

Supplementary Information for

Insertion Reactions of CS₂, COS, PhNCS at Thiolate-Bridged Diiron Centers

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Contents

S Table 1 Selected bond distances (Å) and angles (°) for **2a** and **2b**

S Table 2 Selected bond lengths (Å) and angles (°) for complex **3** and **4**

S Fig. 1 Cyclic voltammogram of **2a** and ferrocene. The scan rate is 0.100V·s⁻¹, and the reference electrode is Ag/AgNO₃.

S Fig. 2 Cyclic voltammogram of **2b** and ferrocene. The scan rate is 0.100V·s⁻¹, and the reference electrode is Ag/AgNO₃.

S Fig. 3 Cyclic voltammogram of **1b**. The scan rate is 0.100V·s⁻¹, and the reference electrode is Ag/AgNO₃.

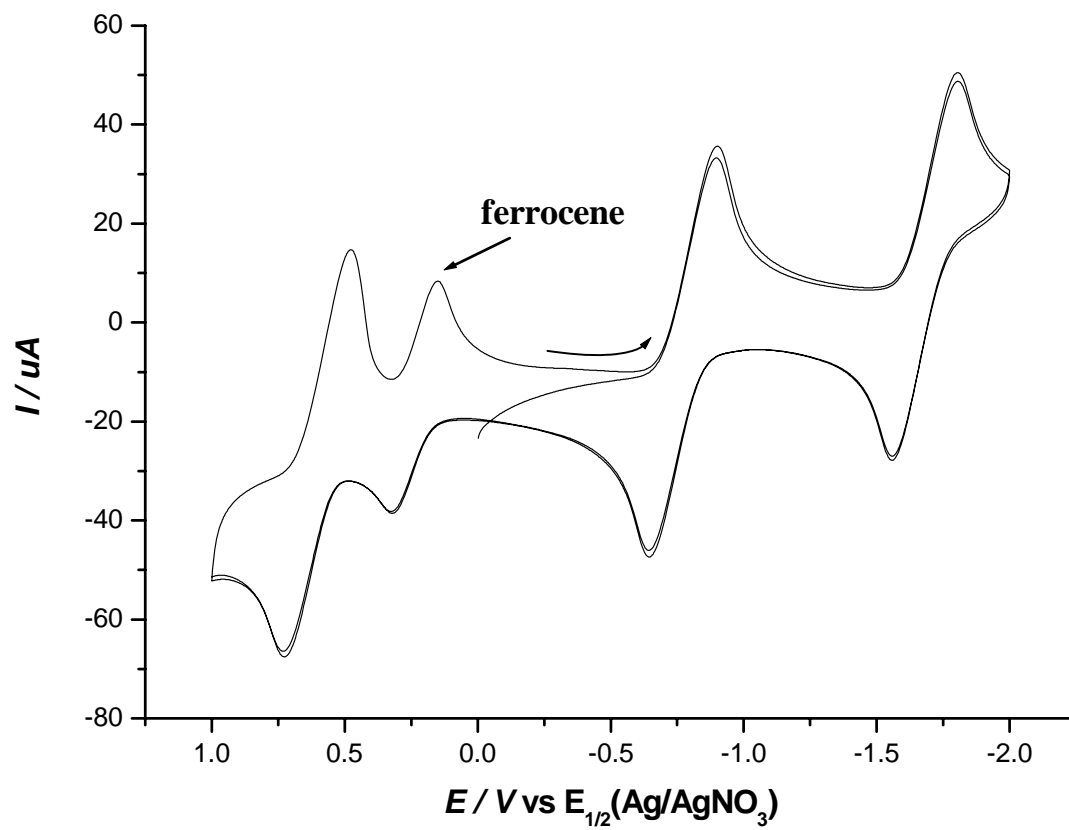
S Table 1

2a			
Fe(1)···Fe(2)	3.141(1)	Fe(1)–S(1)	2.311(2)
Fe(1)–S(2)	2.269(1)	Fe(1)–S(3)	2.184(1)
Fe(2)–S(1)	2.304(2)	Fe(2)–S(2)	2.260(1)
Fe(2)–S(4)	2.193(1)	S(4)–C(25)	1.694(2)
S(5)–C(25)	1.768(2)	S(5)–C(26)	1.813(2)
S(3)–C(25)	1.687(2)		
S(2)–Fe(1)–S(3)	97.0(1)	S(2)–Fe(1)–S(1)	91.4(1)
S(3)–Fe(1)–S(1)	92.1(1)	S(4)–Fe(2)–S(2)	96.3(1)
S(4)–Fe(2)–S(1)	92.4(1)	S(2)–Fe(2)–S(1)	92.5(1)
Fe(2)–S(2)–Fe(1)	87.8(1)	Fe(2)–S(1)–Fe(1)	85.8(1)
S(3)–C(25)–S(4)	129.3(1)	S(3)–C(25)–S(5)	112.1(1)
S(4)–C(25)–S(5)	118.8(1)		
2b			
Fe(1)···Fe(2)	3.350(1)	Fe(1)–S(1)	2.273(1)
Fe(1)–S(2)	2.253(1)	Fe(1)–S(3)	2.179(1)
Fe(2)–S(1)	2.264(1)	Fe(2)–S(2)	2.255(1)
Fe(2)–S(4)	2.162(1)	S(3)–C(23)	1.704(3)
S(4)–C(23)	1.677(3)	S(5)–C(23)	1.764(2)
S(3)–Fe(1)–S(2)	98.3(1)	S(3)–Fe(1)–S(1)	99.0(1)
S(2)–Fe(1)–S(1)	79.7(1)	S(4)–Fe(2)–S(2)	97.9(1)
S(4)–Fe(2)–S(1)	98.9(1)	S(2)–Fe(2)–S(1)	79.9(1)
Fe(2)–S(1)–Fe(1)	95.2(1)	Fe(1)–S(2)–Fe(2)	96.0(1)
S(4)–C(23)–S(3)	129.4(1)	S(4)–C(23)–S(5)	119.5(1)
S(3)–C(23)–S(5)	111.3(1)		

