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Ferrocene mono- and di-sulfonates as building blocks in hydrogen-bonded networks

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Supplementary Information

Figure S1. Structure of compound **1**. The ORTEP view shows the atom-labelling scheme and 30 % thermal ellipsoids.

Figure S2. Structure of compound **2**. The ORTEP view shows the atom-labelling scheme and 30 % thermal ellipsoids.

Figure S3. Structure of compound **3**. The ORTEP view shows the atom-labelling scheme and 30 % thermal ellipsoids.

Figure S4. Structure of compound **4**. The ORTEP view shows the atom-labelling scheme and 30 % thermal ellipsoids.

Table S1. Hydrogen bonding interactions in compounds **1 - 4**.

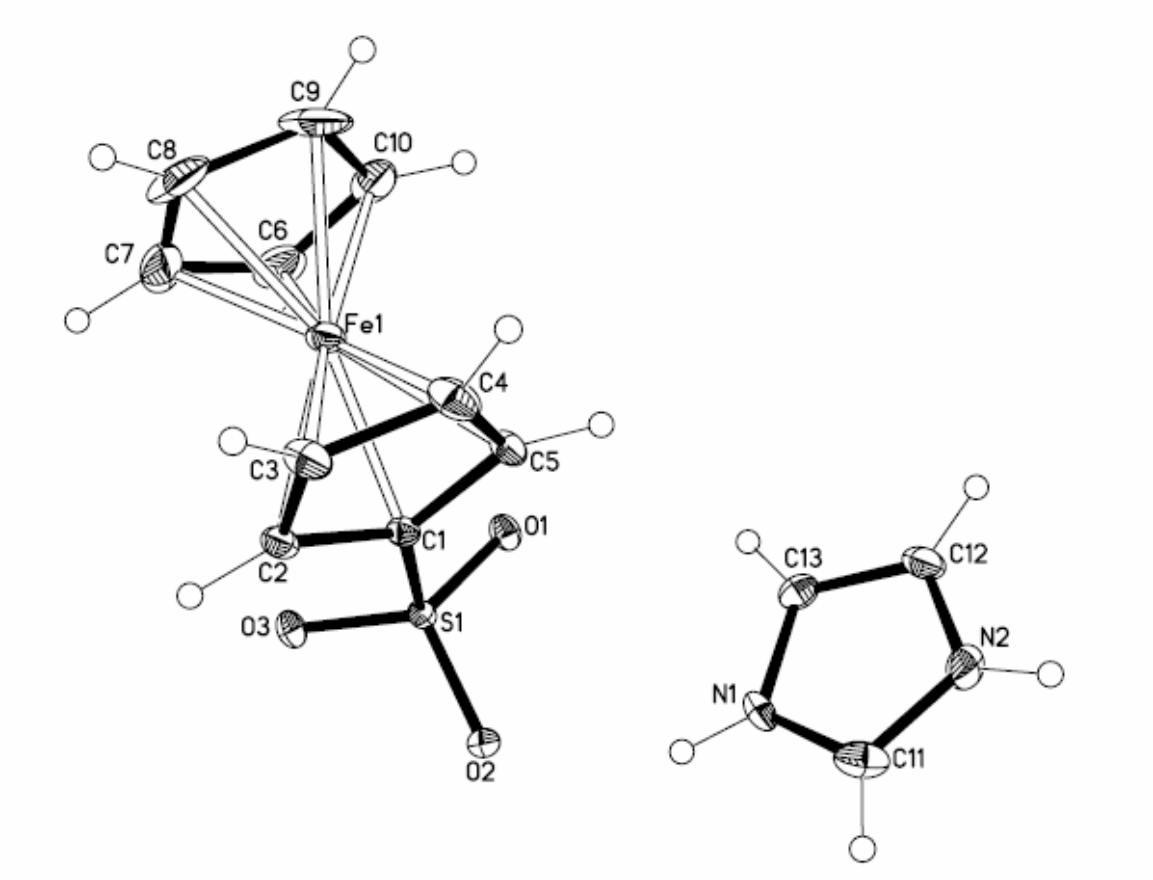


Figure S1

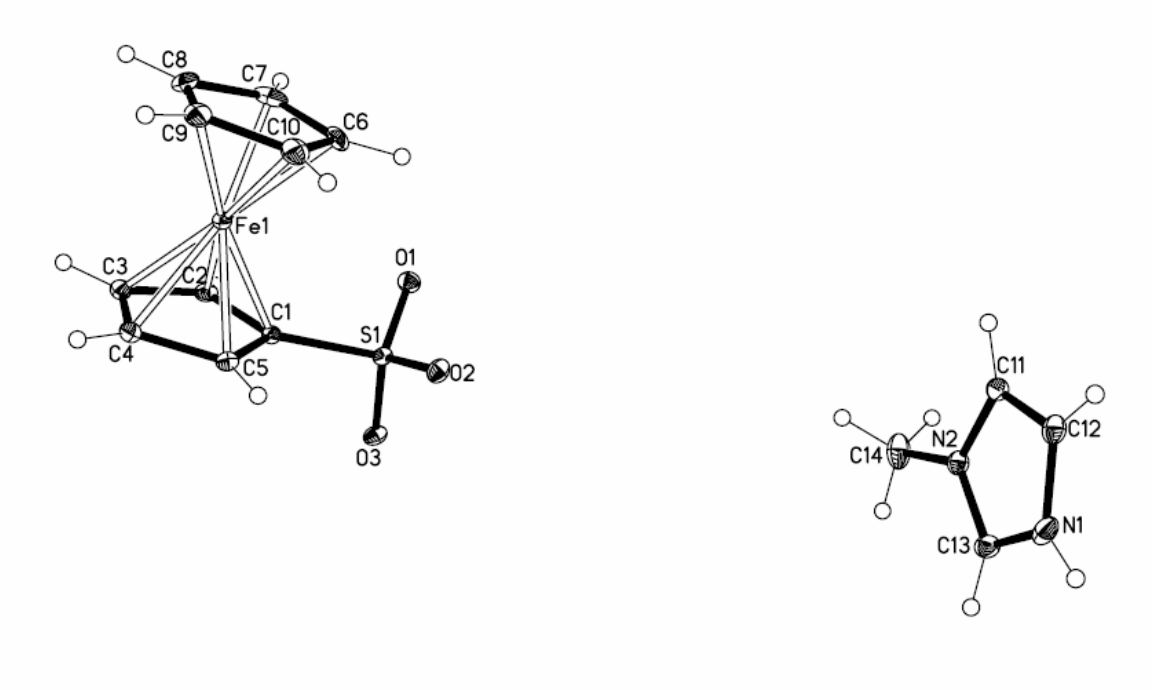
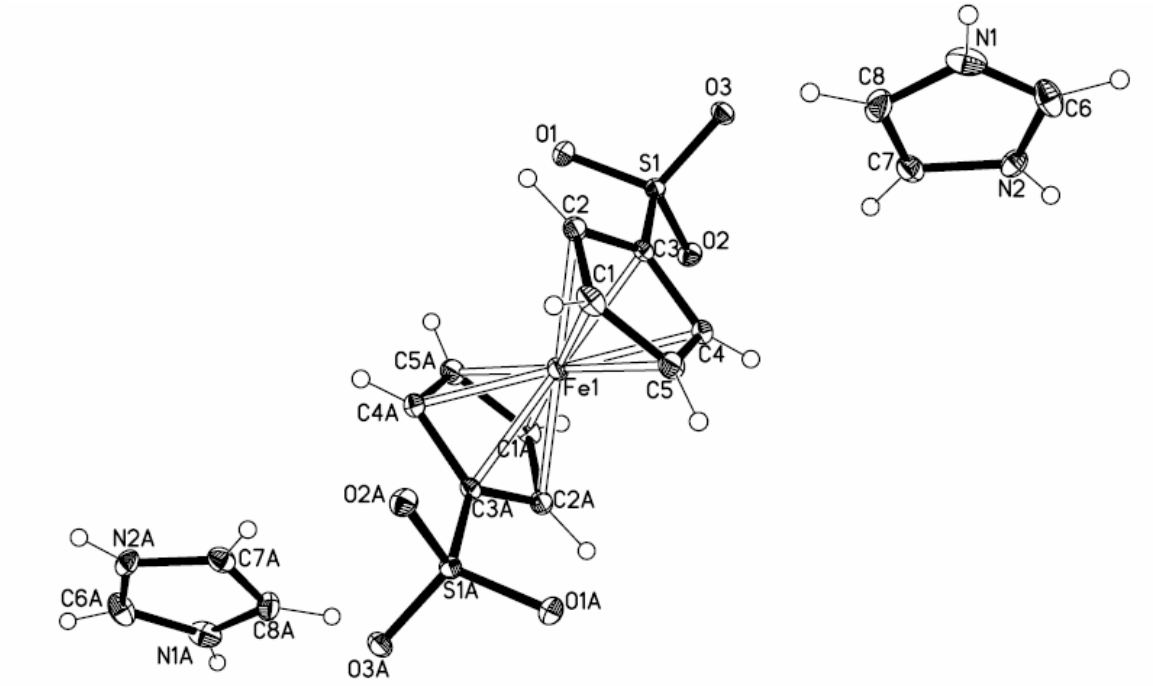


