Supporting Information

Ferrocene-Based Multiple-Stimuli Responsive Organometallogel

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1. Experimental section

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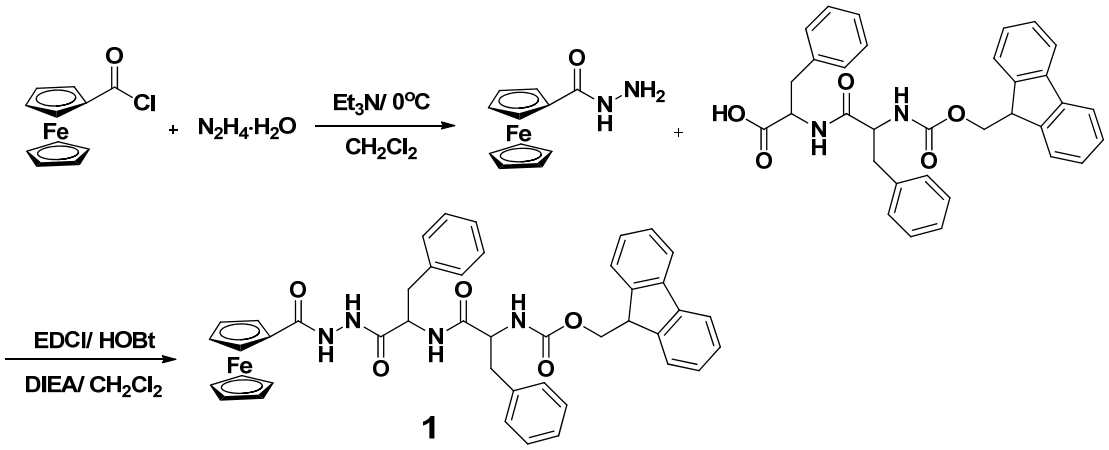
1. Experimental section

1.1 General routes for the preparation of the gelators



1.2 Scanning electronmicrographs (SEM)

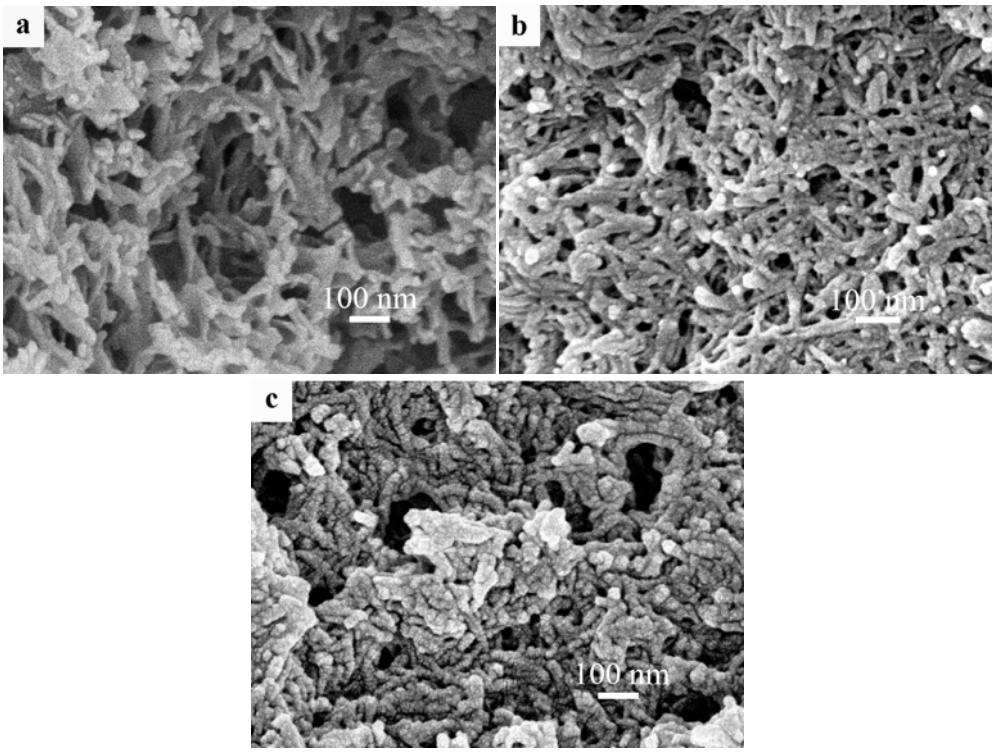


Figure S1. SEM imgaes of gel **1** (26.3 mM) from isopropanol-water mixed solvent with (a) 10% water; (b) 30% water; (c) 50% water.