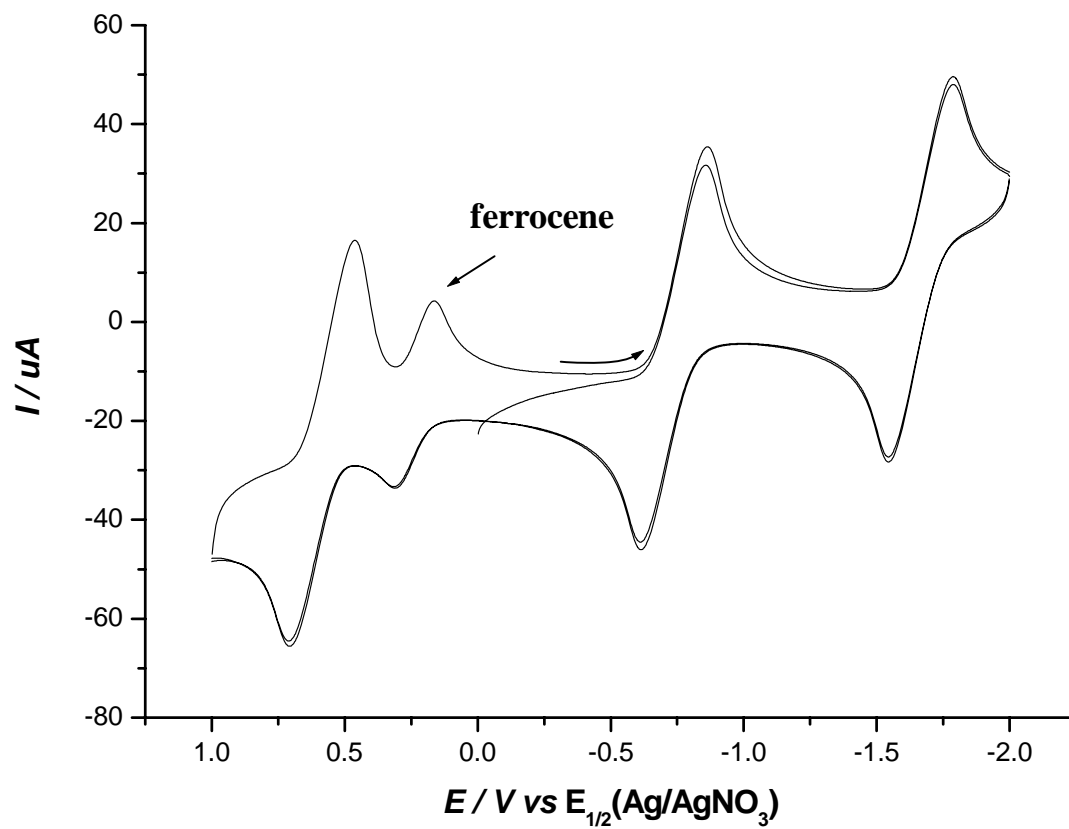
S Table 2

3			
Fe(1)···Fe(1) ^{#1}	3.328(1)	Fe(1)–S(2)	2.135(1)
S(1)–Fe(1) ^{#1}	2.296(1)	S(2)–S(2) ^{#1}	2.033(1)
S(2)–Fe(1)–S(1)	93.6(1)	Fe(1)–S(1)–Fe(1) ^{#1}	93.0(1)
S(2) ^{#1} –S(2)–Fe(1)	107.7(1)	S(1)–Fe(1)–S(1) ^{#1}	76.6(1)
4			
Fe(1)–N(1)	1.989(5)	Fe(1)–S(2)	2.192(1)
Fe(1)–S(3)	2.327(2)	S(1)–C(19)	1.760(5)
S(1)–C(21)	1.821(7)	C(19)–N(1)	1.309(7)
C(11)–N(1)	1.417(8)	C(19)–S(3)	1.711(6)
N(1)–Fe(1)–S(2)	96.4(1)	N(1)–Fe(1)–S(3)	70.2(1)
S(2)–Fe(1)–S(3)	99.3(1)	C(19)–S(1)–C(21)	103.2(3)
C(19)–S(3)–Fe(1)	77.8(2)	N(1)–C(19)–S(3)	110.7(4)
N(1)–C(19)–S(1)	124.5(4)	S(3)–C(19)–S(1)	124.7(3)
C(19)–N(1)–Fe(1)	101.0(4)		

S Fig. 1



S Fig. 2



S Fig. 3