Figure S2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C8
C6
C7
N2
O3
O1
S1
C2
C3
O2
C1
C5A
C4
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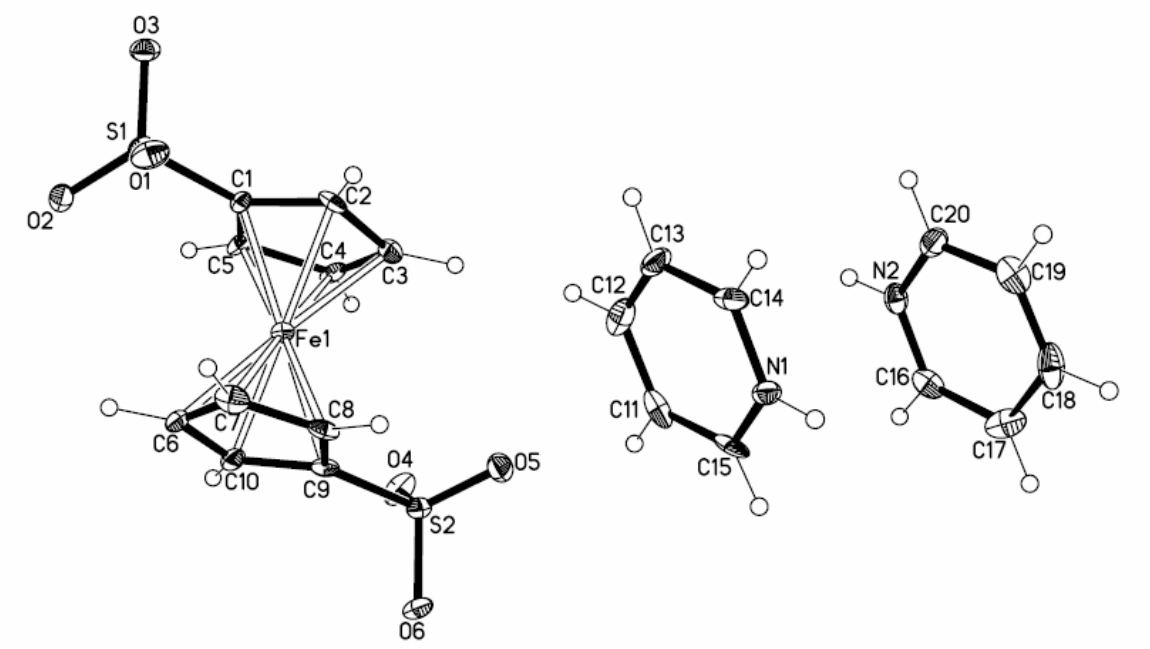
C5
C4A
C1A
O2A
C3A
C2A
N2A
C7A
S1A
C6A
O1A
C8A
N1A
O3A

Figure S3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S1
O1
O2
C1
C2
C5
C4
C3
Fe1
C8
C7
C6
C10
C9
O4
O5
S2
O6
C13
C12
C14
N1
C11
C15
C20
N2
C19
C16
C18
C17

Figure S4

Table S1. Hydrogen bonding interactions[A]

salt	D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
1	N1-H1A	0.88	2.03	151	2.832(3)	O2
	N1-H1A	0.88	2.33	125	2.922(3)	O2 [-x+1, -y+1, -z]
	N2-H2A	0.88	2.22	127	2.842(3)	O3 [x-1, y+1, z]
	N2-H2A	0.88	2.27	126	2.880(3)	O1 [x, y+1, z]
2	N1-H1A	0.88	1.94	151	2.749(3)	O3 [-x+1, -y+1, -z+1]
	N1-H1A	0.88	2.47	124	3.044(3)	O3 [x+1, y, z+1]
3	N1-H1	0.86	2.18	132	2.825(3)	O2 [x, y+1, z]
	N1-H1	0.86	2.35	125	2.924(3)	O1 [x-1, y+1, z]
	N2-H2	0.86	2.03	152	2.820(2)	O3 [x-1, y, z]
	N2-H2	0.86	2.35	125	2.929(2)	O3 [-x+1, -y+1, -z+1]
4	N1-H1A	0.86	1.81	174	2.669(7)	O3 [x+1, y, z+1]
	N1-H1A	0.86	2.83	155	3.631(5)	S1 [x+1, y, z+1]
	N2-H2A	0.86	1.80	177	2.660(7)	O6 [x, y-1, z]
	N2-H2A	0.86	2.86	153	3.641(6)	S2 [x, y-1, z]
	C11-H11	0.93	2.36	142	3.140(9)	O5

[A] D = donor; A = acceptor; distances d in Å; <DHA in deg. The hydrogen atoms have been placed at geometrically estimated positions.