1.3 Transmission electron microscopy (TEM)

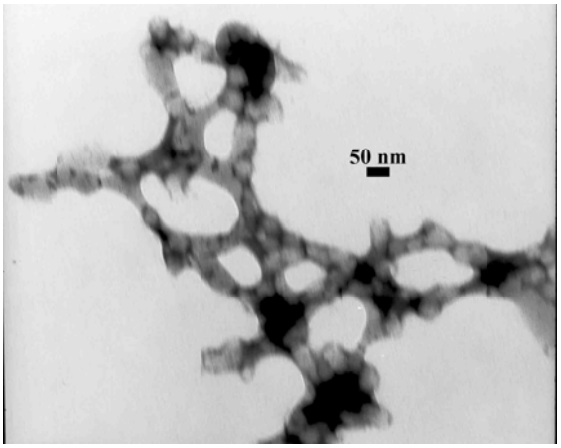


Figure S2. Transmission electron microscopy image of gel **1** from isopropanol-water (v/v=1:1, 2.63mM).

1.4 The concentration-dependent ^{1}H NMR

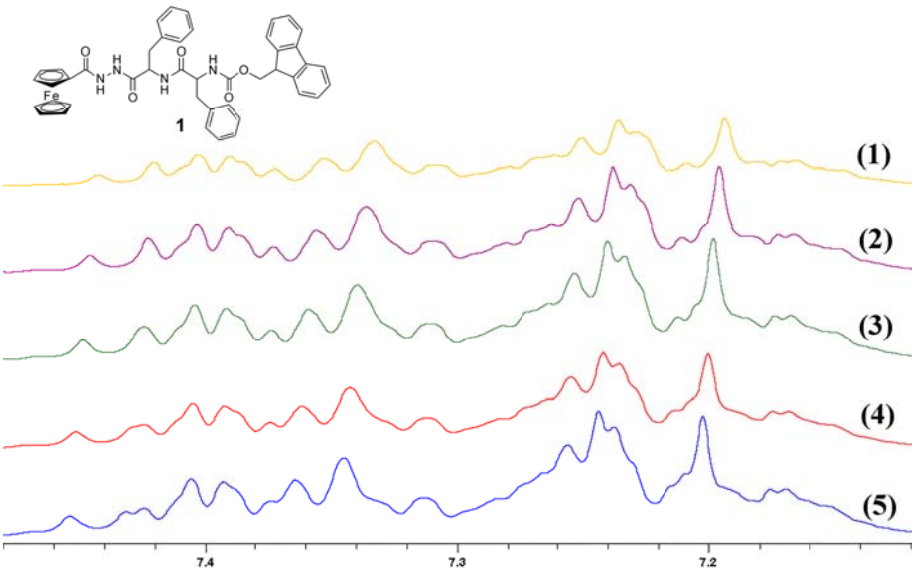


Figure S3. The concentration-dependent ^{1}H NMR (DMSO-*d6*, room temperature), capturing the aromatic proton section: (1) 10 mg/mL, (2) 15 mg/mL, (3) 20 mg/mL, (4) 25 mg/mL, (5) 30 mg/mL.

1.5 Cyclic voltammetric measurements

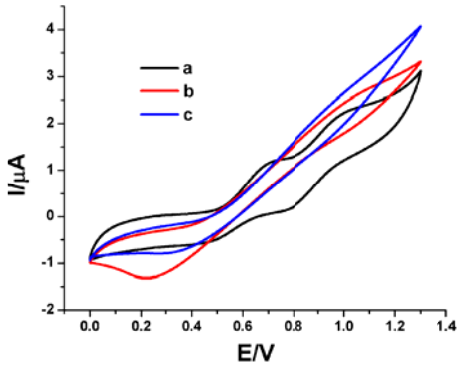


Figure S4. The cyclic voltammograms of the solutions of gelator **2** ((a): 1 mM; (b): 3 mM;

(c): 5 mM).

