

Supporting Information to the Paper

Synthesis and Structural Characterization of Electrochemical Reversible Bisferrocenes Containing Bis(acyl-thiourea)s: Enantiomers and Conformers

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Table S1 Selected bond lengths (Å) for **1**, **2** and **1** (C₆H₆)₂

Compounds	1	2	1 (C ₆ H ₆) ₂
O(1)-C(8)	1.215(5)	1.216(4)	1.217(8)
S(1)-C(7)	1.670(4)	1.669(3)	1.671(7)
C(8)-C(9)	1.465(6)	1.457(5)	1.480(10)
N(2)-C(8)	1.392(5)	1.387(4)	1.373(9)
N(2)-C(7)	1.384(5)	1.393(4)	1.396(9)
N(1)-C(7)	1.314(5)	1.312(4)	1.321(8)
N(1)-C(1)	1.454(5)	1.456(4)	1.449(8)
O(2)-C(20)	1.224(6)	1.225(4)	1.227(9)
S(2)-C(19)	1.667(5)	1.672(4)	1.657(7)
C(20)-C(21)	1.470(6)	1.467(5)	1.469(9)
N(4)-C(20)	1.385(6)	1.386(5)	1.385(9)
N(4)-C(19)	1.400(5)	1.402(4)	1.394(8)
N(3)-C(19)	1.323(5)	1.322(4)	1.335(9)
N(3)-C(2)	1.455(5)	1.455(4)	1.445(8)

Table S2 Selected bond angles (°) for **1**, **2** and **1 (C₆H₆)₂**

Compounds	1	2	1 (C₆H₆)₂
N(2)-C(8)-C(9)	114.9(4)	114.8(3)	115.6(6)
O(1)-C(8)-C(9)	123.6(4)	123.4(3)	122.0(7)
O(1)-C(8)-N(2)	121.5(4)	121.9(3)	122.4(6)
C(7)-N(2)-C(8)	129.8(4)	129.9(3)	129.6(6)
N(1)-C(7)-N(2)	116.3(4)	116.0(3)	115.3(6)
N(2)-C(7)-S(1)	117.0(3)	117.2(3)	117.2(5)
N(1)-C(7)-S(1)	126.7(3)	126.7(3)	127.5(5)
C(7)-N(1)-C(1)	125.4(4)	125.4(3)	124.7(6)
N(4)-C(20)-C(21)	116.3(5)	116.2(3)	115.1(6)
O(2)-C(20)-C(21)	121.2(5)	121.1(4)	121.7(6)
O(2)-C(20)-N(4)	122.5(4)	122.7(3)	123.2(6)
C(20)-N(4)-C(19)	127.9(4)	127.5(3)	127.9(6)
N(3)-C(19)-N(4)	115.5(4)	115.9(3)	116.5(6)
N(4)-C(19)-S(2)	118.6(3)	118.3(3)	118.5(5)
N(3)-C(19)-S(2)	125.9(3)	125.8(3)	125.0(5)
C(19)-N(3)-C(2)	125.4(4)	125.3(3)	124.6(6)

