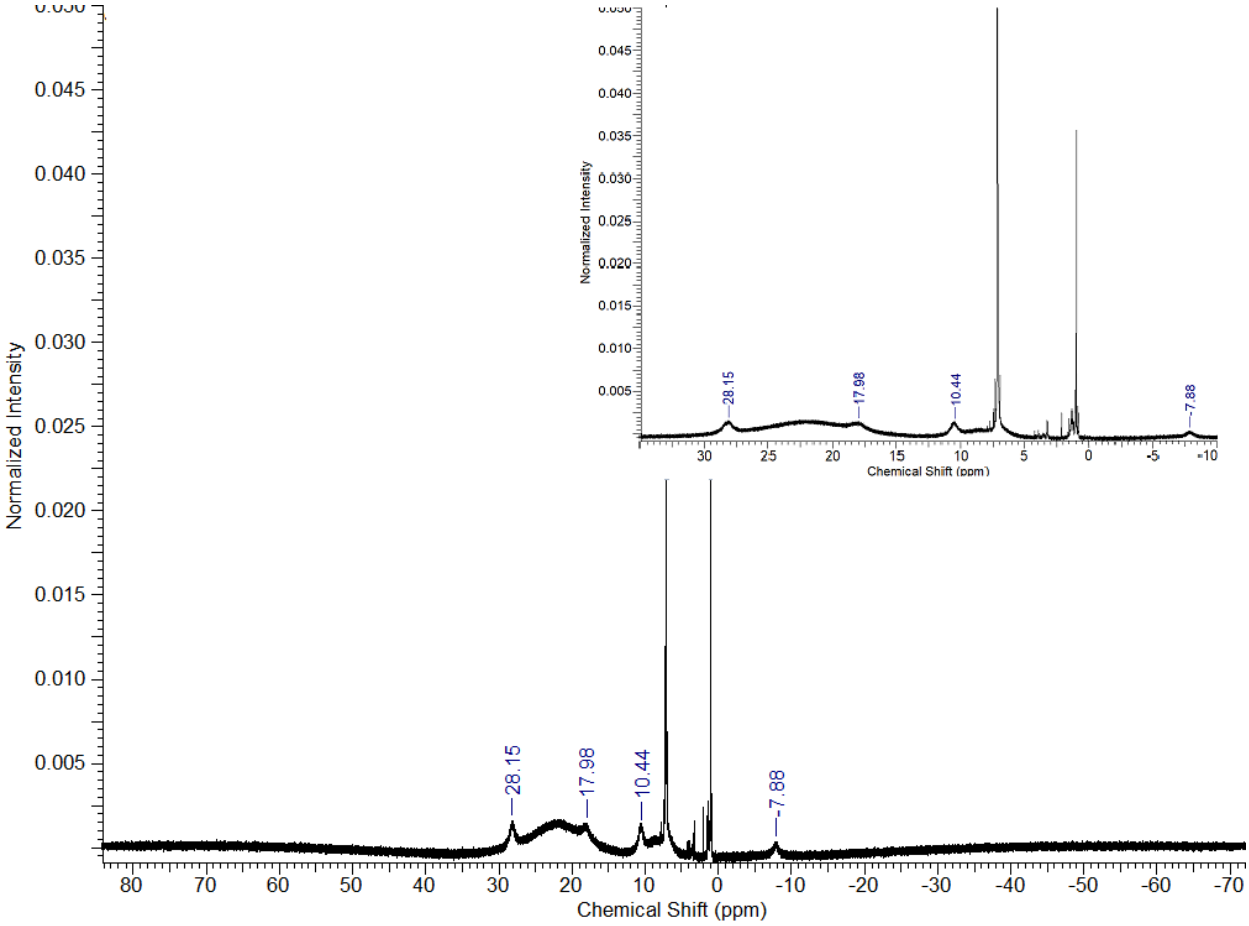


Figure S14: ^{1}H NMR spectrum of **3**.

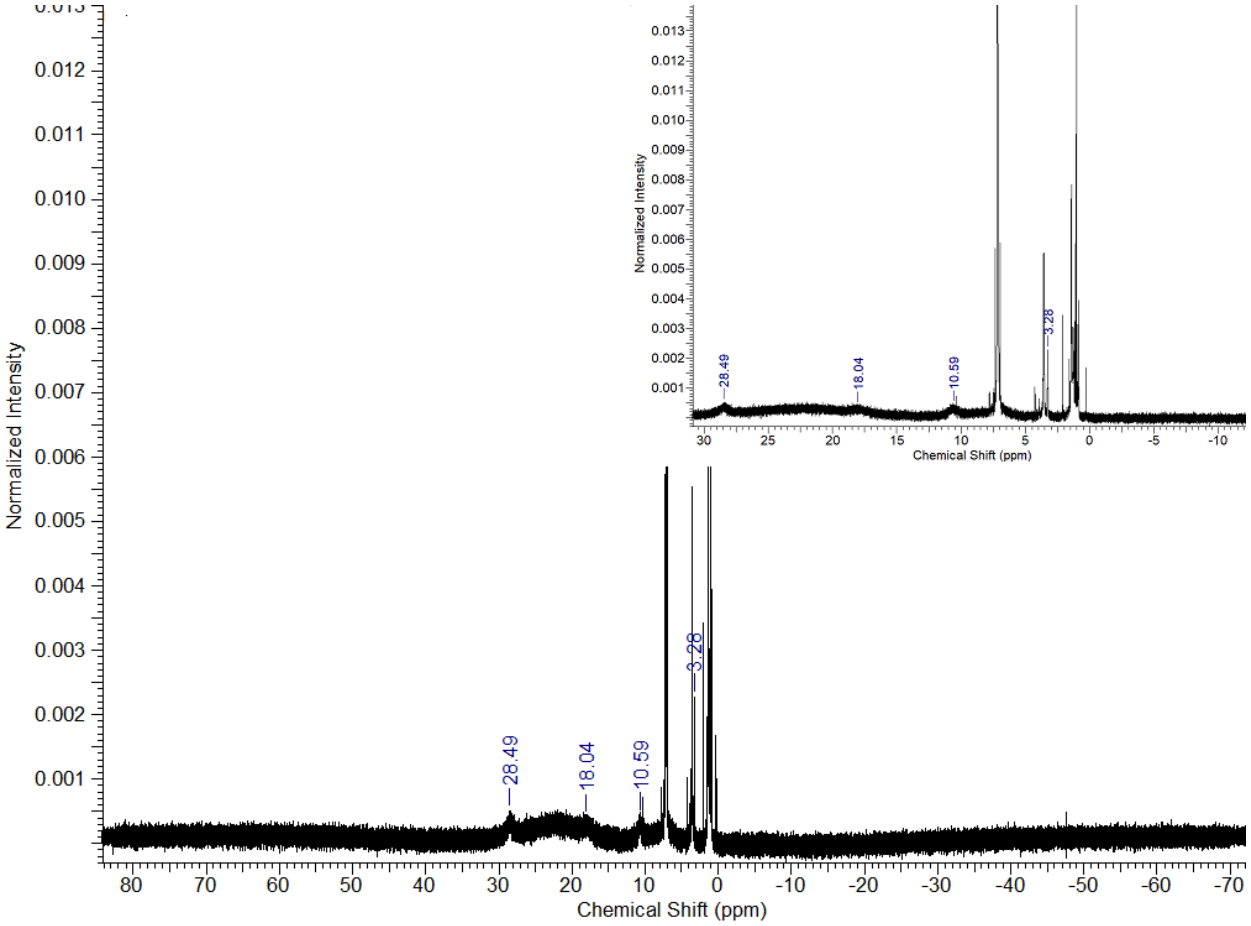


Figure S15: ^{1}H NMR spectrum of **4**.

7. GC-MS spectra

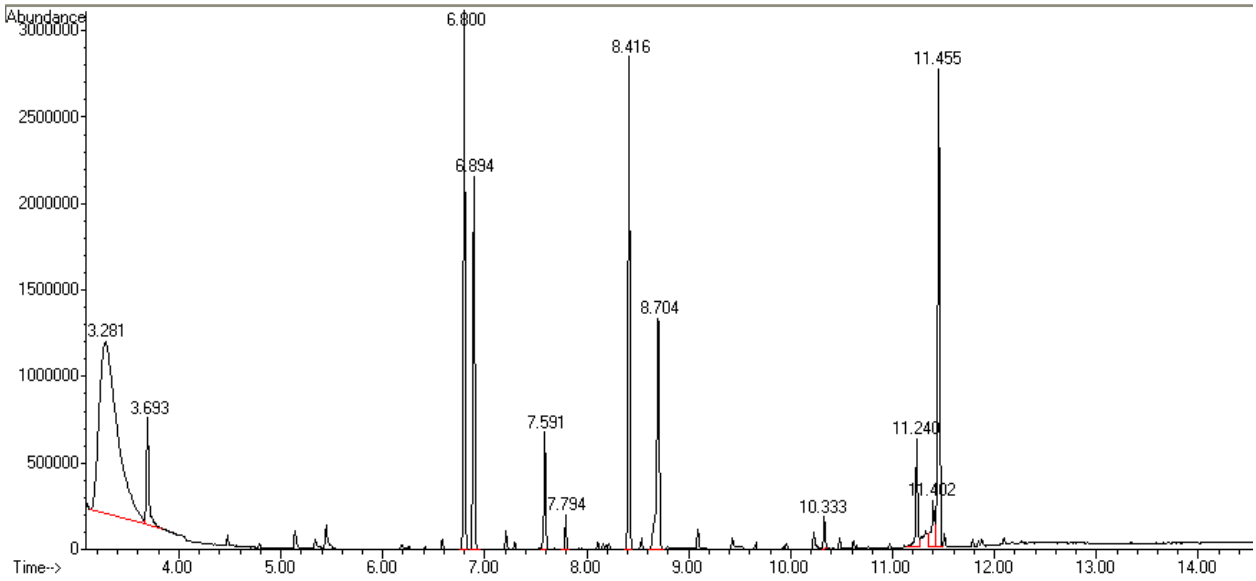


Figure S16. GC taken after stirring **2** at 50 ˚C overnight**.**

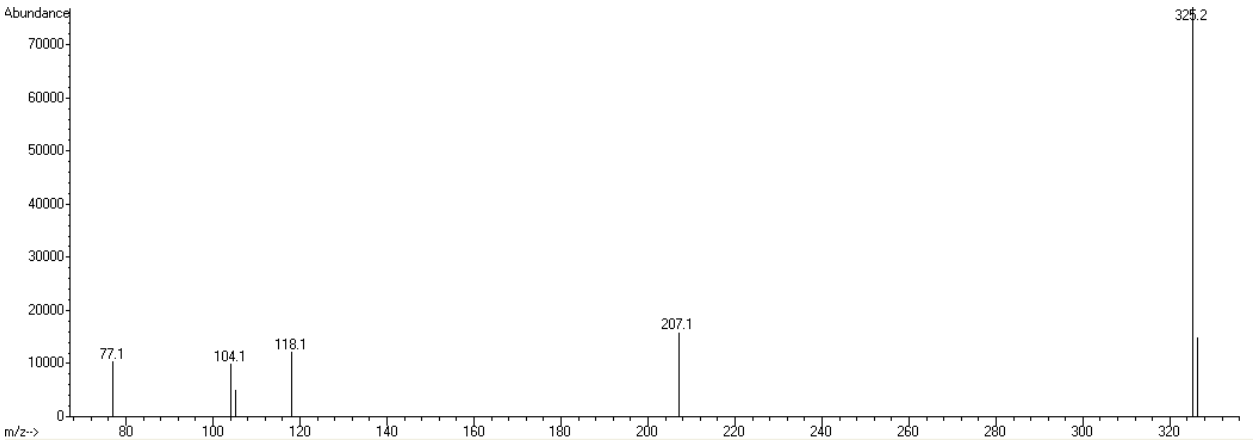


Figure S17. MS of peak at 11.455 in the chromatogram above showing formation of azine**.**

8. Computational Details

DFT calculations were performed using Gaussian 09[4] with default grids and density fitting (when possible). Geometry optimizations at the BP86-D3/def2-SVP level of theory[5–9] were followed by stability calculations[10] to ensure Aufbau electron configurations and harmonic frequency calculations to establish optimized structures as minima.[11] Thermodynamic corrections used standard approximations to estimate enthalpies, entropies, and Gibbs free energies based on the unscaled harmonic frequencies at 298.15 K.[12] Follow-up single point calculations at the B3LYP-D3/def2-TZVP[7,13–16] level of theory simulated the effects of solvent (*n*-hexane) using the SMD implicit solvation model.[17] Triple-zeta free energies were estimated as $G_{TZ} = G_{DZ} - E_{DZ} + E_{TZ}$. Cartesian coordinates are included separately in xyz format, calculated frequencies are listed in **Table S6**, and thermodynamic values are listed in **Table S7**.

Singlet, triplet, quintet, and septet states were probed for the diazoester iron adduct. The metallacycle with the ester coordinated in addition to the diazo moiety (κ^2) was favored. The quintet was found to be lowest in energy (ΔG = 0.0 kcal/mol), followed by the septet (ΔG = 11.1 kcal/mol), triplet (ΔG = 23.6 kcal/mol), and singlet (ΔG = 38.3 kcal/mol). Analysis of the spin density of the quintet state is presented in **Figure S18** and, when combined with the Mulliken spins in **Table S3**, shows this species is best described as a high-spin Fe^{III} ion antiferromagnetically coupled to a diazoester radical anion. An alternative isomer with only the ester coordinated (κ^1) was also calculated for the quintet state. This monodentate form is higher in free energy by 1.34 kcal/mol and is best described as a high-spin Fe^{II} species.

Figure S18. Spin density isosurface plot (iso = 0.002 au) of the lowest energy, S = 2 state of the iron diazoester complex at the BP86-D3/def2-SVP level of theory.