1.6 Redox responsiveness of gel 2

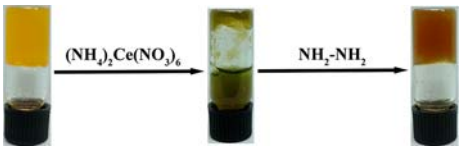


Figure S5. Pictures of the reversible gel–sol phase transition of gel **2** triggered by chemical redox.

1.7 UV–vis spectra of gelator2

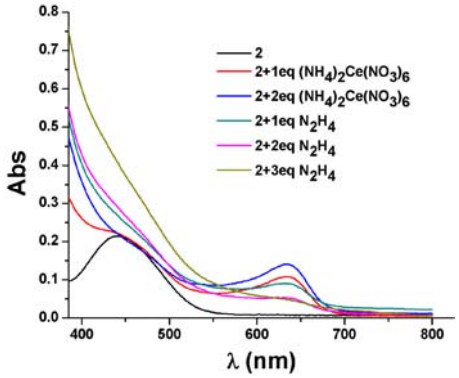
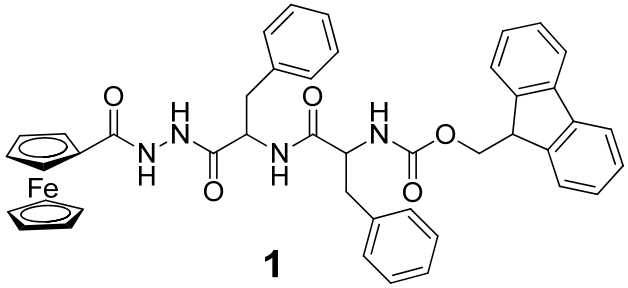


Figure S6. UV–vis spectra of the gelator **2** solution with oxidizing agent and reducing agent (1 mM in isopropanol/water = 3:2).

1.8 *β*-CD responsiveness of gel 2

Figure S7. Gel–sol phase transition of gel **2** (3.01 mM in isopropanol/water = 1:1) triggered by different equivalent of *β*-CD (from left to right, in order, were 0 eq, 1 eq, 2 eq, 3 eq, 4 eq, 5eq).

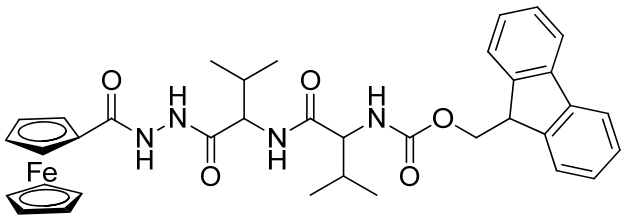
2. Spectral data of the gelators



1

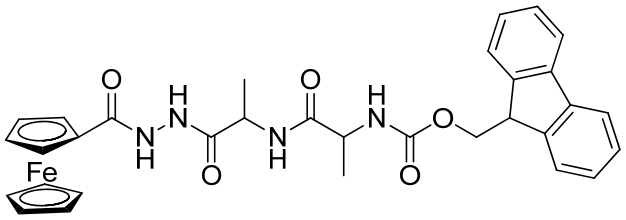
^{1}H NMR (400 MHz,$CDCl_3$) δ = 9.40 (s, 1H), 8.50 (s, 1H), 7.68-7.72 (t, 2H, *J* =

9.5Hz), 7.30-7.46 (m, 5H), 7.05-7.21 (m, 11H), 6.05 (s, 1H), 5.71 (s, 1H),5.04 (s, 1H), 4.82 (s, 1H), 4.72 (s, 1H), 4.03-4.44 (m, 11H), 2.82-3.20 (m, 4H);^{13}C NMR (DMSO-d_6, 100 MHz) δ = 38.1, 39.4, 39.6, 39.8, 40.0, 40.2, 40.4, 40.6, 66.1, 68.6, 70.2,70.8, 70.8, 74.3, 120.5, 127.5, 128.1, 128.4, 128.5, 128.5, 129.7, 129.7, 129.8, 129.9, 138.0, 138.1, 138.5, 138.7, 141.1, 141.2, 141.3, 169.1, 171.3, 171.4, 171.7, 171.8;HRMS(ESI) m/z calculated for $C_{44}H_{40}FeN_4O_5$[M+Na]$^+$783.2240, found 783.2253.