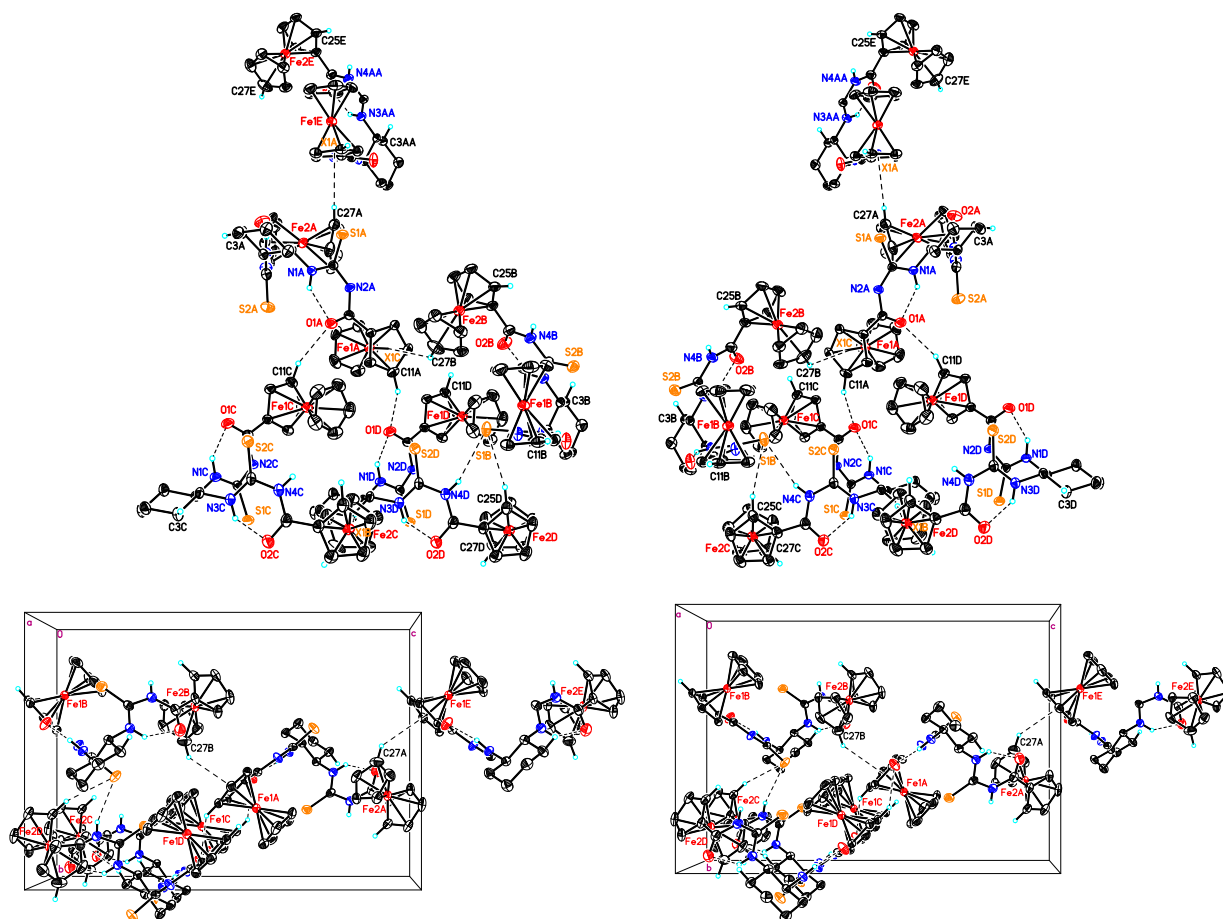


Fig. S1 View of the intermolecular pairs of C-H $\cdots$ O and C-H $\cdots\pi$ (Cg2) cooperating interactions between the adjacent sheets along the *c* axis in compounds **1** (top-left: rotated for clarity; bottom-left: view alone the *a* axis) and **2** (top-right: rotated for clarity; bottom-right: view alone the *a* axis).

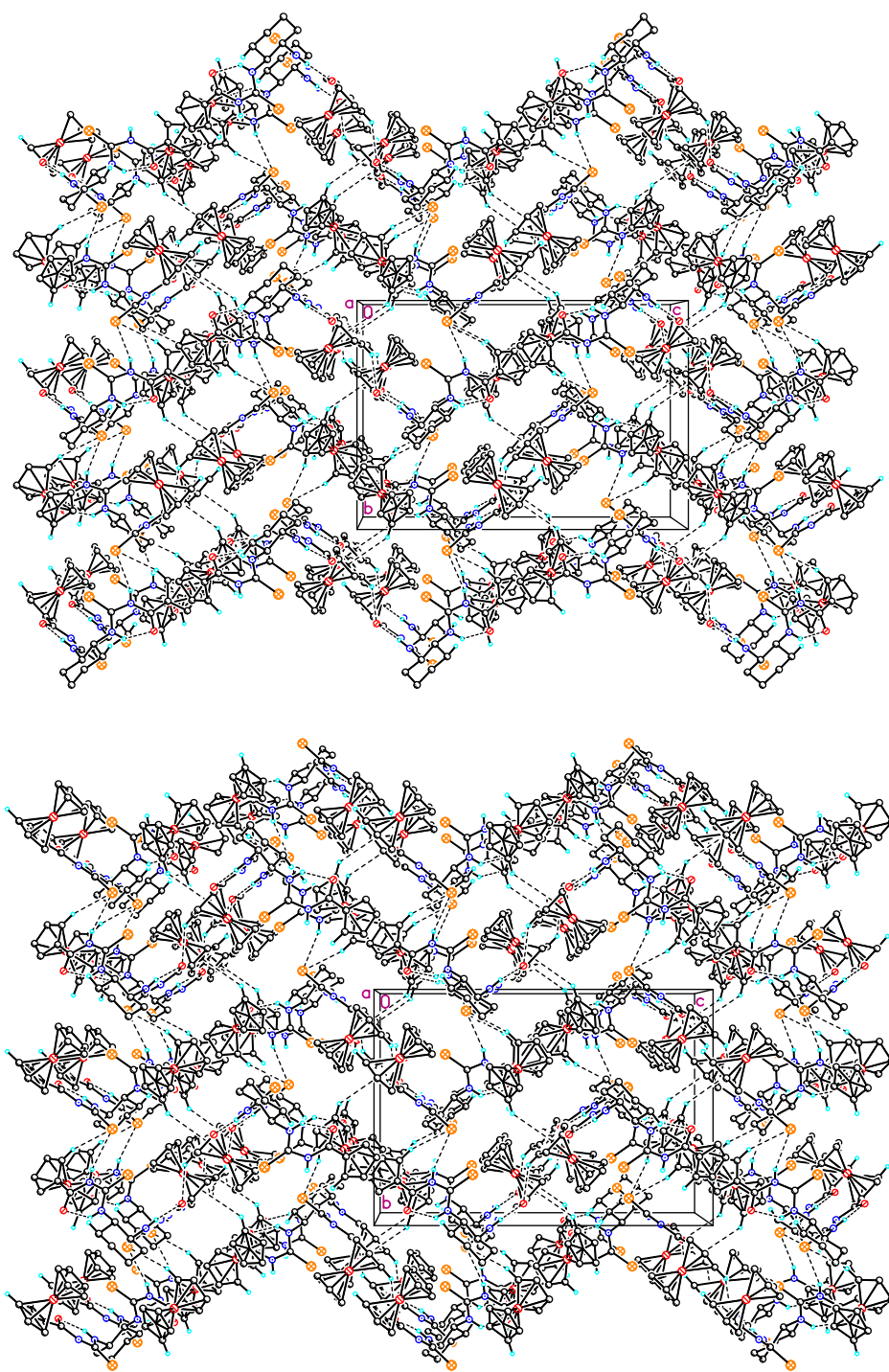


Fig. S2 Projections of the packing structure in compounds **1** (top) and **2** (bottom) in the *bc* plane.