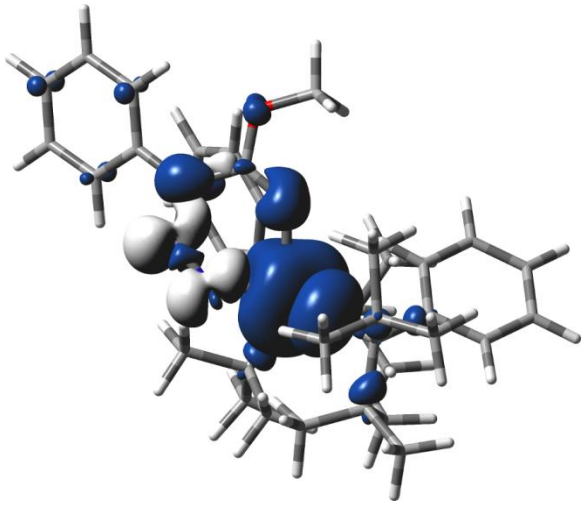
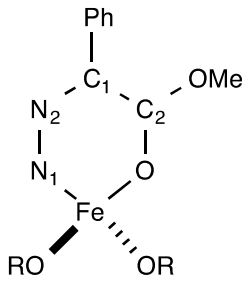


Table S3. Mulliken spins for iron diazoester adducts at the BP86-D3/def2-SVP level of theory.



State	Fe	O_{OR}	O_{OR}	N_1	N_2	C_1	C_2	O
κ^2 $S = 0$	0.06	0.10	–0.09	0.03	–0.01	–0.03	–0.01	–0.03
κ^2 $S = 1$	2.10	0.09	0.00	–0.12	–0.09	0.00	–0.02	0.03
κ^2 $S = 2$	3.45	0.32	0.26	–0.20	–0.13	0.09	0.00	0.07
κ^1 $S = 2$	3.58	0.21	0.18	–0.04	–0.01	0.01	0.00	0.03
κ^2 $S = 3$	3.93	0.37	0.33	0.63	0.28	0.12	0.02	0.09

Singlet through septet states were calculated for the iron carbene resulting from N_2 loss. The quintet was found to be lowest in energy (ΔG = –11.35 kcal/mol vs. quintet diazoester adduct), followed by the septet (ΔG = –10.98 kcal/mol), triplet (ΔG = –8.06 kcal/mol), and finally the singlet (ΔG = 22.18 kcal/mol). Given the sensitivity of density functionals for predicting spin states and the tendency of B3LYP to overstabilize higher spin states,[18] we cannot say conclusively whether the quintet or triplet is favored without experimental verification. Formation of the quintet carbene can occur through two transition states: (i) from the κ^2 diazoester ($\Delta G^{\ddagger}$ = 27.09 kcal/mol) or (ii) from the κ^1 diazoester ($\Delta G^{\ddagger}$ = 29.33 kcal/mol). Loss of N_2 from the κ^2 form is slightly lower in energy, consistent with the equilibrium for this species that slightly favors the κ^2 form over the κ^1 form by 1.3 kcal/mol.

Singlet through undecet states were probed for tetrazene product formed by coupling of two of these iron diazoester adducts. The undecet was predicted to be lowest in energy followed by the singlet, nonet, triplet, quintet, then septet. The undecet and singlet were much lower in energy than the other spin states. Quantitative relative energies of these species, as well as the Mulliken spins at each iron center, are shown in **Table S4**. Based on these Mulliken spins we assign the undecet and singlet as ferro- and antiferromagnetically coupled species with two high-spin Fe^{III} ions. The higher energy states involve spin flips at one or more of the iron centers, with the nonet and triplet corresponding to ferro- and antiferromagnetic coupling between one high-spin and one intermediate-spin Fe^{III} ions. The quintet has one high-spin Fe^{III} antiferromagnetically coupled to a low-spin Fe^{III} ion. The septet has two ferromagnetically coupled intermediate-spin Fe^{III} ions. **Figure S19** shows spin density plots for the two lowest energy states. These spin densities highlight the significant spin polarization in the atoms directly attached to the metal centers, which leads to lower Mulliken spins than might be expected. It is clear from these results that the two magnetic states with high-spin Fe^{III} ions are much more favorable in the low-coordination environment in this product.

The singlet and undecet states are nearly isoenergetic at the BP86-D3/def2-SVP (ΔE = 0.24 kcal/mol) and B3LYP-D3(SMD)/def2-TZVP (ΔE = 0.01 kcal/mol) levels of theory, even though BP86 is known to overstabilize low-spin states while B3LYP overstabilizes high-spin states.[18] The near degeneracy predicted for these states may explain the low magnetic moment observed experimentally since both would be expected to have significant thermal population, but more precise magnetic measurements than Evans' method[3] would be needed to determine this precisely. Because of this we focus our attention on the ferromagnetically coupled state in this manuscript.

Table S4. Relative Gibbs free energies (in kcal/mol) and Mulliken spins for each spin state calculated for the tetrazene coupled product.

State	ΔG	Fe_1	Fe_2
S = 0	0.57	3.88	–3.88
S = 1	26.01	3.90	–2.62
S = 2	41.95	3.89	–0.81
S = 3	45.43	2.76	2.76
S = 4	24.72	3.87	2.74
S = 5	0.00	3.89	3.89

Figure S19. Spin density isosurface plots (iso = 0.002 au) of the antiferromagnetically coupled S = 0 (left) and ferromagnetically coupled S = 5 (right) states of the iron tetrazene complex at the BP86-D3/def2-SVP level of theory.

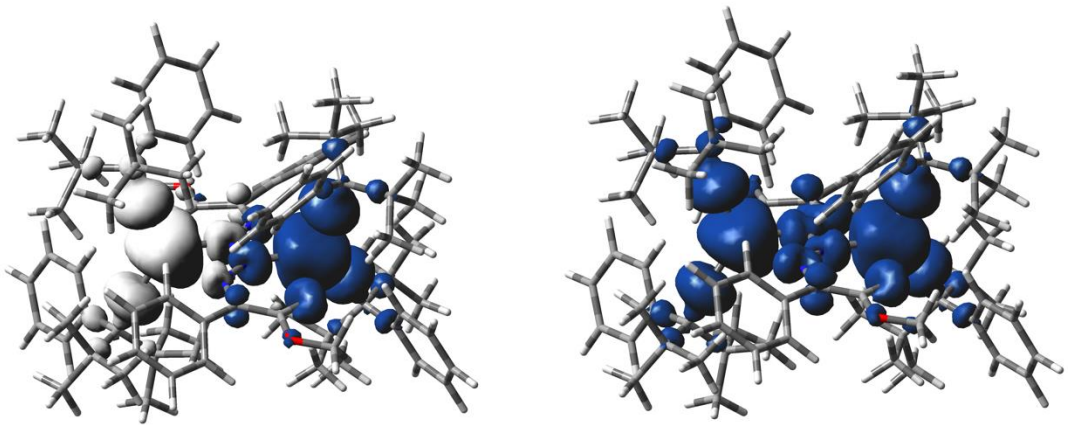


Figure S20. Potential energy scan along the N–N coordinate showing no enthalpic barrier for bond formation on the *S* = 5 surface. Red dots correspond to final SCF energies for constrained geometry optimizations except for the minimum (fully optimized structure) and completely dissociated species (listed at 4.0 Å here, corresponds to twice the *S* = 2 iron diazoester energy). The black curve is a Morse curve fit with D_e = 47.94 kcal/mol, r_e = 1.357 Å, and a = 2.25.

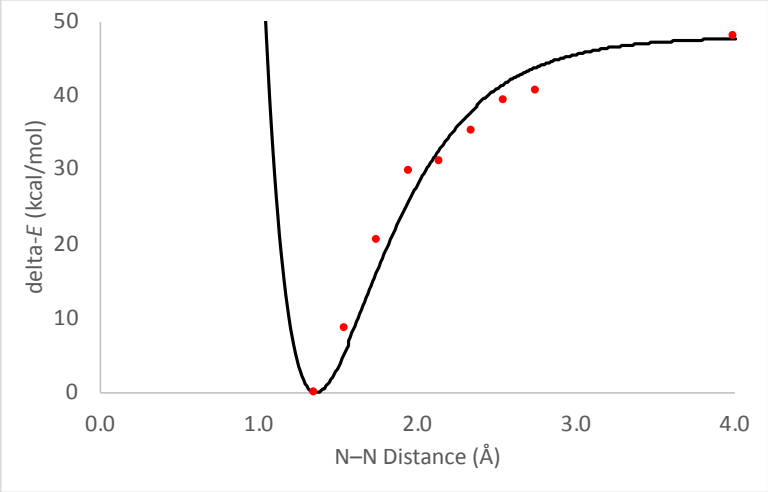
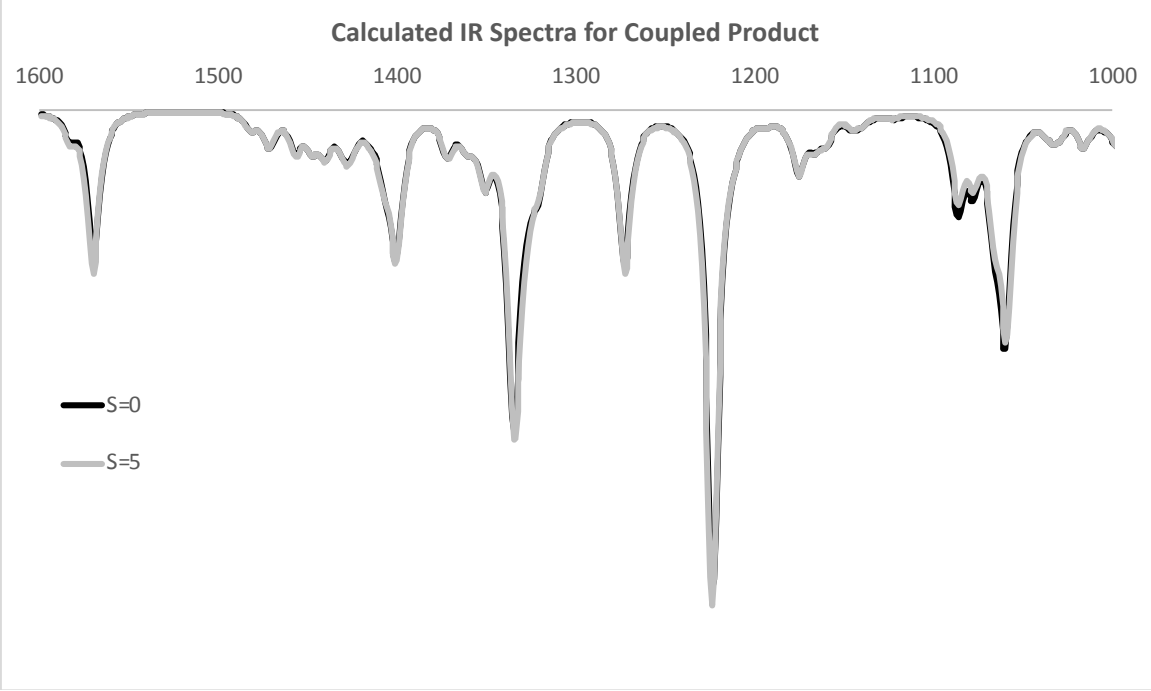


Figure S21. Calculated IR spectra for the *S* = 0 and *S* = 5 states of the reductively coupled iron product at the BP86-D3/def2-SVP level of theory. Unsurprisingly, both produce remarkably similar IR spectra. Line spectra were generated in Gaussian then fit using the default parameters in GaussView.[19]



To understand the contrasting reactivity of this new iron complex with our previously reported work with cobalt and diazoester,[20] we ran similar calculations of the cobalt diazoester and cobalt reductively coupled products. These results are reported below.

Doublet, quartet, and sextet states for the cobalt diazoester adduct were run. In the κ^2 form the quartet is lowest in energy (ΔG = 0.00 kcal/mol), followed by the sextet (ΔG = 17.02 kcal/mol) and the singlet (ΔG = 20.88 kcal/mol). Unlike iron, however, the κ^1 form is favored by 5.30 kcal/mol over the κ^2 form for the quartet. Similar to iron, the κ^2 quartet is best described as high-spin Co^{III} antiferromagnetically coupled to the reduced diazoester, while the κ^1 quartet is best described as a high-spin Co^{II} species. **Table S5** summarizes the Mulliken spin densities of these species.

Table S5. Mulliken spins for cobalt diazoester adducts at the BP86-D3/def2-SVP level of theory. The numbering in the diazoester is the same as for the iron adduct (**Table S3**).

State	Co	O_{OR}	O_{OR}	N_1	N_2	C_1	C_2	O
κ^2 S = 1/2	1.03	0.14	–0.08	–0.11	–0.07	0.06	0.00	0.02
κ^2 S = 3/2	2.40	0.37	0.35	–0.22	–0.16	0.04	0.01	0.07
κ^1 S = 3/2	2.44	0.26	0.20	0.00	0.00	0.00	0.01	0.03
κ^2 S = 5/2	2.74	0.42	0.38	0.68	0.17	0.21	0.01	0.11

We calculated the doublet, quartet, and sextet carbene species. Unsurprisingly, the doublet was found to be lowest in energy (ΔG = –3.54 kcal/mol vs. κ^1 cobalt diazoester adduct), followed by the sextet (ΔG = –2.06 kcal/mol) then the quartet (ΔG = 0.60 kcal/mol). This is consistent with our extensive calculations and spectroscopy of the electronic structure of this compound.[20,21] Transition states for N_2 loss from both the κ^2 diazoester ($\Delta G^{\ddagger}$ = 38.67 kcal/mol) and κ^1 diazoester ($\Delta G^{\ddagger}$ = 37.02 kcal/mol) were located. In contrast to iron, for cobalt the k^1 transition state is favored presumably due to the equilibrium favoring that form over the k^2 form with reduced diazoester.

For the reductively coupled cobalt species, only the singlet and nonet states were calculated. Similar to iron these were found to feature two high-spin Co^{III} ions antiferromagnetically and ferromagnetically coupled to one another. The nonet state is slightly favored in free energy by 2.11 kcal/mol. The driving force to form this reductively coupled species is markedly lower than for iron, with DFT predicting this to only be exergonic by 1.45 kcal/mol. **Figure S22** shows the spin densities for these two species, which are found to have Mulliken spins at the cobalt atoms of 2.71/–2.71 and 2.73/2.73, respectively. Similar to iron, significant spin polarization to the atoms attached to cobalt lowers these values from the ideal of 4.0/–4.0 and 4.0/4.0.

Figure S22. Spin density isosurface plots (iso = 0.002 au) of the antiferromagnetically coupled *S* = 0 (left) and ferromagnetically coupled *S* = 4 (right) states of the cobalt tetrazene complex at the BP86-D3/def2-SVP level of theory.