2

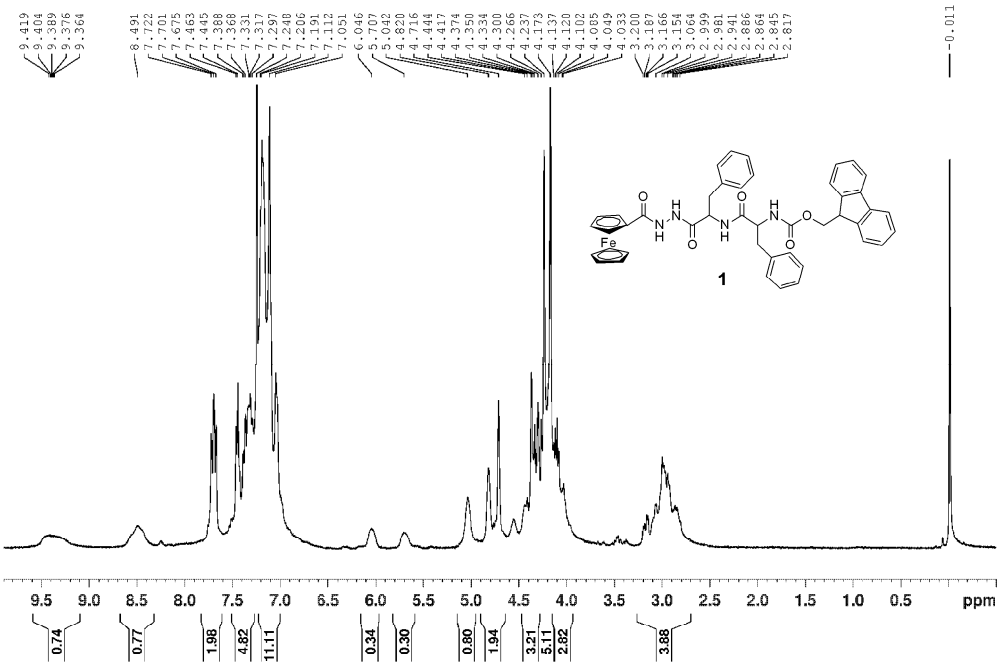
^{1}H NMR (400 MHz,$CDCl_3$) δ = 9.00 (s, 1H), 8.60 (s, 1H), 7.69-7.71 (d, 2H, *J* = 7.0Hz), 7.49-7.56 (m, 5H), 7.16-7.32 (m, 4H), 6.31 (s, 1H), 6.22-6.24 (d, 1H, *J* = 6.3Hz), 4.87 (s, 1H), 4.72-4.75 (d, 2H, *J* = 9.3Hz), 4.12-4.36 (m, 9H), 1.85-2.22 (m, 4H), 0.85-1.03 (m, 12H);^{13}C NMR (DMSO-d_6, 100 MHz) δ = 18.5, 18.7, 18.7, 18.8, 19.8, 19.8, 39.5, 39.7, 39.9, 40.1, 40.3, 40.5, 40.7, 47.1, 47.2, 68.6, 68.9, 70.1, 70.7, 70.8, 74.3, 120.5, 125.7, 125.8, 127.5, 128.1, 141.2, 144.3, 144.4, 169.0, 170.8, 170.9, 171.4, 171.7;HRMS(ESI) m/z calculated for$C_{36}H_{40}FeN_4O_5$[M+H]$^+$665.2421, found 665.2431.

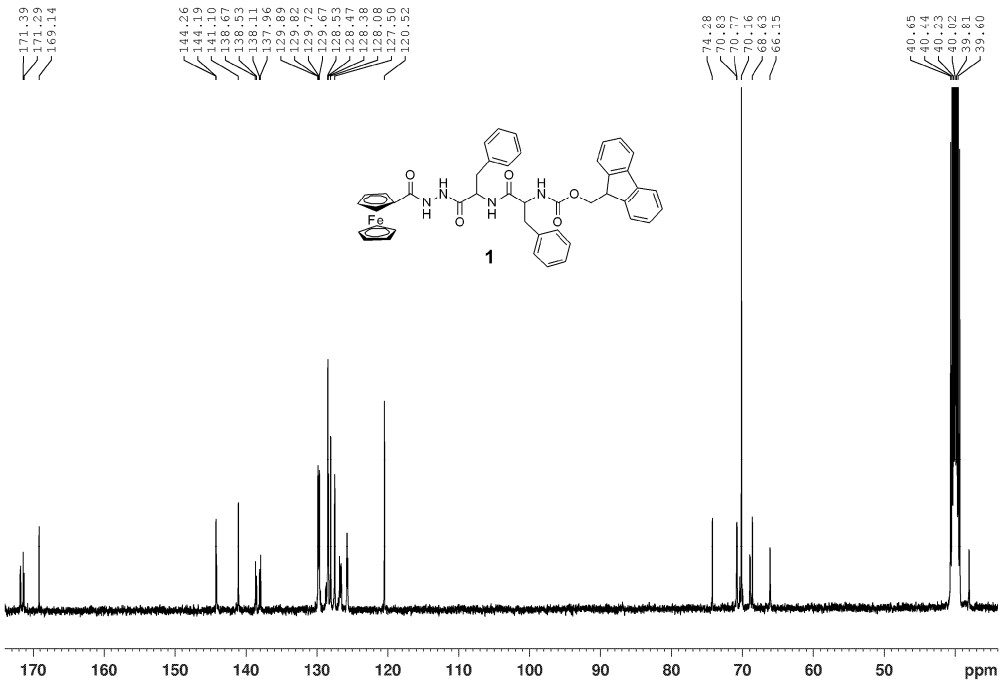


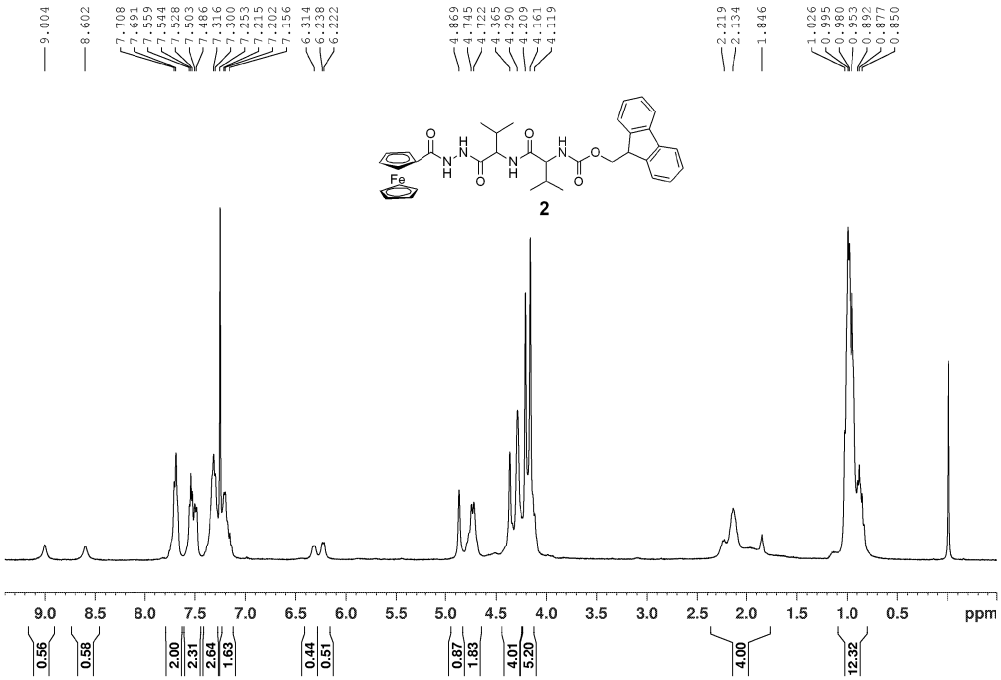
3

^{1}H NMR (400 MHz,$CDCl_3$) δ = 9.21-9.29 (d, 1H, *J* = 34.2Hz), 8.22-8.26 (d, 1H, *J* = 19.0Hz), 7.72-7.75 (t, 2H, *J* = 6.6Hz), 7.53-7.60 (m, 2H), 7.34-7.40 (m, 2H), 7.23-7.30 (m, 2H), 5.89-5.90 (d, 1H, *J* = 6.4Hz),5.63-5.64 (d, 1H, *J* = 4.7Hz),4.67-4.76 (m, 3H), 4.17-4.45 (m,11H), 1.38-1.46 (m, 6H);^{13}C NMR ($CDCl_3$, 100 MHz) δ =14.2, 21.1, 47.0, 60.4, 68.5, 68.6, 70.1, 71.1, 72.3, 76.7, 77.1, 77.4, 120.0, 125.2, 127.1, 127.7, 141.2, 141.3, 143.7, 171.3, 171.4, 173.2, 173.4;HRMS(ESI) m/z calculated for$C_{32}H_{32}FeN_4O_5$[M+Na]$^+$631.1614, found 631.1617.