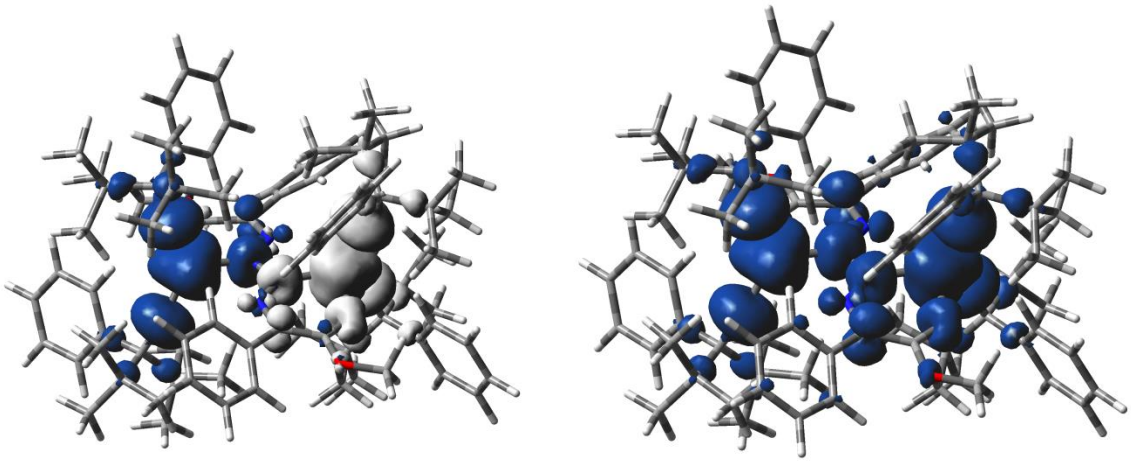


Table S6. Calculated frequencies (cm^{-1}) of all optimized species at the BP86-D3/def2-SVP level of theory. Small imaginary frequencies (< 20 cm^{-1}) were ignored.

N_2

2383.0824

---

diazoester

14.7505 63.0775 93.9036
110.7877 121.0497 136.0788
172.1093 240.8929 296.9553
329.8624 355.8844 400.5201
463.0634 484.3628 498.5987
537.5165 613.2635 665.8637
691.0602 717.3209 752.4658
781.5196 821.8821 896.1133
956.6102 965.4627 979.6147
983.0640 1019.0461 1036.9773
1077.6296 1127.6767 1138.0703
1150.6493 1167.1195 1182.6443
1263.7949 1313.8493 1321.2927
1362.9142 1403.0837 1404.7858
1426.7369 1440.9954 1481.0139
1581.0459 1610.1505 1736.8398
2184.7255 2970.5389 3060.0267
3098.2024 3101.9383 3105.0858
3114.0416 3126.0404 3166.5322

$Fe(OR)_2(k^2$-diazoester)
S=0

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24.2510 33.4607 38.6051
52.9982 56.3513 65.6245
68.2613 71.5715 79.0316
86.8407 94.6181 99.4739
106.0612 109.2949 118.7141
125.9117 130.3536 136.7103
148.6456 153.0675 171.2786
181.5298 182.9529 191.3906
193.5339 202.2756 210.6575
215.6131 221.8136 224.7650
228.2973 232.8159 238.9832
248.2640 250.3385 262.0475
267.4500 272.0261 281.3159
285.1984 291.5583 294.3177
298.2794 300.3265 303.5758
306.7396 312.5991 313.0920
319.7141 324.9568 328.9699
332.5878 338.3142 343.8021
358.5186 361.8113 367.3810
371.8362 380.3346 387.3993
400.3580 402.1200 405.9288
410.8105 413.4866 415.0423
420.2100 429.8943 430.8055
436.5538 444.7355 465.4387
476.5192 481.5097 491.2142
491.6751 508.7697 533.9253
543.5271 547.7096 549.1513
550.9933 557.7502 606.1895
614.6327 615.0721 619.3854
637.4302 653.2773 669.7094
689.2476 698.7438 702.0978
711.6413 717.2574 737.0711
748.8327 761.0434 765.4493
797.8206 799.3929 812.4977
814.7504 817.0680 826.1962
833.2873 850.3180 872.0425
876.3835 889.1366 897.3997
899.9606 902.1908 904.2592
907.3542 907.5276 908.5755
912.7390 913.9982 914.0722
914.8728 915.8883 917.3602
928.1380 929.6084 937.9410
961.0560 961.2340 966.6857
972.4903 973.5459 979.7097
981.1425 981.2504 983.6173
986.7676 988.2810 993.1859
995.6770 999.2697 1002.1705
1006.4596 1006.8350 1015.1721
1018.4431 1022.7701 1027.9664
1034.2806 1034.9354 1036.6139
1072.6667 1074.0882 1077.9187
1125.6552 1132.0468 1136.0220
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3154.9249 3155.1621 3163.4382

$Fe(OR)_2(k^2$-diazoester)
S=1

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90.2220 94.8119 96.6919
100.9109 107.8077 121.7405
125.5963 128.4755 132.0090
148.3225 150.6597 155.7920
177.5357 180.0922 187.3179
192.2320 198.2066 204.8787
213.9044 215.2530 224.1658
230.7570 236.8134 240.8283
245.5687 254.2222 262.7073
264.2600 275.6269 277.5508
280.1707 287.5451 291.3793
293.7855 301.0251 304.6056
309.1454 313.5324 315.6749
322.3266 324.0728 328.6717
330.5133 335.5248 340.3841
347.6459 349.0231 362.3152
375.3552 377.4404 380.2679
398.6822 402.1588 411.0492
411.4045 414.8661 415.3838
417.9363 428.1034 430.0118
435.4055 435.8109 442.0288
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538.9035 546.9907 547.8426
550.1683 551.4442 598.0268
615.2478 615.4781 617.3428
637.9991 649.4809 668.2943
688.9830 697.5590 699.7213
705.4392 716.5138 734.7422
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870.7561 887.1257 894.7562
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3126.4033 3144.1772 3152.7372
3160.0312 3162.1577 3173.4921

$Fe(OR)_2(k^2$-diazoester)
S=2

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96.7110 104.1534 107.5897
115.9056 120.5474 121.0549
135.1186 148.0334 150.2722
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182.8760 193.3874 199.7211
205.7641 213.4705 214.3769
220.9217 230.9752 233.5268
235.1792 250.3945 261.2237
267.6433 279.0333 283.0608
285.9030 288.3977 292.7090
297.4837 304.2932 308.4709
312.5921 316.8623 320.4453
321.6863 324.7421 327.2794
331.9475 332.8748 338.1049
342.3226 347.3147 359.2220
372.8171 377.7194 389.4573
399.3785 403.2936 405.6820
409.6350 412.8368 413.6467
414.1795 417.5990 418.3646
424.5792 426.2733 429.3891
441.6146 449.7793 457.3331
493.1782 497.3222 508.6393
528.2619 545.1592 546.4943
548.8547 551.2026 571.7297
614.4811 614.8419 617.0719
644.1790 649.0095 665.5070
689.6866 706.2562 709.4080
717.1195 719.5362 733.5149
748.4073 756.4686 760.3708
798.4268 799.6331 801.4858
815.9436 817.5961 823.8897
833.8098 841.9212 879.1620
884.7532 885.3849 891.0931
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957.2498 958.6420 964.7182
967.2639 978.9063 980.2733
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989.9391 993.2780 998.6357

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1019.3214	1031.3943	1033.2975
1038.3355	1052.8432	1066.2373
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1352.6003	1356.0761	1361.8634
1364.1457	1365.2711	1366.5394
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2965.8746	2967.7268	2967.8266
2968.0438	2971.1148	2973.6066
2973.7240	2976.1190	2977.4963
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3044.2002	3044.7988	3045.4554
3047.3864	3048.2228	3049.7184
3051.0873	3054.0484	3057.9017
3060.1701	3071.4071	3072.5769
3074.0943	3074.7258	3075.2356
3080.2691	3082.6767	3086.2192
3091.3700	3092.4455	3096.3676
3097.4657	3098.8194	3099.0833
3099.3228	3105.2052	3106.9104
3108.9951	3110.5606	3112.1283
3116.0449	3119.6338	3124.2540
3124.4914	3131.9560	3147.4607
3150.9680	3153.6992	3163.5747

$Fe(OR)_2$(k^1-diazoester)
S=2

15.1295	20.7234	32.6973
38.6783	40.5406	44.9034
51.9378	57.3418	61.4749
69.1258	71.8720	80.6625
85.0222	89.3109	93.4466
99.7185	101.6824	105.1149
106.8420	109.2683	114.6423
116.2064	123.0183	127.1880
131.5934	135.7909	148.5297
171.1104	176.0447	185.8427
188.1770	202.3706	210.5571
222.6743	230.3484	233.4443
237.2236	247.3465	249.7666
253.3848	262.8970	268.6362
277.2622	279.6199	291.0982
291.7168	293.0421	296.7047
298.2609	307.7433	312.1187
317.2369	319.5332	322.3514
326.5395	331.4755	333.4081
336.3273	343.5244	344.3743
348.7088	372.6222	383.7775
389.4706	393.3522	402.6176
406.3016	409.6045	413.6835
415.8583	419.6228	421.9851
423.9122	426.2346	426.6916
432.7772	444.0459	456.9053
493.2708	494.8656	509.6592
540.1372	542.3962	543.3805
546.3777	550.5569	551.1406
611.7386	614.9069	617.7035
637.2697	649.3460	653.2685
689.3313	704.9425	706.0378
708.8447	716.9430	732.2655
739.8408	744.4486	758.5244
788.9185	796.5750	799.7103
807.1717	814.7118	818.7459
834.2907	838.8246	877.5526
882.3318	883.6820	887.6985
890.4357	900.3762	903.7345
906.1286	906.5936	909.2599
911.5557	912.1986	914.1871
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923.2296	924.7890	929.4270
931.8728	949.2198	959.6651
965.1295	977.2424	977.9239
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1017.5950	1028.8149	1031.5403
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1137.5602	1146.0099	1147.6761
1149.1302	1154.9897	1160.7761
1163.5966	1167.5611	1169.4779
1174.0929	1178.4369	1181.2268
1183.4059	1188.8747	1192.9189
1203.2065	1207.6678	1211.7232
1217.5347	1219.6834	1275.1024
1278.1334	1278.6743	1317.1398
1317.5197	1319.1851	1322.2760
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1328.0676	1331.0565	1348.5482
1350.6756	1352.3540	1356.8265
1359.1823	1362.0326	1364.7807
1365.5917	1391.2714	1392.5675
1394.2320	1396.5594	1403.5158
1405.9589	1406.4633	1407.4630
1409.1548	1412.1618	1414.7318
1416.3959	1418.2476	1419.0318
1420.3510	1421.0061	1422.0439
1424.4794	1425.2095	1426.1319
1427.6781	1429.5704	1431.9431
1433.7844	1434.5121	1436.2550
1439.7348	1444.3176	1451.7625
1454.5010	1469.5256	1471.7971
1474.2082	1560.7369	1587.3121
1588.1443	1592.1088	1609.2275
1609.8870	1629.4406	2155.1395
2960.9271	2961.0334	2962.7558
2963.0912	2963.2001	2963.7535
2964.3137	2969.1336	2969.2567
2970.1737	2971.6429	2976.7683
2982.0787	3032.6403	3039.5162
3040.1588	3040.5176	3040.6268
3043.2682	3045.0856	3047.2277
3048.0602	3048.8839	3056.5704
3059.5816	3067.7410	3068.2849
3075.6678	3080.7172	3081.3701
3081.4964	3083.4270	3087.0853
3088.6426	3091.5703	3093.2056
3093.4657	3094.7314	3099.0578
3102.1742	3103.4811	3105.6212
3109.3954	3114.5526	3115.9323
3117.4223	3118.4333	3123.9425
3129.5124	3134.3744	3143.2317
3146.0853	3153.6199	3177.5038

$Fe(OR)_2$(k^2-diazoester)
S=3

-14.2809	11.5575	19.4784
20.6930	29.6938	31.6240
34.8460	50.0230	54.8941
59.8298	65.1373	67.8322
77.5115	79.3963	87.6101
93.6138	96.2162	98.4483
105.4095	116.3261	127.4578
129.1771	139.0639	141.5812
158.5820	171.1726	176.1965
186.9554	196.4478	208.3398
209.0455	219.0209	222.1467
232.3807	244.0156	252.7630
257.3097	258.6135	267.6939
269.8938	274.0964	279.4304
282.6169	283.4730	292.8693
294.6077	297.8472	301.2378
303.3011	305.1315	318.0175
320.4675	324.1312	326.8239
328.9967	332.9304	335.4728
336.8952	350.2738	354.4759
367.3678	371.6602	375.9199
384.7134	388.4898	401.6266
402.1692	408.4148	411.3045
412.4675	414.5880	415.0312
416.2394	419.3848	431.0114
434.1734	434.8999	466.6191
470.9403	493.8915	496.7118

519.5362 542.8161 547.6453
549.2967 553.6974 573.7292
614.1508 615.6138 618.4895
637.3866 641.0649 659.4776
690.2962 704.7974 707.7611
716.6988 731.8731 740.7208
744.4371 752.6314 759.7846
796.1792 796.8276 797.8243
810.7193 811.7104 824.4327
836.0027 839.3225 876.7846
882.3998 885.3485 886.9179
900.6941 901.0304 902.0414
902.8039 908.2685 909.8831
911.4057 911.9494 915.7642
916.4403 917.9870 919.0092
920.2847 929.4478 930.7987
957.8793 962.6523 966.6177
968.3198 977.9535 983.5156
984.0070 985.2701 986.1417
988.6010 991.8621 992.7538
994.9766 997.5439 1002.9892
1004.7034 1006.2202 1010.3880
1016.3305 1028.7914 1029.3200
1035.3034 1052.4443 1060.6580
1072.0767 1077.2428 1082.8094
1122.3259 1132.2948 1132.8508
1135.4399 1143.7328 1148.1723
1148.7457 1159.0333 1160.6808
1162.9819 1164.3560 1166.4388
1172.0300 1174.6509 1180.5375
1181.9927 1189.6454 1191.9605
1198.1567 1202.5846 1207.9771
1214.2861 1219.0459 1267.6869
1277.4965 1279.3551 1306.8565
1314.6504 1321.0385 1324.3899
1325.4341 1328.8783 1329.1778
1330.4680 1335.9365 1340.1882
1351.7158 1355.3501 1359.5071
1362.0520 1362.7917 1364.4997
1364.8977 1395.5381 1397.5021
1399.8870 1400.7823 1404.9251
1407.2095 1407.7103 1410.0224
1410.4638 1411.8593 1412.8802
1413.7591 1414.7014 1416.9828
1423.7136 1424.3734 1424.5130
1425.4236 1427.2237 1427.9716
1429.2410 1430.2122 1432.5244
1433.6441 1435.3995 1439.1968
1443.8091 1446.2091 1449.1652
1450.9807 1471.2731 1474.2296
1482.8813 1508.9302 1579.6431
1587.6282 1589.1953 1608.6366
1610.0117 1610.9749 1711.2312
2922.4355 2959.6407 2961.9011
2963.8712 2964.4947 2966.3349
2967.0355 2968.5884 2969.2750
2972.4215 2973.7814 2976.1224
2977.6665 3009.9647 3035.5914
3038.6099 3043.7070 3044.7120
3045.3010 3046.6363 3048.3530
3048.5326 3050.5646 3051.2794
3057.2782 3060.4446 3069.8244
3071.3087 3071.5173 3072.7592
3077.2582 3078.7155 3082.1234
3085.5643 3086.2997 3090.9601
3094.3636 3096.6356 3097.6663
3098.0808 3103.4448 3105.5680
3106.0033 3107.9790 3110.4705
3117.3748 3118.3291 3120.1380
3124.3943 3143.1710 3153.6138
3155.3012 3155.3799 3196.5996

$Fe(OR)_2$(carbene)
S=0

1.6091 11.8968 20.3961
22.6392 31.6068 43.5056
51.4273 55.6081 65.5174
68.9323 76.8173 78.0497
82.9545 85.4816 88.1363
96.9114 101.7704 110.9157
111.7703 121.6429 122.7931
131.4140 141.5988 156.9615
168.1696 185.5903 194.6765
198.7063 200.0645 206.7923
210.4599 220.8265 224.8382
230.3206 239.4918 241.0854
254.5381 262.5321 272.8432
276.0534 278.9793 287.4617
293.6770 296.2355 300.4335
302.8067 306.4935 311.6650
314.6721 317.0652 323.0235
326.9587 328.5060 329.1477
336.1414 337.5706 345.5667
347.8286 375.2603 377.3903
385.3731 394.7931 400.3120
405.5200 407.4612 411.5503
417.6197 418.0540 421.8259
426.7231 432.9523 440.5633
447.3164 457.0262 487.6385
495.9920 509.2965 533.2743
546.8181 548.8482 550.6149
554.2589 607.0653 613.2928
614.9077 631.0121 649.8682
654.6195 680.9793 712.0493
714.1900 721.5355 727.3479
738.6705 751.7429 755.5260
765.7592 792.7913 798.2041
799.2184 816.8361 820.4782
824.7917 844.0682 846.7671
884.2627 887.3393 892.1627
894.4083 896.7061 902.3496
903.2515 906.2922 907.3689
908.9035 909.4864 911.7997
912.2513 913.0715 918.7228
919.3830 920.7507 922.8590
933.7681 934.3189 945.1679
957.0520 968.0252 970.3497
976.0888 979.7469 982.0278
982.0474 983.8741 988.8725
994.5221 995.6987 996.9022
998.0917 1005.0673 1008.0846
1011.1683 1012.1596 1022.2343
1024.1173 1028.1543 1035.1277
1038.1230 1051.2694 1075.2935
1081.0794 1083.5017 1122.2268
1132.9787 1135.4475 1136.4964
1151.7271 1152.4103 1154.8959
1158.4394 1161.4044 1165.2283
1166.5337 1169.1471 1174.7100
1175.5811 1182.4209 1183.0572
1187.0526 1191.1122 1192.0962
1207.9513 1210.0989 1217.9838
1222.6820 1278.8579 1288.1974
1288.8668 1311.2796 1322.0144
1322.1289 1322.9099 1323.9544
1326.3825 1327.9728 1335.6681
1336.3491 1354.0551 1354.1997
1356.0535 1362.7891 1363.6314
1364.9703 1366.6036 1393.4477
1395.4791 1396.1563 1396.4871
1397.2993 1403.0014 1403.4201
1407.1308 1410.2586 1411.4159
1414.1028 1415.1191 1416.5149
1417.1727 1421.1543 1422.6576
1423.7728 1424.3018 1425.0138
1427.9109 1428.3622 1429.0316
1429.1031 1430.4894 1432.3540
1435.1585 1443.4766 1446.1456
1450.8235 1451.7898 1467.9457
1477.2338 1477.4770 1567.2750
1587.9229 1588.5113 1597.3676
1608.0790 1609.8706 1666.9230
2958.8287 2962.3299 2963.0954
2965.9179 2968.7867 2969.0263
2969.8289 2970.1337 2972.4281
2973.3015 2976.2514 2976.9518
2985.2742 3033.6829 3040.8460
3042.9619 3045.0270 3047.4359
3048.0597 3048.1227 3049.5926
3051.1028 3053.2514 3054.4167
3058.1808 3068.7273 3072.2009
3075.5414 3078.1620 3079.4931
3080.0633 3081.4430 3085.9810
3091.3564 3093.2720 3095.8570
3096.0859 3096.3881 3097.1228
3098.6732 3099.0040 3100.4944
3106.2557 3107.7979 3108.8884
3116.7356 3117.7123 3118.5894
3120.5819 3124.1178 3130.7359
3146.2813 3146.8854 3155.6824

$Fe(OR)_2$(carbene)
S=1

-5.7977 15.1024 23.1570
24.4468 31.7369 41.3346
46.6691 61.3926 65.2629
69.8714 74.8410 81.5360
83.1771 86.0749 90.4210
92.0813 98.5224 113.8400
116.0811 126.3383 128.6529
132.2406 139.2902 155.2568
162.0965 185.9349 192.5456

196.1417 200.9301 210.1570
217.3382 223.1151 229.5728
237.9493 240.1639 249.2181
251.9330 259.9821 267.5812
272.5409 279.7537 281.8245
284.2897 291.4512 292.1884
301.4230 309.0720 309.5515
312.1505 315.9237 317.4085
325.1979 328.6922 329.7893
332.3824 335.0057 342.3469
346.8098 372.5015 376.4313
381.1611 391.2926 399.8437
400.4635 404.2874 414.4156
414.7948 416.4354 419.8295
421.7776 425.8261 438.5177
442.7294 448.9164 483.8576
493.3822 508.7476 515.0596
542.5805 548.3398 550.7714
553.0926 606.3225 614.0900
615.3276 627.5963 648.0471
657.3568 688.8990 708.5382
712.9989 717.2556 721.2655
738.0480 744.9641 747.4561
762.1381 774.6891 795.6370
800.0911 814.7953 821.0641
831.1121 844.3343 849.3520
878.8575 885.9426 891.8455
893.2677 898.2246 903.2126
904.7030 906.2989 907.5693
909.9102 910.5642 912.0713
913.4140 914.2246 917.1243
918.4878 920.7253 925.9477
926.8096 932.3071 933.9641
963.7315 965.5283 970.6882
978.0218 980.0335 983.6923
985.2231 985.8558 989.5930
994.9296 995.5184 996.9506
999.1079 1002.0800 1007.9827
1011.4290 1012.0945 1024.0292
1027.3320 1029.0915 1038.1513
1048.7976 1052.6259 1077.7458
1080.9369 1089.3557 1124.5705
1131.8714 1132.7124 1136.9117
1148.1952 1154.0408 1154.3184
1160.1186 1161.7725 1163.6598
1166.4933 1166.8362 1174.4366
1176.3309 1181.7200 1183.0392
1188.2359 1189.3195 1192.1786
1207.1358 1208.0162 1219.4886
1220.6495 1268.0744 1284.2693
1285.6831 1310.3278 1319.5639
1321.5341 1322.5941 1324.5837
1327.5879 1333.6801 1335.4141
1340.1589 1352.5407 1353.0014
1353.2789 1361.9567 1365.0770
1365.1956 1367.1228 1394.1836
1395.3640 1396.1470 1397.3413
1397.7327 1403.3711 1403.5804
1407.6512 1410.9475 1411.7908
1414.4698 1414.9107 1417.2197
1418.3043 1420.0552 1422.1253
1422.7932 1423.3334 1425.2364
1426.0499 1428.4314 1428.8185
1429.5314 1431.4474 1432.7184
1433.8965 1439.9556 1445.2240
1451.6003 1451.9548 1466.3485
1467.0393 1474.8962 1562.8689
1582.3043 1588.3371 1594.9090
1602.5933 1608.7260 1664.3637
2960.9899 2961.9065 2963.9817
2964.0211 2964.7637 2965.3317
2966.3447 2967.1791 2967.8593
2968.6117 2970.2925 2973.3874
2977.7932 2981.6132 3031.4026
3039.7643 3042.3067 3042.9006
3043.5499 3045.1255 3046.4502
3047.1435 3048.1242 3050.3900
3051.1430 3065.3198 3065.9685
3067.8550 3070.6182 3072.3360
3073.4881 3075.3083 3076.9916
3083.3779 3083.9298 3093.9759
3095.4415 3096.7161 3098.0746
3100.9158 3101.1698 3101.4962
3103.3210 3103.8010 3109.1496
3111.8435 3116.2946 3117.2301
3122.3718 3130.7666 3138.4826
3141.7325 3151.8175 3170.0687

$Fe(OR)_2$(carbene)

S=2

-21.2134 11.2077 12.3866
28.7618 30.2910 36.5047
42.8156 46.4337 49.7782
52.3950 61.2244 62.6344
77.0721 85.0901 87.9359
91.7866 93.7550 96.4414
102.6356 108.4181 115.1287
125.4157 147.1664 153.7348
161.1619 169.5252 174.8991
181.2620 194.8996 208.9568
212.4749 223.1358 230.2893
233.0991 241.7989 252.7062
259.8144 268.5157 271.7269
274.7660 282.8888 287.7457
292.0120 298.5514 299.0732
301.0160 304.8669 308.8905
312.3908 322.8272 325.0006
326.3417 328.0427 331.8754
334.3333 334.7573 338.7666
350.8334 363.7076 367.4899
379.3884 392.6099 396.1969
400.5578 406.7768 412.7142
414.3039 416.3162 417.2564
420.2823 423.0451 430.5421
431.3536 434.1216 445.5826
492.0533 496.5367 498.0772
543.3420 545.4162 548.5097
550.0645 605.2679 614.4456
614.9928 635.7405 642.8152
646.7202 671.6119 679.0293
706.0069 706.5385 713.3294
730.4843 740.7870 750.1845
761.5018 763.6772 797.9679
800.3036 814.5651 819.1845
820.9556 836.5502 837.2488
841.3877 876.4548 882.5906
883.8154 892.4660 904.2877
905.6402 906.5843 908.5948
909.7694 909.9348 912.7031
913.6636 915.7430 916.2105
917.1692 922.0788 922.1999
929.8261 933.1819 940.3698
961.8860 965.0176 969.5942
982.1737 983.3175 983.4896
983.6621 986.1749 993.2713
995.3021 995.7503 996.8802
1002.4952 1003.9664 1004.9698
1009.8184 1012.2876 1019.7870
1028.8334 1031.4033 1042.1847
1053.9950 1070.3241 1073.5454
1079.5839 1095.2571 1122.0877
1133.7332 1133.8309 1135.2736
1149.8138 1150.1461 1152.2181
1156.4541 1161.5976 1163.3761
1165.4843 1166.3022 1173.1432
1175.4753 1182.1314 1182.9772
1190.9849 1193.5672 1205.5981
1209.8691 1215.6543 1220.9142
1250.5677 1277.8388 1281.6666
1284.1815 1322.1662 1323.7511
1325.0340 1327.2511 1329.8675
1331.6851 1333.5056 1336.9360
1352.8158 1352.9486 1355.1025
1361.5500 1362.9999 1364.7166
1366.0084 1370.3363 1393.1912
1394.8003 1400.1785 1400.3578
1404.3425 1405.2085 1407.5184
1409.6652 1410.5942 1413.7189
1415.9597 1416.4308 1418.6191
1420.4697 1423.4082 1424.4747
1424.6938 1427.2215 1427.6564
1428.8798 1428.9653 1429.3915
1432.9527 1434.5999 1436.4055
1439.8764 1442.1565 1444.3848
1452.4191 1455.2371 1462.6599
1474.1736 1475.6931 1493.4506
1561.7930 1588.0994 1588.8247
1594.4967 1609.4476 1609.9563
2957.3137 2962.3479 2963.0518
2964.2217 2965.3429 2966.3437
2966.7132 2968.5341 2969.8319
2971.7075 2972.2495 2974.8568
2978.7533 3035.9623 3036.3941
3038.8650 3042.5212 3043.3607
3043.3837 3045.2874 3048.2649
3049.5307 3050.1798 3053.4230
3061.2587 3062.5663 3064.3528
3073.2019 3074.2284 3075.5338
3076.9350 3077.3684 3078.0387
3091.0348 3092.5162 3092.6854
3095.1853 3095.3775 3098.8845
3099.5984 3102.3736 3102.9060
3105.1141 3108.3966 3112.5651
3117.2327 3117.4875 3118.6005

3124.8520 3140.3984 3140.7755
3141.2598 3151.6773 3153.3889

$Fe(OR)_2$(carbene)
S=3

-17.7046 -3.2925 12.6722
17.7626 21.4424 32.7956
36.3881 43.6999 50.8367
61.3399 63.9168 72.6017
78.7929 82.6720 87.2784
92.2979 98.4274 107.2990
109.1273 114.6312 126.5811
133.0428 148.5399 157.1537
159.8882 171.2444 177.8993
184.2571 190.6675 209.1294
212.0118 215.4184 222.6909
235.4552 240.8576 246.3390
255.5754 257.7028 267.5567
268.3667 277.0272 279.9605
286.7303 289.6166 291.8279
298.3574 300.5417 310.2245
314.4890 317.3783 318.2236
321.9789 323.9051 324.9925
327.9878 329.7759 333.6724
342.3864 344.4627 374.1412
378.6092 395.6030 400.3236
403.7367 410.0065 412.8407
415.3298 416.8647 417.9735
421.1106 422.6211 429.1316
434.9657 450.2151 466.8812
494.0444 496.4943 499.3890
544.1418 546.1306 549.8882
551.1646 602.2118 614.0202
615.1267 638.9793 644.8546
649.4210 668.9547 691.4844
703.5236 708.3468 710.5947
715.3929 725.3845 746.4335
749.8313 766.2219 796.8987
797.8146 813.5479 813.9675
815.7735 829.1868 833.5448
839.1506 880.9829 884.5732
887.5419 888.9657 901.3599
902.0564 904.1064 904.3239
905.7371 908.0224 908.3466
910.9263 912.9587 913.3862
914.1211 914.5826 917.1889
929.1458 929.7147 937.5278
960.1327 961.9245 965.7491
974.9629 978.2273 980.3093
981.5510 987.1662 990.0213
990.8100 991.3208 991.5123
992.8859 1000.8861 1004.0456
1007.6586 1013.0379 1016.6381
1028.9706 1031.0345 1033.7433
1049.1892 1061.7033 1076.0823
1078.5097 1084.5575 1124.0410
1131.6740 1133.0448 1134.9131
1144.5922 1150.1800 1152.5670
1157.6320 1161.2424 1163.3842
1164.1602 1165.1280 1174.9875
1176.1357 1179.1157 1181.8015
1186.7228 1190.6989 1202.7966
1208.1717 1216.3538 1216.9131
1258.2655 1279.1185 1282.0231
1290.5129 1319.4277 1320.7580
1323.7070 1323.8432 1326.6951
1327.9776 1333.0032 1334.7240
1350.3407 1352.8221 1353.1471
1362.1184 1363.1022 1364.1490
1364.9197 1376.7661 1389.5673
1392.1685 1394.7140 1395.0801
1397.8372 1400.6655 1404.0994
1405.0015 1409.7201 1412.2602
1413.3858 1414.1514 1415.9485
1417.0675 1419.9735 1421.5178
1422.2512 1424.1516 1426.4140
1426.8862 1427.6216 1428.3348
1431.2347 1432.1341 1433.4768
1434.6933 1439.2586 1443.3788
1449.0157 1451.7412 1473.6733
1474.8861 1483.6713 1491.0483
1543.3831 1580.7203 1587.3435
1587.9200 1608.8632 1609.9394
2944.3854 2956.8553 2959.1014
2961.7680 2964.1246 2964.6799
2967.0096 2969.2226 2970.1771
2970.4395 2970.7134 2974.8512
2975.1950 3020.4216 3026.8921
3037.7589 3039.6766 3044.6292
3044.6667 3046.1211 3046.5038
3047.9159 3048.0728 3051.1073
3051.9046 3065.6022 3067.2141
3071.0211 3072.0712 3072.9291
3074.0776 3081.9395 3085.4388
3088.7052 3092.8934 3093.1233
3096.7809 3096.8405 3096.9232
3099.1496 3102.7110 3102.8713
3105.1190 3105.8792 3106.7037
3116.8573 3116.9597 3117.1084
3123.8742 3125.1578 3145.2761
3148.2215 3150.1155 3171.8430

$Fe(OR)_2(k^2$-diazoester)
N2 loss TS
S=2

-79.5461 -3.6213 12.7431
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1192.1374	1195.2629	1196.3663
1205.6078	1206.8148	1207.7943
1209.6677	1213.2392	1216.8251
1217.6716	1218.2778	1219.8363
1255.7062	1271.8126	1278.8712
1280.2178	1282.3718	1283.1541
1284.1200	1302.3349	1320.9516
1322.3061	1322.7890	1323.4633
1324.2851	1326.1129	1326.8317
1327.1119	1327.5822	1327.8818
1329.4479	1331.3148	1332.6290
1334.1784	1334.8266	1335.0664
1336.4798	1340.5364	1349.4505
1350.2681	1352.4790	1353.2288
1353.3220	1361.1650	1362.3500
1363.9671	1364.5800	1364.7402
1365.0929	1367.4987	1367.7340
1369.9783	1376.3979	1394.3366
1394.3860	1396.2040	1396.6037
1397.9629	1399.3129	1402.2300
1403.1768	1403.7021	1405.6189
1406.4558	1407.2630	1407.6391
1408.8127	1411.0831	1411.6268
1411.8719	1412.6732	1413.6853
1414.5400	1414.8210	1415.9340
1416.7365	1417.5149	1418.8717
1419.7697	1420.3880	1421.3611
1421.5906	1421.9876	1423.1662
1423.8970	1424.5366	1425.3361
1425.7578	1426.5615	1426.6935
1427.7182	1428.0458	1428.4877
1429.5006	1429.8959	1431.4336
1432.5223	1433.4513	1433.8392
1434.6687	1435.9197	1438.0213
1439.5676	1441.1630	1442.9061
1443.2137	1445.4314	1447.4949
1449.8722	1450.8977	1452.1384
1453.9335	1457.5149	1467.1943
1473.2272	1474.0137	1474.2430
1476.1869	1480.3350	1482.8944
1486.4860	1567.9272	1579.9619
1582.2945	1587.2847	1587.7572
1588.3148	1589.4191	1592.5493
1608.3735	1610.2455	1610.3390
1610.5182	1611.6300	1612.7133
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2965.4846	2966.7996	2966.8762
2967.2408	2967.7782	2968.1373
2968.1620	2968.8731	2968.9242
2970.7536	2972.1922	2972.6774
2973.4757	2973.7225	2974.3343
2976.1611	2976.5012	2981.0810
2981.8366	2981.8554	2986.3703
2994.1921	3007.2790	3041.0517
3042.2681	3042.7022	3043.3441
3044.6389	3044.8661	3045.1238
3045.6333	3046.0410	3046.9198
3047.5236	3048.2885	3048.5678
3048.9865	3049.4361	3054.3803
3056.7142	3058.5360	3064.0934
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3072.9350	3074.1908	3076.5863
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3084.5639	3085.9494	3086.0655
3089.4975	3091.0480	3092.6071
3093.2168	3094.3319	3094.5486
3095.6001	3096.2194	3097.8373
3098.4813	3099.2134	3100.7781
3101.4613	3102.5584	3103.6076
3105.3859	3106.5012	3106.8098
3107.4539	3107.5843	3109.3394
3109.3809	3111.6560	3112.3712
3112.6053	3114.6617	3117.1726
3118.5167	3120.0724	3120.4189
3121.5721	3125.2627	3129.9011
3131.6332	3147.0215	3149.4433
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3156.2236	3160.7883	3165.1339
3166.0416	3194.9244	3226.0665

2$_{Fe}$

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61.5701	62.9557	65.3544
67.8915	69.3014	72.4592
74.2524	75.6303	79.6325
83.7532	89.9828	92.5633
93.5931	95.8138	97.6264
99.6915	103.4397	105.1960
106.9359	109.1012	115.3517
116.4513	120.8890	122.5829
122.9596	127.5593	129.8762
133.6709	136.4754	143.9579
144.4784	153.2795	161.3055
164.3962	176.9438	179.7207
180.8718	182.8231	184.9853
188.8612	191.7332	196.5268
200.0145	201.7405	207.9969
214.3585	218.3634	219.5129

220.7473 224.4231 225.6838
229.4126 233.3610 238.3455
240.7967 242.1699 245.4522
248.5999 250.1554 252.5181
255.3469 259.1635 264.2511
268.5324 269.7531 270.9378
272.4337 276.1798 280.6224
281.2054 282.3305 283.6124
287.6481 289.2307 291.8402
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309.2619 310.7258 315.2446
315.9419 319.1259 319.8032
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329.5150 331.7181 331.9388
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616.5285 617.7445 617.9736
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647.9674 648.0476 666.4193
687.5815 691.2162 692.0667
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838.6389 844.3212 847.9180
874.1908 878.0071 878.3797
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891.3617 896.6147 901.9979
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3107.8146 3108.7774 3109.2047
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3170.7786 3190.9686 3210.4406

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42.6743 43.1680 47.9271
48.2139 49.8008 52.4387

54.8379	56.2514	57.4423	740.0189	744.7648	747.2255	1335.0246	1337.6316	1339.4850
64.0198	65.2291	66.3322	747.5056	749.3063	751.0277	1349.6265	1350.6538	1353.2965
72.7108	74.6196	75.7809	768.2604	776.1339	798.0050	1354.1725	1360.2972	1361.7049
77.4372	81.1594	82.3524	799.5226	801.2071	802.3086	1363.5145	1364.1986	1365.1127
83.6271	84.6298	89.1017	804.1836	817.9919	819.6239	1365.4544	1365.7539	1368.1797
91.6659	93.5050	95.9328	819.7602	821.8781	827.8254	1369.3892	1369.6674	1391.8122
99.5578	107.5524	109.0458	831.1049	833.6778	836.7842	1392.3891	1395.5643	1396.5277
109.7468	115.4963	116.6664	840.1986	842.4341	847.5276	1396.8882	1400.3293	1401.6774
120.7730	121.1975	125.0583	871.1176	875.9598	878.4631	1402.2426	1403.6560	1404.0491
126.3026	127.6961	130.1832	879.1995	884.3981	884.4522	1405.6778	1407.4752	1407.9697
132.2365	136.9930	140.5452	894.7376	895.4997	905.3231	1408.6039	1408.8436	1410.8369
141.5346	146.8404	154.0055	905.6136	906.7801	908.2000	1411.1053	1411.7825	1412.4128
163.2483	169.0653	172.8871	908.4125	910.1999	910.4161	1414.0649	1414.1517	1415.5872
179.1234	181.3680	183.7953	910.7100	911.1982	911.4383	1416.1119	1416.7534	1416.8607
187.2667	191.9303	192.7721	913.2350	914.1188	914.3679	1417.5003	1420.0791	1420.6639
194.3137	200.9661	204.1842	915.8223	916.1292	916.8937	1420.9796	1421.2776	1421.5609
208.7843	211.5610	212.0603	917.1082	918.0404	918.1532	1422.6725	1423.2651	1424.4334
217.6562	219.8608	222.7245	918.2791	922.0522	922.7501	1426.0095	1426.0333	1426.6676
223.9882	228.3309	234.9085	924.8132	925.6646	927.1395	1427.5608	1427.6137	1428.3111
236.5329	240.4092	241.7430	929.5719	930.5722	934.0057	1429.0665	1429.6161	1430.2944
242.8378	244.7728	251.1084	934.3228	935.4909	937.2052	1431.8453	1432.5970	1434.2872
253.6595	256.8941	258.1028	962.9860	963.4109	964.9170	1435.5268	1436.4720	1437.3596
263.2348	264.2166	272.0323	967.4939	967.9025	968.9247	1439.0099	1439.8132	1441.7557
274.2430	275.5075	278.3713	969.7083	977.6147	980.0589	1444.5415	1445.6580	1447.5307
279.9487	283.5955	284.6400	981.4235	981.9562	982.8772	1448.7801	1450.0793	1455.0549
285.4765	287.5554	289.6090	984.0544	986.0992	986.4677	1455.3027	1456.9238	1473.1832
292.8820	295.5286	295.9970	987.2769	988.3393	988.3589	1474.7650	1475.4198	1475.7287
298.6406	301.8064	303.9770	989.9843	990.0118	991.1185	1476.8242	1479.3892	1484.7152
311.3463	313.0672	313.7042	993.1702	996.0477	997.2078	1486.5664	1577.1635	1580.5986
315.6441	316.3394	319.4973	999.1126	999.5236	1000.7064	1587.0763	1588.0364	1588.4116
320.2750	323.0231	325.2382	1001.9490	1003.2145	1006.7260	1588.6454	1588.8417	1594.5487
327.8507	329.5583	331.0529	1008.5547	1010.1190	1012.2647	1609.0214	1610.0769	1610.4949
332.5649	335.2748	337.4659	1013.7130	1014.4195	1014.6592	1610.9719	1611.7717	1613.7502
339.6325	342.1872	342.4448	1015.0020	1021.4527	1023.3526	2963.2048	2964.3169	2965.8500
343.8759	346.5178	348.5797	1027.4144	1029.8020	1032.2167	2965.8650	2965.9087	2966.1297
351.7295	353.6552	366.0283	1033.6305	1034.6885	1037.8268	2966.1490	2966.4891	2966.5119
366.6996	374.5093	376.1841	1040.8368	1043.5541	1045.2651	2968.4486	2969.5740	2970.4348
376.9205	381.1645	382.2080	1073.6079	1075.8247	1077.2654	2970.8755	2971.3106	2971.6395
386.9176	388.7739	392.7114	1078.0562	1078.2303	1079.5047	2971.9472	2974.5439	2976.5067
400.6031	401.1151	402.7741	1117.7249	1126.1096	1131.5975	2979.1945	2980.8827	2981.7657
404.3465	406.6871	407.4481	1131.6826	1134.9390	1135.5197	2985.7688	2986.3600	2986.9368
408.5596	413.8747	414.4061	1135.5584	1135.9056	1148.1801	2988.8072	3019.5972	3040.3112
416.7374	419.1659	419.8602	1148.2509	1148.7534	1149.3040	3040.7281	3041.8309	3043.2271
421.2391	422.1765	423.4067	1157.5933	1159.2085	1160.0297	3044.0446	3044.4241	3044.9724
425.1412	427.4811	431.0319	1160.8181	1161.7846	1162.4813	3046.2623	3047.3978	3047.7819
432.0112	432.6282	433.3711	1162.8403	1164.0106	1164.3184	3048.2458	3048.6352	3048.7856
436.2233	438.9819	440.1107	1165.0500	1167.4741	1167.6464	3048.8920	3051.8549	3052.5222
444.1267	448.6116	453.1554	1173.2852	1174.0741	1174.4536	3055.2370	3063.7516	3066.4864
461.2360	462.0661	489.3228	1179.3063	1180.8591	1182.1365	3066.9494	3067.2702	3067.3676
493.3380	495.6526	497.1235	1183.0109	1184.1211	1193.0961	3069.0020	3070.3879	3071.7315
499.4390	502.9495	533.1630	1194.1803	1194.8015	1195.3532	3074.2865	3076.5038	3077.0666
539.2913	546.0401	546.9314	1203.9154	1205.8671	1207.0092	3078.5306	3078.8588	3079.9139
547.4881	548.9786	550.0621	1208.0617	1212.7950	1216.1854	3080.1317	3082.1538	3083.4025
552.2731	553.5570	555.1933	1218.2908	1220.6252	1222.5954	3085.9491	3086.0576	3086.8872
613.3643	614.5221	615.2941	1224.5920	1270.4280	1279.0921	3090.4337	3090.5116	3092.8482
615.9128	617.9757	619.1060	1283.0455	1283.1147	1283.2752	3094.5838	3094.6990	3096.8870
640.0141	642.1316	644.3671	1286.2882	1304.2092	1316.7476	3098.0751	3099.2325	3099.4852
647.0007	647.2839	655.2251	1318.7089	1319.9912	1320.7712	3100.6476	3101.6038	3102.0632
692.3996	693.7815	700.8148	1321.5803	1324.2175	1325.1024	3102.2221	3103.3444	3104.1526
705.4298	707.0144	707.4376	1326.3814	1326.9771	1327.4524	3104.3952	3105.9481	3107.2927
710.6069	713.6203	716.9183	1328.7108	1330.2978	1330.6632	3107.5332	3108.1827	3109.9460
721.0237	732.8618	734.3232	1331.8189	1332.7283	1334.1023	3110.4393	3113.0426	3114.0642

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2$_{Fe}$
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$Co(OR)_2(k^2$-diazoester)
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$Co(OR)_2(k^2$-diazoester)
S=3/2

-14.0621 7.0117 15.3367
24.6374 25.0651 35.4085
36.9220 43.5476 49.4552
51.9842 57.0985 71.9521
73.2725 77.7380 80.5759
83.5626 90.7488 95.6135
102.0138 111.5797 120.7274
130.4637 138.7496 153.6396
168.2112 171.6794 178.7404
185.1071 194.3299 195.7232
203.0880 211.9827 216.0235
222.1417 227.8971 234.0092
240.1420 249.3247 256.6547
261.7535 269.6858 276.4824
279.6817 282.5132 286.7171
292.0175 297.4176 305.6627
308.7916 317.1469 319.8215
321.4024 324.8689 330.6491
333.5509 334.5058 341.6860
344.6108 346.0743 353.8911
360.1507 375.7046 384.7925
394.3223 398.0326 401.4696
402.9421 409.9856 412.3915
412.8470 415.6843 419.8870
423.3185 424.5597 426.5140
432.1386 451.4126 472.5771
492.4222 494.8897 503.9496
534.4516 542.3662 543.8422
545.6994 547.1393 560.0984
614.2239 615.1364 619.3436
642.0755 647.9616 662.3204
691.1970 702.6642 707.2219
719.8348 720.2708 740.8012
743.2512 757.4401 759.9219
796.2226 798.2892 801.4199
812.5539 815.1607 824.9706
834.8752 835.1101 875.9273

877.0946 879.8281 882.4674
900.9028 901.3997 902.8156
905.3644 905.4055 909.5552
910.8551 912.0895 912.8107
914.0014 916.6189 916.9822
917.7765 927.1519 928.4222
958.0546 960.7255 965.0964
967.8557 978.6306 978.8748
983.8688 986.0330 988.2618
990.4215 991.7920 992.3118
995.4020 997.3644 1001.2534
1002.6763 1008.3923 1009.8566
1017.9843 1030.2175 1032.2146
1038.2538 1059.8492 1063.5000
1073.2404 1080.3277 1085.6048
1125.6706 1132.3711 1135.0688
1136.2930 1143.3754 1152.3859
1153.1054 1160.9245 1161.1271
1161.7582 1163.0288 1166.6631
1172.8374 1174.9734 1181.5951
1184.7960 1192.0007 1193.9793
1206.2579 1209.1142 1210.5983
1213.8005 1216.5606 1277.6372
1279.1846 1287.1613 1318.2470
1319.0572 1319.8193 1322.7361
1325.4079 1326.6788 1328.4687
1330.5251 1333.0460 1346.0825
1350.5655 1351.8627 1357.5089
1361.9884 1364.1252 1364.4479
1365.0379 1391.2213 1395.0504
1395.2455 1396.5013 1403.1134
1406.0335 1406.8137 1409.3317
1409.7908 1412.8063 1413.9666
1414.9543 1416.0654 1416.6294
1417.8707 1421.4836 1422.8564
1424.6388 1426.5950 1426.8757
1427.5946 1429.5321 1431.2555
1432.3880 1433.9915 1442.0504
1443.2910 1444.4722 1449.3211
1450.5755 1473.5960 1476.0097
1485.0318 1544.9903 1581.6862
1588.0962 1588.3759 1609.5281
1611.1093 1611.7278 1774.3307
2961.3438 2962.0292 2963.9787
2964.7098 2965.0401 2965.6938
2968.5125 2968.6587 2971.7541
2973.1242 2975.9984 2976.5925
2979.1659 3039.7063 3042.1994
3042.6208 3042.7668 3044.7053
3045.5449 3045.8471 3048.7722
3048.9558 3051.2689 3059.7973
3063.3459 3067.4447 3071.5592
3071.8075 3072.9642 3074.5344
3076.5291 3077.5561 3083.4693
3085.4122 3087.2396 3090.2805
3095.5815 3097.3177 3098.4165
3101.8161 3102.3001 3103.7559
3105.8909 3107.4531 3110.4221
3115.0400 3119.1929 3119.9375
3124.1478 3131.3391 3149.4103
3157.0699 3157.1165 3236.3656

$Co(OR)_2(k^1$-diazoester)

S=3/2

-11.6233 16.4454 26.4333
28.4533 33.6276 39.2222
44.8868 53.3254 56.2338
60.9171 63.7442 69.9723
75.3349 80.4066 81.4677
83.2328 92.3696 95.6547
102.8197 108.9542 113.7928
120.8042 127.1814 135.7774
136.3866 144.4665 157.3122
177.1232 179.4556 188.4081
202.4681 204.9199 206.2696
214.7570 221.7555 229.6452
233.4674 247.5989 250.3965
258.3835 262.1547 264.6970
274.6092 278.7818 281.8631
285.2986 292.4498 295.1156
296.7521 303.7753 310.9910
312.7136 316.2727 318.1627
323.1458 326.0858 328.8787
331.5706 339.9546 342.1319
344.6937 361.9139 365.9765
378.9932 387.3462 400.1074
401.8731 402.5233 409.0578
414.6396 415.0939 421.9962
424.0097 425.8295 430.8226
435.6536 462.7722 472.0932
492.7412 496.5519 498.7445
531.3036 537.9249 541.2069
547.0947 547.9350 549.0276
609.9180 615.1201 615.3531
641.3974 648.9124 662.6531
691.8895 697.1629 702.7102
703.5069 706.4328 738.6836
739.3937 744.4845 761.1612
793.9579 796.6833 800.2243
810.2744 814.8555 817.5415
833.1195 833.7000 877.1600
882.3596 882.6857 885.7613
886.7829 900.2958 901.4674
903.8058 904.5359 907.2624
908.4027 910.7435 913.3960
914.1398 916.1657 919.5908
921.5338 923.4563 928.5630
932.7376 940.0212 958.1026
959.9734 971.5577 976.9576
977.4941 982.1977 986.2216
990.6527 993.3658 993.5292
996.6032 998.6899 1002.9073
1006.2606 1008.3521 1009.1141
1023.0810 1028.9638 1029.2537
1051.4416 1060.0505 1067.9345
1075.7057 1081.4694 1100.0488
1126.6333 1131.0561 1131.9258
1138.4483 1139.3178 1142.2553
1153.4282 1159.2458 1160.3757
1161.6640 1167.1389 1167.3554
1174.6754 1176.3086 1181.8551
1182.7544 1189.7478 1190.5970
1203.6683 1208.1815 1208.3708
1214.6302 1216.2534 1274.8170
1275.6400 1281.7039 1314.1603
1315.5120 1317.5137 1320.7920
1325.4883 1325.6509 1326.0597
1329.5640 1332.8686 1347.6155
1351.0576 1354.1984 1356.0932
1360.1139 1363.7143 1365.0883
1368.1222 1389.4149 1392.9635
1395.1925 1396.2442 1401.2107
1406.2260 1408.3073 1408.5033
1409.2953 1411.2777 1411.7735
1413.8587 1415.5982 1418.0850
1418.8573 1420.6223 1421.5946
1422.8618 1425.2070 1425.6548
1427.1615 1428.3653 1429.6352
1433.4486 1434.3102 1436.0986
1441.9783 1443.9771 1446.1706
1450.8804 1471.1241 1472.4145
1481.3885 1579.5575 1587.0564
1587.5520 1603.0829 1608.8355
1609.2395 1631.9037 2170.3521
2945.0680 2959.5142 2959.7918
2962.3431 2962.7077 2962.8503
2964.6063 2966.8418 2970.0273
2971.7939 2972.9718 2973.3673
2978.7207 3025.3599 3036.8535
3038.0817 3038.4065 3042.6970
3042.7632 3044.0751 3045.1808
3046.7993 3048.5477 3050.1081
3061.0001 3067.9899 3068.6488
3069.8656 3072.2289 3072.2888
3076.6797 3080.1919 3083.1629
3088.8078 3090.3531 3091.3998
3092.0084 3094.4023 3100.7633
3102.0266 3103.7171 3104.3653
3106.3131 3113.3770 3116.1953
3116.7392 3117.2871 3121.7022
3125.7686 3130.5837 3146.8231
3147.9397 3151.5035 3161.9949

$Co(OR)_2(k^2$-diazoester)

S=5/2

-11.1808 8.6831 16.1414
22.0547 29.3944 32.5050
36.6379 43.6938 51.5270
59.4508 64.1087 67.0224
73.3529 79.3067 87.7128
91.0511 93.8248 96.5743
106.8758 117.4699 121.2791
136.2744 138.3976 147.5570
165.2709 173.5117 180.9687
195.1430 197.7136 205.3212
211.3411 219.6650 226.2667
228.9510 236.7905 245.9868
253.1966 259.4593 265.6380
271.9100 273.2175 279.8667
281.9639 286.2260 290.2736
295.6483 299.9156 301.0604
304.6677 306.5650 318.1363

323.9971 324.6676 325.3022
329.7071 330.4929 336.3502
337.7080 342.9032 360.1112
367.1907 376.4101 379.8473
393.6424 396.1855 400.0524
402.0869 406.3073 409.0411
411.1655 412.5282 415.4941
416.1091 422.3808 431.5993
432.5732 437.6063 454.1152
484.2255 495.0878 497.4956
523.1384 545.4472 547.4988
548.7320 552.3069 573.7197
613.6863 615.1884 617.6921
636.6431 639.5943 664.0604
687.1079 704.7950 705.2486
720.8154 729.0195 739.0017
743.0434 753.7746 763.5617
797.2368 798.4758 800.6350
812.1242 814.1424 823.8391
836.0127 836.8305 872.3293
878.4758 878.8692 881.8771
902.0543 903.8833 905.1278
905.9775 906.9843 908.9237
913.9092 915.2314 915.9791
916.2167 919.1483 919.6282
922.5687 926.8928 927.9360
959.9282 963.1306 963.9911
967.9811 979.7022 981.8004
982.4937 986.3565 987.8447
991.0660 991.8658 995.1394
995.7552 997.3890 1002.2460
1004.8666 1009.6346 1012.0309
1015.4001 1029.5447 1030.0080
1033.4852 1053.8927 1057.6474
1072.6467 1076.9792 1079.4310
1122.4861 1132.5890 1133.5220
1135.8142 1146.0738 1147.4916
1148.7999 1159.0542 1159.2473
1160.8725 1161.3691 1162.0475
1169.7483 1172.2405 1181.1481
1184.4814 1190.2442 1193.0454
1193.4081 1204.1488 1211.1416
1214.8929 1216.6846 1259.3208
1281.0578 1281.4517 1304.4726
1324.8750 1325.3393 1326.8309
1327.1251 1329.1988 1330.1616
1332.4162 1334.7063 1336.1746
1353.9439 1355.5576 1362.4825
1363.0156 1363.5100 1363.8345
1364.2723 1398.3659 1398.9489
1399.9849 1400.2761 1404.0200
1405.6832 1408.1382 1409.4751
1409.9695 1412.1219 1413.6967
1414.7857 1416.1180 1417.2799
1422.3602 1424.0746 1425.3836
1425.9321 1426.4899 1428.5879
1430.1150 1430.2511 1431.6335
1433.8937 1435.3045 1437.6218
1439.8409 1447.2422 1450.5967
1450.7595 1471.4233 1473.4619
1478.9243 1520.8058 1573.9032
1587.1879 1588.7042 1598.3772
1609.2229 1609.8141 1623.9966
2963.3411 2963.4324 2963.6654
2964.6721 2967.3914 2967.6240
2968.0771 2969.2415 2972.2964
2974.6474 2975.2403 2976.1517
2978.9379 3042.2849 3042.5322
3042.8511 3044.6803 3046.1426
3046.4331 3047.0172 3049.0271
3049.5219 3049.7041 3051.3625
3058.0619 3063.5172 3070.5953
3070.7396 3070.9614 3072.9506
3076.1765 3078.9223 3084.3860
3087.3287 3088.9959 3091.8514
3094.2680 3096.3925 3098.5952
3102.6368 3103.3739 3105.7265
3106.2315 3107.4582 3109.3741
3118.5222 3119.3070 3119.9057
3127.6617 3149.0539 3156.5696
3156.8064 3165.5838 3187.2576

$Co(OR)_2$(carbene)
S=1/2

-7.6731 15.1914 25.1070
29.1688 34.5528 41.5676
50.4206 57.9912 63.2889
70.7316 74.7441 78.8814
82.7307 90.0452 91.5563
95.6225 101.7703 108.5394
119.1158 124.1793 126.2808
129.1721 140.2445 150.9676
171.9346 185.0096 191.9551
196.8459 199.1210 202.2313
216.0053 220.6357 226.6880
231.1276 240.7922 244.0816
246.1086 259.5279 265.2832
271.6191 278.2071 282.3519
285.1133 295.4470 300.1580
303.5005 307.4126 311.6210
312.5591 315.3097 318.0212
326.4673 329.9157 331.2017
332.1185 333.5826 345.3371
351.7741 359.5053 379.0734
380.6071 386.9125 396.8441
401.5861 402.4595 414.3636
416.0490 418.3535 423.0950
423.7213 436.8838 439.5167
444.7858 473.8318 483.0231
501.6922 507.8813 529.7810
542.8563 547.7150 549.5327
557.0820 607.2366 613.6450
614.6161 627.0046 648.8329
658.8289 687.0957 702.1841
710.8856 714.8789 718.5550
730.6290 740.1912 746.6212
759.2262 765.3918 793.8773
798.3695 813.2757 815.8004
831.4639 837.3469 844.7426
881.3263 885.1211 889.8204
892.4098 898.6181 905.2549
906.2070 906.9193 907.5600
909.8038 910.4424 911.1513
912.0658 916.1447 917.5951
918.2379 920.5949 922.5301
923.4238 928.0633 932.5491
953.2299 967.6060 971.4497
974.7917 979.9380 980.2543
981.4840 982.3318 985.7253
988.9717 992.9199 994.6505
997.1755 1001.3557 1008.7734
1010.4537 1011.4203 1023.7461
1025.9454 1027.1061 1037.7239
1039.6222 1055.7453 1075.6526
1078.1564 1093.1162 1124.7828
1131.4938 1132.4667 1137.0185
1146.0676 1152.1262 1154.2249
1158.6512 1160.7632 1162.0517
1163.9503 1167.2090 1172.3653
1174.3566 1180.5241 1181.2701
1187.2607 1189.4625 1191.2768
1204.0116 1205.8873 1218.0887
1218.2646 1265.2804 1280.3687
1284.5478 1309.6153 1321.7433
1323.9371 1323.9576 1325.3616
1328.9323 1331.9530 1335.4061
1336.6519 1351.3597 1351.7406
1354.1793 1363.8468 1364.5285
1365.1908 1367.1871 1393.5791
1396.2246 1396.6000 1397.7214
1400.3539 1401.8976 1407.5940
1409.7205 1411.3835 1412.2399
1412.9798 1415.2657 1416.1270
1419.8298 1420.7637 1421.8465
1422.7521 1423.0003 1424.5443
1427.0623 1427.8112 1428.3135
1429.5229 1431.6231 1434.2753
1434.4537 1445.5528 1447.0797
1449.1476 1453.1295 1465.2732
1470.6142 1472.9430 1563.3409
1583.9908 1586.6911 1596.1680
1606.5644 1606.9504 1671.2192
2961.8578 2962.5188 2964.6623
2965.9769 2966.6821 2967.0152
2967.9737 2969.2373 2970.5629
2971.6046 2972.4928 2972.7362
2978.9403 2980.7046 3038.3973
3040.4269 3041.3972 3043.5043
3044.6522 3045.9637 3046.5719
3049.2166 3049.4819 3051.9159
3053.9662 3068.0126 3070.3090
3070.9499 3071.2728 3073.6324
3076.4432 3077.7537 3079.7554
3083.0880 3085.9115 3092.4258
3095.1287 3096.7807 3099.4341
3099.6993 3100.1681 3101.4716
3102.2506 3103.5146 3110.5098
3112.2950 3114.2686 3116.7523
3122.6083 3127.7865 3139.5367
3140.0725 3155.8927 3165.6567

$Co(OR)_2$(carbene)
S=3/2

-14.1825	5.8313	16.3536
29.4653	33.2103	38.4208
42.7409	49.1144	55.0294
70.7751	73.8021	76.9982
78.3259	80.7525	88.4617
90.1952	96.0047	97.5360
102.7548	108.7253	116.6344
121.8267	128.3172	146.6024
166.5235	178.9112	185.4408
190.6953	198.3749	206.8806
210.5685	221.0655	224.4227
227.3109	229.5935	242.0284
244.1998	257.5079	268.8469
272.4912	274.7858	276.6994
280.9764	286.3794	295.0592
301.8990	305.8388	311.6070
313.4319	315.3842	320.4351
321.7018	326.8724	329.6161
332.3276	335.1062	342.2505
349.0179	351.1837	367.7606
377.9294	396.9041	397.9679
400.4935	403.9880	411.0481
411.9576	419.7278	420.5088
426.5595	427.7595	432.3217
440.8689	452.7650	463.4435
493.9159	498.5847	512.1707
545.0161	547.2979	547.6160
552.9412	604.6683	612.8060
615.0003	624.3770	647.5903
648.6407	681.3223	693.2986
707.1229	710.3258	713.1506
728.1967	744.8119	747.5633
751.3992	765.0481	796.9221
800.2513	814.0126	818.7764
821.3115	838.8610	845.7294
874.2526	877.7165	881.2453
883.1977	893.8604	903.6775
905.3462	905.4536	905.6043
908.5348	910.8143	911.1891
913.9695	914.4203	915.7351
916.0837	918.8673	920.8831
921.9056	927.0770	929.0039
959.1972	964.7544	969.2588
980.0082	981.1489	982.0883
983.0040	986.4189	990.7034
992.2382	994.8875	996.2252
996.6201	1002.7764	1004.6298
1009.8533	1011.4907	1020.6567
1027.0848	1030.9357	1037.4284
1046.1096	1059.4609	1073.8342
1078.6278	1086.0063	1122.0506
1130.9730	1133.7373	1135.9336
1145.5087	1146.3279	1152.5426
1154.8616	1160.1010	1164.5777
1165.2341	1166.2627	1170.5456
1171.7581	1181.3347	1181.6807
1182.6095	1190.1363	1191.2473
1209.0091	1209.0903	1212.1683
1216.7967	1277.2998	1280.2625
1283.5428	1308.2001	1321.4827
1321.7332	1324.5669	1327.6751
1328.2503	1331.9977	1334.2323
1336.7130	1351.5632	1354.0761
1356.2609	1362.4432	1364.5715
1365.4409	1365.9944	1394.0798
1395.5799	1396.2640	1396.8950
1398.2736	1403.2914	1406.3669
1407.3576	1408.6134	1412.0593
1412.9651	1415.5434	1415.9615
1417.2527	1421.3368	1422.0033
1422.9156	1424.0589	1425.1736
1426.7646	1426.9235	1427.3574
1429.5640	1432.1178	1433.9064
1434.5426	1444.1468	1447.6732
1449.3471	1453.5301	1463.7071
1472.7543	1475.4869	1561.9878
1585.2626	1589.3239	1594.9262
1605.6986	1608.6791	1671.7824
2958.5935	2962.4457	2964.4361
2964.9150	2965.6522	2966.2908
2967.6916	2969.8579	2970.8813
2971.8721	2975.3847	2979.4497
2980.5249	3036.7871	3041.8620
3042.6056	3045.3587	3047.9666
3048.2225	3049.2827	3050.4755
3051.9189	3052.3816	3054.2755
3060.6473	3061.6126	3067.2675
3071.5785	3074.4808	3076.6140
3078.0643	3083.7235	3085.6073
3086.1550	3087.5786	3087.9404
3095.3777	3095.4715	3098.8660
3099.2764	3103.4686	3106.3427
3107.7545	3107.8312	3116.2547
3117.3997	3118.7218	3119.5845
3125.6518	3132.4011	3142.5937
3153.3181	3154.0359	3164.0555

$Co(OR)_2$(carbene)
S=5/2

-12.0070	11.6105	13.4951
23.3435	26.1847	38.5129
39.8585	50.6129	59.6762
67.7050	70.1169	74.4777
80.6506	83.3317	91.2037
96.6277	105.0238	110.4189
112.4143	119.3377	133.2225
139.9036	152.8165	155.4519
171.2624	175.3906	185.3143
188.8835	207.4908	213.0809
216.4087	222.6113	229.7818
245.6784	247.0297	254.7887
260.0146	263.0709	273.2844
274.0517	282.9192	287.5838
291.1003	296.1026	299.0457
301.1220	306.8926	315.5412
316.7852	317.6517	321.7679
324.6898	326.5523	328.3534
329.1412	332.1084	337.1767
343.4439	350.4241	375.2514
379.6052	395.9075	400.9026
402.3315	409.9325	411.9302
415.1827	417.8401	418.7218
421.2015	422.8488	428.1893
431.0592	443.4125	467.5653
495.1563	496.0780	499.0590
543.1272	544.8404	548.1578
550.6021	602.8479	614.1137
615.2723	636.5630	644.4049
649.4166	669.8407	688.1714
703.9030	706.2016	711.3889
712.9180	728.7927	745.3554
749.8840	765.7178	798.2641
798.7347	813.5103	815.3520
817.0167	823.6972	831.3679
837.1609	879.0398	880.2119
883.1027	883.7648	901.9848
902.6655	902.9209	905.2894
906.1016	911.3130	911.9239
913.1287	914.3864	915.4315
917.5014	918.1841	920.3494
925.5580	926.2708	934.8797
957.4808	961.0312	962.2937
975.0026	978.7044	979.7662
980.1892	987.2289	989.4037
991.0058	991.5270	994.5500
999.8148	1003.1272	1005.0612
1008.7122	1013.9335	1016.9241
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1079.3634	1082.5845	1123.9496
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1148.7017	1149.7590	1151.8634
1157.9898	1161.8255	1162.4964
1163.1335	1164.9111	1172.7235
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1189.8793	1194.4660	1207.6405
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1325.2487	1327.0398	1328.1161
1329.6877	1333.4217	1334.8730
1350.5048	1351.8518	1353.9585
1361.8551	1362.3166	1363.5796
1365.2972	1376.5375	1395.5856
1395.8030	1396.7543	1399.8326
1405.4629	1405.8087	1406.3098
1407.7399	1412.1987	1413.3524
1415.8488	1416.8095	1417.3602
1418.6332	1422.3035	1422.3549
1424.5071	1424.9423	1426.5614
1427.5543	1428.9323	1429.8726
1431.8557	1433.3535	1434.5368
1434.9785	1442.4967	1447.4042
1450.8881	1453.7353	1474.0130
1474.7863	1478.9846	1489.6329
1544.1169	1581.0476	1587.3364
1588.4932	1609.3903	1610.2938
2955.7076	2960.4490	2964.0949
2965.6024	2965.8039	2966.4184
2967.2666	2967.5924	2970.6100
2970.7776	2972.5238	2977.9503
2979.7171	3034.0054	3039.3610
3041.2770	3043.5708	3045.3858

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3049.1819 3049.6015 3060.9219
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3068.8273 3072.8757 3073.8740
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3113.0234 3117.7357 3120.5971
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3149.3580 3153.7334 3169.1712

$Co(OR)_2(k^2$-diazoester)
N2 loss TS
S=3/2

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81.1507 88.5371 97.5034
101.8501 105.4589 110.2998
117.2034 121.4329 124.1134
132.0736 148.5658 162.3630
172.9780 176.6757 185.4939
187.6229 195.1271 207.6917
212.7597 219.3876 230.9116
235.9097 242.8598 246.9186
253.9450 260.8493 263.1511
269.5024 270.8921 278.6734
282.9009 283.9938 288.8699
294.9866 297.4103 300.3790
304.7441 307.9078 313.3194
320.9180 321.1316 327.6570
333.2904 334.4240 335.8195
344.3156 350.5065 356.4066
363.9779 374.8235 379.8213
384.3417 389.5971 394.1707
406.7784 409.0333 411.3833
415.4871 418.8192 422.4208
426.3194 432.1910 434.8981
438.6956 443.4241 477.4436
493.6399 499.1437 543.4548
546.2122 546.7520 549.1741
550.0276 600.4589 614.7942
616.9085 638.3791 641.1430
641.9771 664.3328 685.0311
705.1460 706.0732 726.4856
738.0688 742.4464 752.3877
753.4216 797.7179 798.4842
806.7123 811.6227 813.0010
813.8920 836.4327 838.0754
875.7740 877.4048 880.9644
882.2292 899.9199 900.1453
903.6995 907.3046 908.0679
909.9210 910.6425 913.4622
914.4933 916.2516 917.2886
917.7625 921.6068 924.2471
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1608.5324 1610.7576 2079.6959
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3154.1801 3155.3532 3160.3360

$Co(OR)_2(k^1$-diazoester)
N2 loss TS
S=3/2

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72.6148 79.6294 81.9431
86.6302 93.1082 96.1318
98.5655 106.1428 112.2723
117.4719 120.0744 123.9417
129.2418 133.0285 141.9575
162.9243 171.5718 176.3667
182.7961 192.9623 204.6365
207.6790 212.2142 218.7769
225.4320 231.6896 239.8675
246.5087 246.8907 253.8840
266.1238 269.9820 274.6496
279.9912 285.3509 288.7445
296.0910 299.8349 301.1398
305.4751 311.5657 314.4841
316.2123 318.7902 324.2002
327.8390 331.4723 332.6009
336.1478 343.1176 349.4284
359.8364 368.9007 377.3619
388.9608 400.5489 403.5185
406.1755 412.8181 414.0080
417.0292 418.5592 424.9799
428.8931 430.3011 433.8121
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495.5163 496.5559 543.5759
544.1426 548.3998 549.6615
565.7766 598.3738 614.9933
616.1867 641.5830 649.5193
653.7364 684.7278 705.6951
706.9549 710.3367 716.7542
739.3330 745.9048 746.4120
762.2058 797.9969 799.0343
812.3693 815.2504 816.8763
818.2744 836.2110 842.7965
875.1443 881.2950 882.1119
887.7544 888.5248 903.8168
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909.7033 910.9742 911.2377
915.9275 917.5386 917.8620
919.2115 921.2776 925.1570
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977.6981 979.7498 983.4677
988.7640 992.3567 995.1182
995.5120 998.3123 1000.3000
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1010.3183 1011.9896 1030.9091
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1475.4322 1529.0512 1541.2120
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1608.8460 1609.7570 2197.6357
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58.9816 61.9765 63.1457
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95.3672 98.4515 104.2248
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119.5772 125.2452 127.8542
128.0717 130.3844 138.5444
140.5929 142.7574 143.2624
164.5845 170.7844 178.4078
179.0285 179.7923 180.9512
183.8243 185.6245 188.3757
190.7085 196.1890 198.1857
202.5015 207.0320 212.6353
215.2656 223.3816 227.5539
232.4915 236.2087 238.6147
241.2287 241.3884 244.0216
244.6089 247.7717 247.9839
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267.5068 270.5228 274.7507
274.9263 277.7371 279.9716
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305.2057 306.1764 314.1595
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1455.9933	1457.3064	1459.5421
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1474.6659	1474.8986	1479.9399
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2966.5313	2966.6196	2966.9775
2967.0038	2968.2425	2968.2768
2970.3739	2970.4013	2970.5179
2970.6691	2974.0212	2974.0610
2977.2569	2977.3190	2980.6450
2982.0001	2983.1662	2983.2104
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3040.8827	3041.4007	3041.4297
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3044.7508	3045.1652	3045.2860
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3081.8804	3082.0171	3082.0607
3082.1206	3085.8613	3085.8811
3086.2053	3086.2829	3088.7443
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3095.1297	3095.1317	3097.1421
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S=4

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65.1419	67.7527	72.6585
73.5038	74.9169	77.6224
80.0890	84.3725	86.6599
89.7980	91.0305	94.5114
94.7722	98.4580	104.0617
104.2838	107.2334	108.5564
111.1088	114.5349	119.3507
120.6957	125.8183	128.1600
128.4118	130.5860	137.9630
140.5380	142.5468	143.0998
164.6570	169.7658	177.7857
178.6616	180.2806	181.4960
183.5425	185.9697	188.7614
191.0372	196.6587	199.4227
203.1401	207.0656	212.9891
215.5472	224.6347	228.0057
232.5241	236.3960	240.1251
242.7172	243.3038	244.9263
246.0961	248.3184	249.2336
252.0142	254.6444	256.6347
263.6942	266.0731	268.0858
268.7692	270.9727	274.7818
275.5703	278.4875	280.7479
282.4489	284.5585	284.6646
287.9090	288.4315	294.3075
295.7437	301.1137	302.4509
305.2112	306.1400	313.9494
315.7310	319.4070	322.6935
323.0360	326.5988	326.8118
327.5611	328.2675	328.6178
331.1133	331.3223	332.3709
337.6352	340.1812	340.4654
342.2993	347.6354	347.7426
353.5273	356.0668	365.3472
365.7799	367.8472	369.2765
372.3490	374.6945	379.5448
381.0812	384.0887	392.3298
395.1515	399.3928	401.2981
401.3600	404.0898	405.3397
405.7587	406.2267	413.0356
414.2654	415.2891	415.6296
417.5396	421.2175	422.1010
423.7781	424.0135	427.6717
427.9058	428.4812	430.6935
431.0882	436.0967	438.5083
439.2956	440.8404	441.5066
451.9180	473.4818	490.9659
491.5174	494.6098	494.8049
504.8545	517.8648	536.0691
541.6232	546.0807	546.1502
546.5277	546.7182	548.6881
548.9316	549.0852	550.4260
613.4608	614.3563	616.2436
616.2587	616.7768	616.8689
642.0433	642.2635	644.8197
644.8781	647.1834	656.3583
689.8076	690.7372	702.6750
702.7337	711.9910	713.2356
718.1370	721.3371	722.0826
722.5675	735.4989	738.0065
738.2653	743.8497	744.0642
746.5860	746.7066	751.0173
768.1897	777.0361	800.0084
800.2221	801.7752	803.2083
817.0000	818.2859	818.5197
819.5256	821.3123	827.7836
828.4780	831.5978	832.0063
840.8856	841.6535	842.6714
874.9850	875.0119	876.1729
876.8534	880.7664	880.9342
884.9534	885.4781	904.3734
904.4405	905.4329	906.7279
907.8187	908.8063	910.2904
910.3706	910.6207	910.6892
913.3163	913.6149	913.8273
914.1361	915.1781	915.5261
916.7306	919.4062	919.6724
919.7401	919.8510	924.2661
924.5786	925.1067	925.1711
925.6211	928.9438	928.9871
933.1747	933.2835	960.9122
960.9796	961.1811	961.3041
965.3299	969.3042	969.6835
980.4766	980.7129	980.8199
981.0224	982.2850	986.4950
986.5646	986.8764	987.8650
988.4935	988.5309	991.1376
994.6961	994.8550	996.6255
997.2788	997.6583	999.1741
1000.3687	1001.3235	1001.5754
1002.8904	1003.1702	1006.9459
1007.1825	1011.8565	1012.9646
1013.6575	1013.7350	1015.6976
1024.7054	1031.0098	1031.1091
1033.2572	1034.1552	1037.1416
1039.6021	1051.5187	1053.0261
1055.5372	1057.7766	1075.2308
1077.8510	1078.0897	1078.5556
1080.9545	1081.7274	1099.2027
1120.7432	1120.9546	1132.6753
1132.7039	1136.0383	1136.0673
1136.9262	1137.1962	1142.0686
1142.1233	1147.2112	1147.5527
1158.1447	1159.3422	1159.6583
1161.1838	1161.3671	1163.1447
1163.2147	1164.4611	1164.5655
1164.8901	1167.3184	1167.5286
1171.7259	1173.0014	1174.5792
1176.7999	1182.9700	1183.7429
1186.6849	1186.7528	1194.5863
1194.7678	1195.3595	1195.6284
1209.4328	1210.5465	1210.6534
1211.7124	1214.4671	1216.2501
1216.5021	1216.8356	1217.5367
1255.2411	1272.9922	1279.6549
1279.7112	1280.2588	1286.7175
1286.8829	1314.0666	1315.8007
1322.3655	1322.4089	1322.9371
1323.5031	1325.4630	1325.4943
1326.9233	1327.0961	1329.1585
1329.4574	1329.9974	1330.6528
1331.6029	1331.9243	1332.2547
1332.5059	1334.7103	1347.0667

1352.7724	1353.1305	1353.1954
1353.2801	1360.3514	1360.7161
1361.7352	1361.8258	1364.2120
1364.3095	1364.5206	1364.7424
1371.2998	1373.3000	1389.7186
1394.4422	1394.6326	1397.6410
1397.8955	1398.7342	1400.9512
1401.1034	1403.4717	1404.4891
1404.5734	1406.2569	1409.0496
1409.2040	1409.8389	1410.3958
1411.1294	1411.5761	1412.9122
1413.8930	1414.1187	1414.7517
1415.0727	1416.0012	1416.7032
1417.3831	1418.2740	1418.6281
1420.0944	1421.0065	1421.7444
1423.8212	1424.4537	1424.8562
1425.4028	1426.2123	1426.6441
1427.1009	1427.8814	1428.1522
1428.6082	1430.0759	1430.1346
1430.5511	1431.8844	1433.1741
1435.4352	1436.1801	1436.2161
1436.6649	1437.4099	1440.1698
1444.1827	1445.0801	1446.3139
1447.8087	1449.0180	1449.9931
1455.3543	1457.1484	1457.3046
1463.6443	1473.5022	1473.5767
1474.5168	1474.7712	1480.0998
1480.3067	1565.8196	1572.3921
1582.4659	1582.5387	1587.7070
1587.8023	1587.8447	1588.0284
1609.4220	1609.4588	1609.5397
1609.5450	1610.3981	1611.0287
2961.0086	2961.0182	2963.4304
2963.4726	2964.0182	2964.0367
2966.5061	2966.5508	2967.1713
2967.1973	2968.4631	2968.4990
2969.8525	2969.9801	2970.5030
2970.5448	2974.4654	2974.5074
2976.9282	2976.9968	2980.3502
2981.8330	2983.6295	2983.6643
2995.5787	2998.7098	3041.0158
3041.0378	3041.5506	3041.5828
3042.9644	3043.0711	3045.0554
3045.0983	3045.5646	3045.6644
3046.4240	3046.4589	3048.2562
3048.2974	3048.5687	3048.6313
3051.4071	3051.8439	3066.6667
3066.8497	3066.8725	3067.6204
3067.7174	3067.7699	3073.1909
3073.3745	3074.0533	3074.0911
3076.1463	3076.1958	3078.1553
3078.2626	3079.2734	3079.3118
3081.3523	3081.5322	3082.3593
3082.3791	3085.4320	3085.4929
3086.5811	3086.6616	3088.6780
3090.0517	3094.7961	3094.9177
3095.2918	3095.3041	3097.1908
3097.1966	3100.3895	3100.3941
3106.0046	3106.0172	3109.5692
3109.5895	3111.7526	3111.7656
3112.2249	3112.2343	3118.5032
3118.5254	3119.4435	3119.5629
3121.0485	3121.0698	3123.0851
3123.1030	3126.6803	3128.7329
3137.8164	3137.8233	3156.0696
3156.0777	3158.8489	3158.8957
3166.2115	3166.2389	3171.8941
3171.9050	3204.3687	3204.4793

Table S7. BP86-D3/def2-SVP SCF energies, enthalpies, and free energies, and B3LYP-D3/def2-TZVP (+SMD) single point energies, of all optimized species. All energies are listed in hartrees.

Species	Spin	$E(SCF)_{BP86}$	H_{BP86}	G_{BP86}	$E(SCF)_{B3LYP}$	G_{B3LYP}
N_2	0	-109.443545	-109.434811	-109.456577	-109.567669	-109.580701
diazoester	0	-607.288937	-607.122520	-607.175786	-607.961327	-607.848176
$Fe(OR)_2(k^2$-diazoester)	0	-3191.641586	-3190.761678	-3190.890634	-3193.740625	-3192.989673
$Fe(OR)_2(k^2$-diazoester)	1	-3191.650498	-3190.770635	-3190.901369	-3193.762256	-3193.013127
$Fe(OR)_2(k^2$-diazoester)	2	-3191.664509	-3190.784379	-3190.916029	-3193.799213	-3193.050733
$Fe(OR)_2(k^1$-diazoester)		-3191.645831	-3190.764952	-3190.900738	-3193.793684	-3193.048591
$Fe(OR)_2(k^2$-diazoester)	3	-3191.628980	-3190.750073	-3190.884598	-3193.777309	-3193.032927
$Fe(OR)_2$(carbene)		-3082.178879	-3081.309113	-3081.441885	-3084.171686	-3083.434692
$Fe(OR)_2$(carbene)		-3082.208534	-3081.340476	-3081.468497	-3084.222917	-3083.482880
$Fe(OR)_2$(carbene)		-3082.194471	-3081.326570	-3081.458392	-3084.224200	-3083.488121
$Fe(OR)_2$(carbene)		-3082.183566	-3081.317521	-3081.446647	-3084.224445	-3083.487526
$Fe(OR)_2(k^2$-diazoester) N_2 loss TS		-3191.596904	-3190.720856	-3190.856335	-3193.748138	-3193.007569
$Fe(OR)_2(k^1$-diazoester) N_2 loss TS		-3191.602721	-3190.725117	-3190.862486	-3193.744235	-3193.004000
$\mathbf{2}_{Fe}$		-6383.405793	-6381.641108	-6381.875901	-6387.671660	-6386.141768
$\mathbf{2}_{Fe}$		-6383.391240	-6381.623592	-6381.857914	-6387.634557	-6386.101231
$\mathbf{2}_{Fe}$		-6383.380472	-6381.613920	-6381.844996	-6387.611294	-6386.075818
$\mathbf{2}_{Fe}$		-6383.372746	-6381.605416	-6381.841645	-6387.601380	-6386.070279
$\mathbf{2}_{Fe}$		-6383.392692	-6381.625026	-6381.860063	-6387.635905	-6386.103276
$\mathbf{2}_{Fe}$		-6383.405414	-6381.640670	-6381.876417	-6387.671673	-6386.142676
$Co(OR)_2(k^2$-diazoester)		-3310.696862	-3309.817020	-3309.947584	-3312.807235	-3312.057957
$Co(OR)_2(k^2$-diazoester)		-3310.704852	-3309.825264	-3309.960809	-3312.835267	-3312.091224
$Co(OR)_2(k^1$-diazoester)		-3310.694383	-3309.814999	-3309.949576	-3312.844483	-3312.099676
$Co(OR)_2(k^2$-diazoester)		-3310.672451	-3309.793381	-3309.928244	-3312.808302	-3312.064095
$Co(OR)_2$(carbene)		-3201.257963	-3200.389974	-3200.517298	-3203.265273	-3202.524608
$Co(OR)_2$(carbene)		-3201.235649	-3200.367755	-3200.499041	-3203.254629	-3202.518021
$Co(OR)_2$(carbene)		-3201.228915	-3200.361386	-3200.491802	-3203.259373	-3202.522260
$Co(OR)_2(k^2$-diazoester) N_2 loss TS		-3310.638035	-3309.762062	-3309.897051	-3312.779043	-3312.038059
$Co(OR)_2(k^1$-diazoester) N_2 loss TS		-3310.643172	-3309.765701	-3309.903334	-3312.780513	-3312.040675
$\mathbf{2}_{Co}$		-6621.486066	-6619.720223	-6619.954695	-6625.729660	-6624.198289
$\mathbf{2}_{Co}$		-6621.484627	-6619.717730	-6619.956969	-6625.729312	-6624.201654

9. Mössbauer data

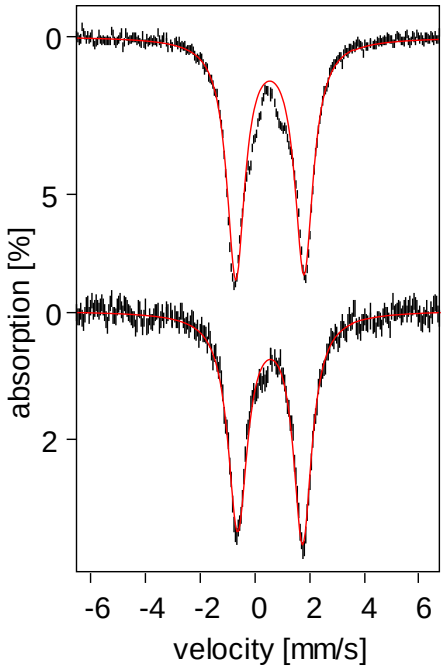

Figure S23. Zero-field Mössbauer spectra recorded at 80 K for **3** (top) and **4** (bottom). The solid red lines are simulations obtained using the parameters listed in Table S1.

Table S8. Zero-field Mössbauer parameters obtained at 80 K for complex **2**, **3**, and **4**.

Complex	**δ** [mm/s]	**ΔE_Q** [mm/s]	**Γ_L** [mm/s]	**Γ_R** [mm/s]	**%**
2	0.55	2.52	0.68	0.75	97
3	0.56	2.50	0.80	0.82	96
4	0.57	2.38	0.86	0.81	100

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