3. ^{1}H NMR and ^{13}C NMR Spectras of the gelators



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0.980
0.933
0.882
0.877
0.850
Fe
2
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0.58
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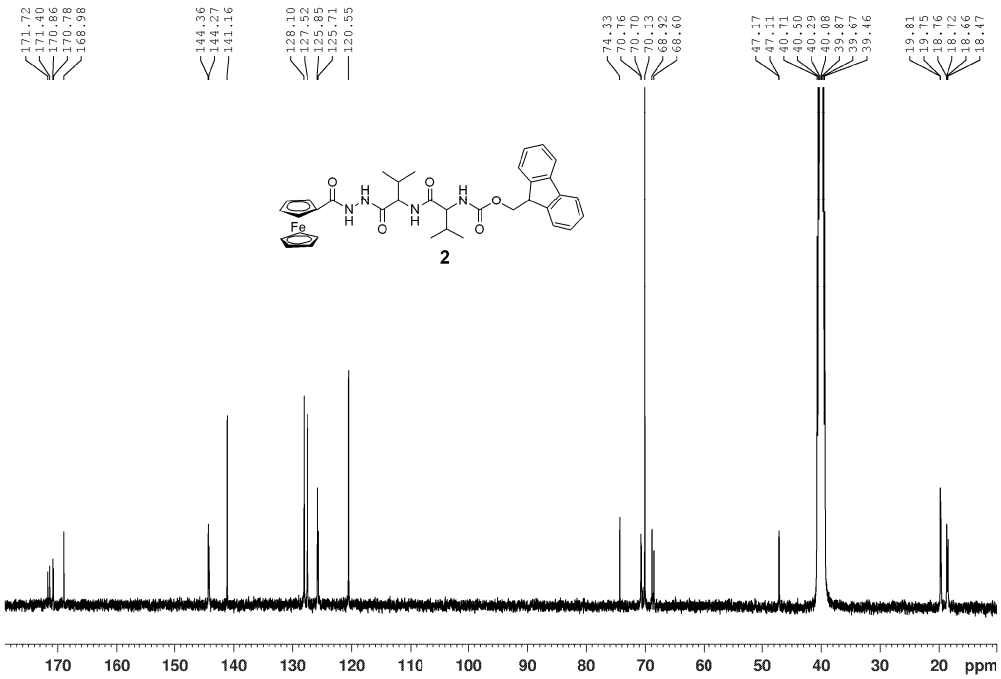
5.20
4.00
12.32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40.71
40.50
40.29
40.08
39.87
39.67
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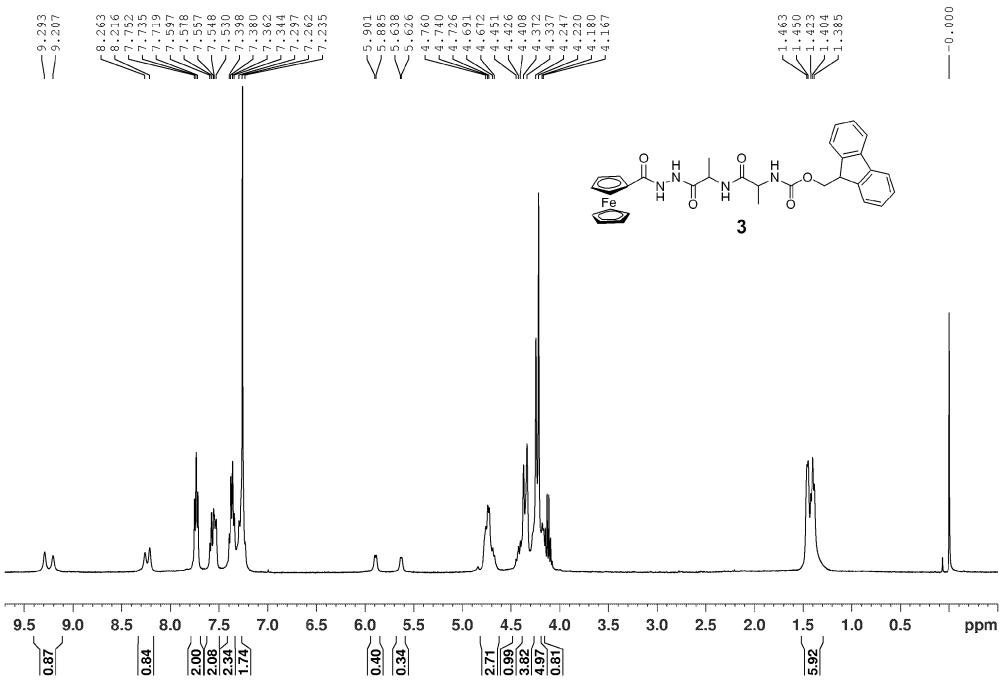
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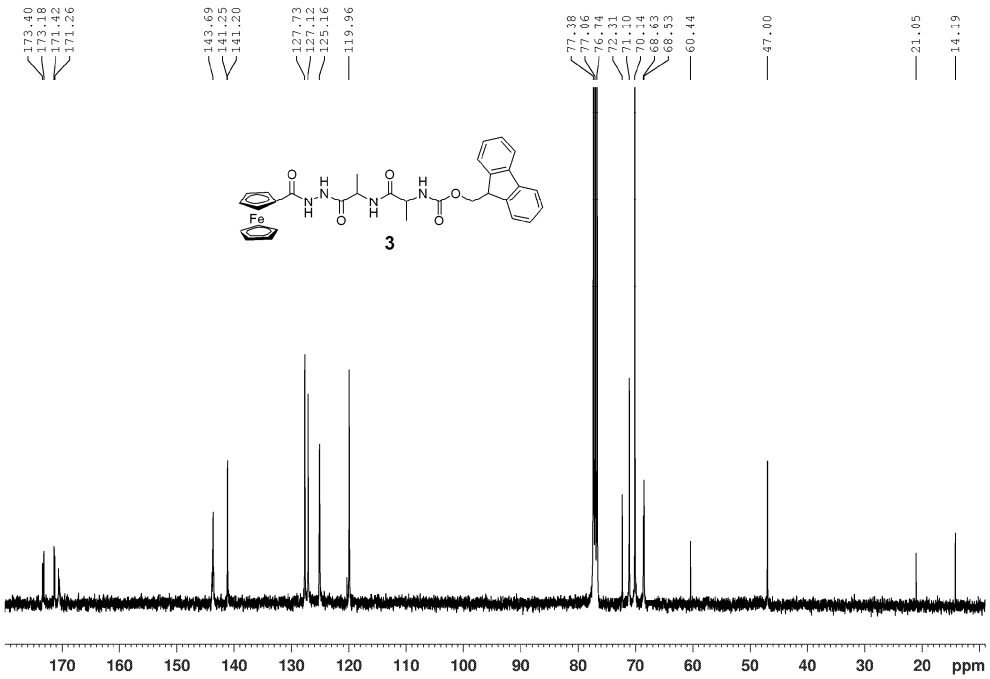
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14.19
Fe
3
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm