Supplementary Material (ESI) for Soft Matter

SUPPORTING INFORMATION

Ferrocene Based Organometallic Gelators: A Supramolecular Synthon Approach

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Physico-chemical data for the salts

1. **Butylammoniumferrocinedicarboxylate 1_3:** m.p. 198-200^{0}C. Anal. Calc. for $C_{20}H_{32}FeN_2O_4$: C, 57.15; H, 7.67; N, 6.66. Found: C, 56.74; H, 7.37; N, 6.29. FT-IR (KBr): 3387, 2960, 2929, 2874, 2796, 2681, 2598, 2571, 2212, 1641, 1525, 1460, 1384, 1348, 1329, 1298, 1184, 1074, 1031, 1020, 931, 914, 848, 825, 810, 775, 744, 594, 559, 499, 484, 410 cm^{-1}. ^{1}H NMR(CD_3OD) (300MHz) δ = 4.67 (4H, s, Ferrocene Proton), 4.25 (4H, s, Ferrocene Proton), 2.92 (4H, t, J = 7.42 Hz, $^+NH_3CH_2CH_2(CH_2)_1CH_3$), 1.67-1.60 (4H, m, $^+NH_3CH_2CH_2(CH_2)_1CH_3$), 1.46-1.39 (4H, m, $^+NH_3CH_2CH_2(CH_2)_1CH_3$), 0.97 (6H, t, J = 7.23Hz, $^+NH_3CH_2CH_2(CH_2)_1CH_3$).

2. **Pentylammoniumferrocenedicarboxylate 1_4:** m.p. 190^{0}C. Anal. Calc. for $C_{22}H_{36}FeN_2O_4$: C, 58.93; H, 8.09; N, 6.25. Found* C, 57.25; H, 7.84; N, 5.84. FT-IR (KBr): 3421, 3022, 2956, 2931, 2870, 2137, 1647, 1575, 1473, 1386, 1357, 1344, 1209, 1182, 1051, 1022, 821, 788.91, 561, 513, 482 cm^{-1}. ^{1}H NMR(CD_3OD) (500MHz) δ = 4.68 (4H, s, Ferrocene Proton), 4.25 (4H, s, Ferrocene Proton), 2.91 (4H, t, J = 7.5Hz, $^+NH_3CH_2CH_2(CH_2)_2CH_3$), 1.68-1.65 (4H, m, $^+NH_3CH_2CH_2(CH_2)_2CH_3$), 1.39-1.36 (8H, m, $^+NH_3CH_2CH_2(CH_2)_2CH_3$), 0.94 (6H, t, J = 6.75, $^+NH_3CH_2CH_2(CH_2)_2CH_3$). **this is the best results obtained among the several samples tested for elemental analysis*.

3. **Hexylammoniumferrocenedicarboxylate 1_5:** m.p. 164-167^{0}C. Anal. Calc. for $C_{24}H_{40}FeN_2O_4$: C, 60.50; H, 8.46; N, 5.88. Found: C, 60.67; H, 8.40; N, 5.30. FT-IR (KBr): 3385, 3090, 3005, 2951, 2931, 2856, 2202, 1633, 1548, 1518, 1473, 1458, 1386, 1338, 1184, 1101, 821, 790, 667, 513 cm^{-1}. ^{1}H NMR(CD_3OD) (300MHz) δ = 4.67 (4H, s, Ferrocene Proton), 4.25 (4H, s, Ferrocene Proton), 2.91 (4H, t, J = 7.29 Hz, $^+NH_3CH_2CH_2(CH_2)_3CH_3$), 1.66-1.64 (4H, m, $^+NH_3CH_2CH_2(CH_2)_3CH_3$), 1.35 (12H, m, $^+NH_3CH_2CH_2(CH_2)_3CH_3$), 0.90 (6H, br S, $^+NH_3CH_2CH_2(CH_2)_3CH_3$).

4. **Heptylammoniumferrocenedicarboxylate 1_6:** m.p. 155^{0}C. Anal. Calc. for $C_{26}H_{44}FeN_2O_4$: C, 61.90; H, 8.79; N, 5.55. Found: C, 61.50; H, 8.18; N, 5.13. FT-

IR (KBr): 3111, 2960, 2928, 2854, 2783, 2686, 2600, 2551, 2212, 1647, 1626, 1518, 1460, 1383, 1338, 1184, 1024, 823, 808, 785, 553, 501, 412 cm^{-1}. ^1H NMR(CD_3OD) (300MHz) δ = 4.67 (4H, s, Ferrocene Proton), 4.25 (4H, s, Ferrocene Proton), 2.91 (4H, t, J = 7.44Hz, $^+NH_3CH_2CH_2(CH_2)_4CH_3$), 1.66-1.64 (4H, m, $^+NH_3CH_2CH_2(CH_2)_4CH_3$), 1.36-1.32 (16H, m, $^+NH_3CH_2CH_2(CH_2)_4CH_3$), 0.89 (6H, br S, $^+NH_3CH_2CH_2(CH_2)_4CH_3$).

5. **Nonaylammoniumferrocenedicarboxylate 1_8:** m.p. 137^{0}C. Anal. Calc. for $C_{30}H_{52}FeN_2O_4$: C, 64.28; H, 9.35; N, 5.00. Found: C, 64.26; H, 8.45; N, 4.68. FT-IR (KBr): 3111, 2958, 2922, 2852, 2783, 2683, 2573, 2220, 1647, 1626, 1519, 1460, 1383, 1338, 1184, 1024, 823, 808. 785, 555, 501, 418 cm^{-1}. ^1H NMR (CD_3OD) (300MHz) δ = 4.67 (4H, s, Ferrocene Proton), 4.25 (4H, s, Ferrocene Proton), 2.91 (4H, t, J = 7.32Hz, $^+NH_3CH_2CH_2(CH_2)_6CH_3$), 1.66 (4H, br S, $^+NH_3CH_2CH_2(CH_2)_6CH_3$), 1.35-1.29 (24H, br S, $^+NH_3CH_2CH_2(CH_2)_6CH_3$), 0.88 (6H, m, $^+NH_3CH_2CH_2(CH_2)_6CH_3$).

6. **Decylammoniumferrocenedicarboxylate 1_9:** m.p. 138-140^{0}C. Anal. Calc. for $C_{32}H_{56}FeN_2O_4$: C, 65.29; H, 9.59; N, 4.76. Found: C, 65.28; H, 9.80; N, 5.17. FT-IR (KBr): 3109, 3091, 2947, 2916, 2852, 2794, 2681, 2578, 2224, 1653, 1629, 1518, 1460, 1384, 1338, 1184, 1120, 1024, 908, 823, 806, 785, 719, 555, 501, 435, 418 cm^{-1}. ^1H NMR(CD_3OD) (300MHz) δ = 4.67 (4H, d, J = 1.8Hz, Ferrocene Proton), 4.25 (4H, d, J = 1.8Hz, Ferrocene Proton), 2.90 (4H, t, J = 7.32Hz, $^+NH_3CH_2CH_2(CH_2)_7CH_3$), 1.65 (4H, br S, $^+NH_3CH_2CH_2(CH_2)_7CH_3$), 1.29 (28H, br S, $^+NH_3CH_2CH_2(CH_2)_7CH_3$), 0.88 (6H, m, $^+NH_3CH_2CH_2(CH_2)_7CH_3$).

7. **Undecylammoniumferrocenedicarboxylate 1_{10}:** m.p. 136-138^{0}C. Anal. Calc. for $C_{34}H_{60}FeN_2O_4$: C, 66.22; H, 9.81; N, 4.54. Found: C, 65.62; H, 9.09; N, 4.39. FT-IR (KBr): 3111, 3091, 2958, 2918, 2852, 2787, 2681, 2578, 2218, 1651, 1626, 1564, 1516, 1460, 1383, 1338, 1184, 1024, 954, 908, 823, 808, 785, 719, 553, 501, 414 cm^{-1}. ^1H NMR(CD_3OD) (500MHz) δ = 4.66(4H, s, Ferrocene Proton), 4.24 (4H, s, Ferrocene Proton), 2.90 (4H, t, J = 7.50Hz, $^+NH_3CH_2CH_2(CH_2)_8CH_3$), 1.65-1.64 (4H, m, $^+NH_3CH_2CH_2(CH_2)_8CH_3$), 1.35-1.28 (32H, m, $^+NH_3CH_2CH_2(CH_2)_8CH_3$), 0.88 (6H, t, J = 6.5, $^+NH_3CH_2CH_2(CH_2)_8CH_3$).

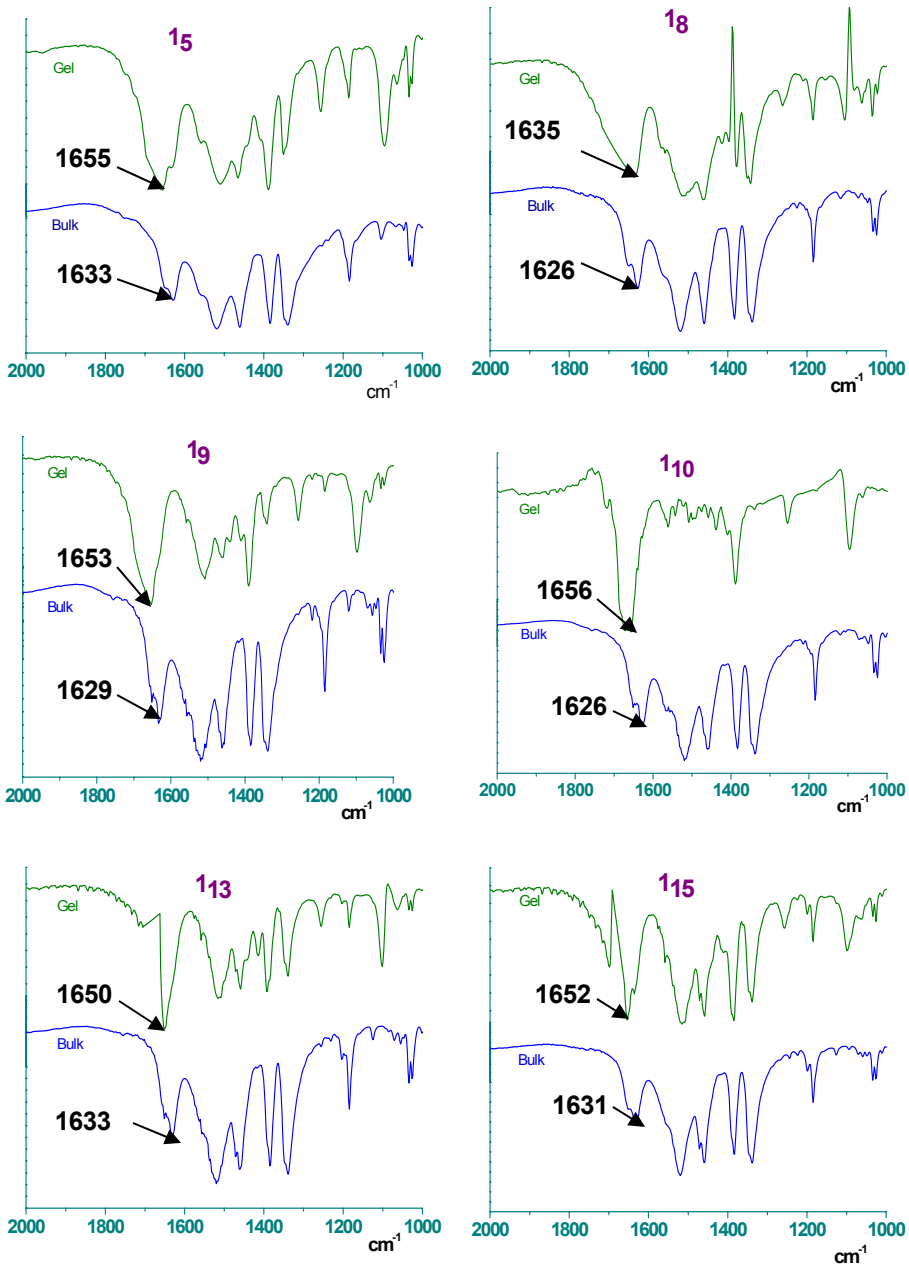
8. **Dodecylammoniumferrocenedicarboxylate 1_{11}:** m.p. 142-146^{0}C. Anal. Calc. for $C_{36}H_{64}FeN_2O_4$: C, 67.06; H, 10.01; N, 4.34. Found: C, 67.31; H, 9.80; N, 4.26. FT-IR (KBr): 3109, 3091, 2916, 2852, 2789, 2685, 2565, 2225, 1629, 1519, 1460, 1384, 1338, 1184, 1122, 1033, 806, 785, 555, 501, 418 cm^{-1}. ^1H NMR(CD_3OD) (300MHz) δ = 4.68(4H, s, Ferrocene Proton), 4.25 (4H, s, Ferrocene Proton), 2.90 (4H, t, J = 7.5Hz, $^+NH_3CH_2CH_2(CH_2)_9CH_3$), 1.65-1.63 (4H, m, $^+NH_3CH_2CH_2(CH_2)_9CH_3$), 1.35-1.28 (36H, m, $^+NH_3CH_2CH_2(CH_2)_9CH_3$), 0.89(6H, t, J = 6.16, $^+NH_3CH_2CH_2(CH_2)_9CH_3$).

9. **Tridecylammoniumferrocenedicarboxylate 1_{12}:** m.p. 138-141^{0}C. Anal. Calc. for $C_{38}H_{68}FeN_2O_4$: C, 67.84; H, 10.19; N, 4.16. Found: C, 67.35; H, 9.81; N, 4.28. FT-IR (KBr): 3111, 3091, 2958, 2918, 2852, 2787, 2677, 2576, 2218, 1647, 1627, 1519, 1460, 1383, 1338, 1184, 1024, 825, 808, 785, 553, 501, 418 cm^{-1}. ^1H NMR(CD_3OD) (500MHz) δ = 4.68(4H, s, Ferrocene Proton), 4.25 (4H, s, Ferrocene Proton), 2.89(4H, t, J = 7.5Hz, $^+NH_3CH_2CH_2(CH_2)_{10}CH_3$), 1.66-1.62 (4H, m, $^+NH_3CH_2CH_2(CH_2)_{10}CH_3$), 1.36-1.28 (40H, m, $^+NH_3CH_2CH_2(CH_2)_{10}CH_3$), 0.89(6H, t, J = 6.5, $^+NH_3CH_2CH_2(CH_2)_{10}CH_3$).

10. Tetradecylammoniumferrocenedicarboxylate 1_{13}: m.p. 134-138^{0}C. Anal. Calc. for $C_{40}H_{72}FeN_2O_4$: C, 68.55; H, 10.35; N, 4.00. Found: C, 68.74; H, 10.73; N, 3.98. FT-IR (KBr): 3109, 3093, 3080, 2916, 2852, 2796, 2677, 2573, 2225, 1633, 1516, 1460, 1384, 1338, 1184, 1124, 1026, 956, 823, 806, 783, 717, 555, 501, 482, 418 cm^{-1}. ^{1}H NMR(CD_3OD) (500MHz) δ = 4.68(4H, s, Ferrocene Proton), 4.25 (4H, s, Ferrocene Proton), 2.89(4H, t, J = 7.50Hz, $^+NH_3C\mathit{H}_2CH_2(CH_2)_{11}CH_3$), 1.65-1.61 (4H, m, $^+NH_3CH_2C\mathit{H}_2(CH_2)_{11}CH_3$), 1.36-1.28 (44H, m, $^+NH_3CH_2CH_2(C\mathit{H}_2)_{11}CH_3$), 0.89(6H, t, J = 6.75, $^+NH_3CH_2CH_2(CH_2)_{11}C\mathit{H}_3$).

11. Pentadecylammoniumferrocenedicarboxylate 1_{14}: m.p. 131^{0}C. Anal. Calc. for $C_{42}H_{76}FeN_2O_4$: C, 69.21; H, 10.51; N, 3.84. Found: C, 69.16; H, 10.23; N, 3.82. FT-IR (KBr): 3111, 3090, 3078, 2958, 2916, 2852, 2787, 2677, 2584, 2214, 1629, 1519, 1458, 1384, 1336, 1199, 1182, 1028, 806, 783, 553, 501 cm^{-1}. ^{1}H NMR(CD_3OD) (500MHz) δ = 4.67(4H, s, Ferrocene Proton), 4.24 (4H, s, Ferrocene Proton), 2.89(4H, t, J = 7.5Hz, $^+NH_3C\mathit{H}_2CH_2(CH_2)_{12}CH_3$), 1.68-1.62 (4H, m, $^+NH_3CH_2C\mathit{H}_2(CH_2)_{12}CH_3$), 1.37-1.27 (48H, m, $^+NH_3CH_2CH_2(C\mathit{H}_2)_{12}CH_3$), 0.89(6H, t, J = 6.75, $^+NH_3CH_2CH_2(CH_2)_{12}C\mathit{H}_3$).

12. Hexadecylammoniumferrocenedicarboxylate 1_{15}: m.p 131^{0}C. Anal. Calc. for $C_{44}H_{80}FeN_2O_4$: C, 69.81; H, 10.65; N, 3.70. Found: C, 69.61; H, 10.53; N, 3.81. FT-IR (KBr): 3109, 3091, 3080, 2916, 2852, 2796, 2681, 2573, 2225, 1631, 1519, 1460, 1384, 1338, 1184, 1030, 806, 783, 717, 555, 501, 489, 416 cm^{-1}. ^{1}H NMR(CD_3OD) (300MHz) δ = 4.68(4H, s, Ferrocene Proton), 4.25 (4H, s, Ferrocene Proton), 2.90(4H, t, J = 7.45Hz, $^+NH_3C\mathit{H}_2CH_2(CH_2)_{13}CH_3$), 1.65 (4H, m, $^+NH_3CH_2C\mathit{H}_2(CH_2)_{13}CH_3$), 1.35-1.28 (52H, m, $^+NH_3CH_2CH_2(C\mathit{H}_2)_{13}CH_3$), 0.89(6H, t, J = 5.95, $^+NH_3CH_2CH_2(CH_2)_{13}C\mathit{H}_3$).



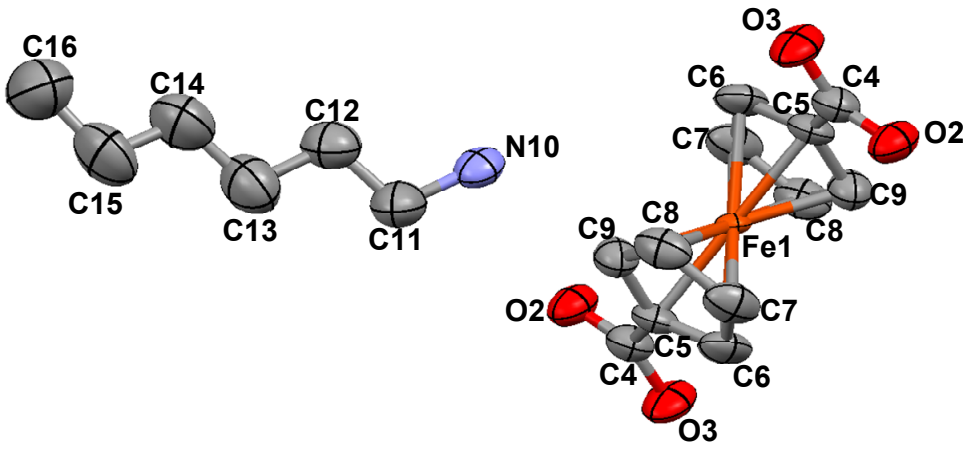
FT-IR of 5 wt % DMF gels (olive) and the corresponding salt as synthesized (blue)

X-ray single crystal data.

Data were collected using MoKα (λ = 0.7107 Å) radiation on a BRUKER APEX II diffractometer equipped with CCD area detector. Data collection, data reduction, structure solution/refinement were carried out using the software package of SMART APEX. All structures were solved by direct method and refined in a routine manner. In most of the cases, nonhydrogen atoms were treated anisotropically. All the hydrogen atoms were geometrically fixed. CCDC (CCDC No. 795748-795753) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB21EZ, UK; fax: (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

Molecular Plots and Hydrogen Bonding Parameters for the compounds

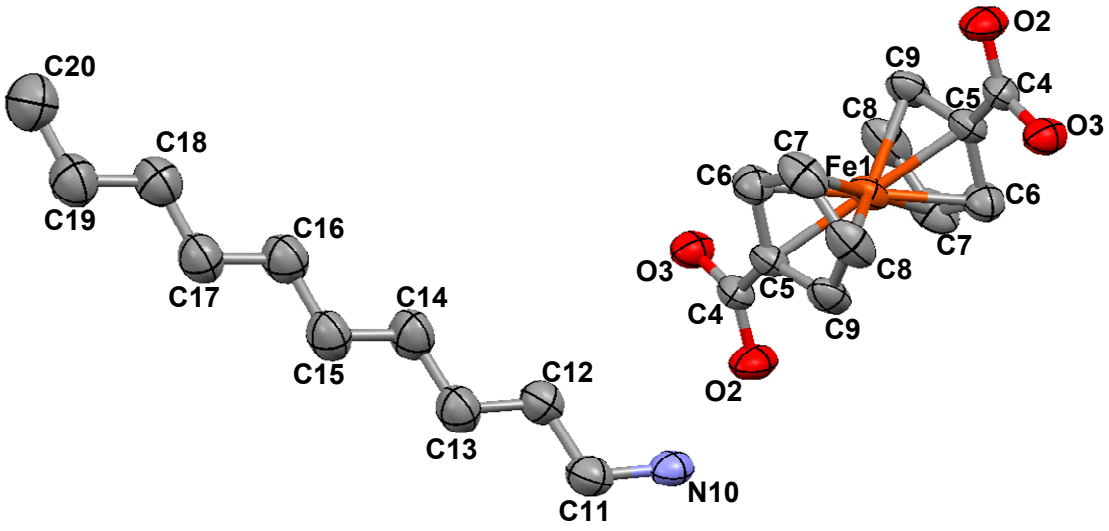
Compound: 1_5



Hydrogen bonding parameters

D*—H···*A	***D*—H**	**H···*A***	***D*···*A***	***D*—H···*A***
1_5				
N10—H10A···O3^{i}	0.89	1.82	2.700 (8)	168.3
N10—H10B···O2^{ii}	0.89	1.92	2.770 (8)	160.0
N10—H10C···O2^{iii}	0.89	1.87	2.727 (8)	160.0
Symmetry codes: (i) x+1, y, z; (ii) -x+1, -y+1, -z+2; (iii) x, y, z.				

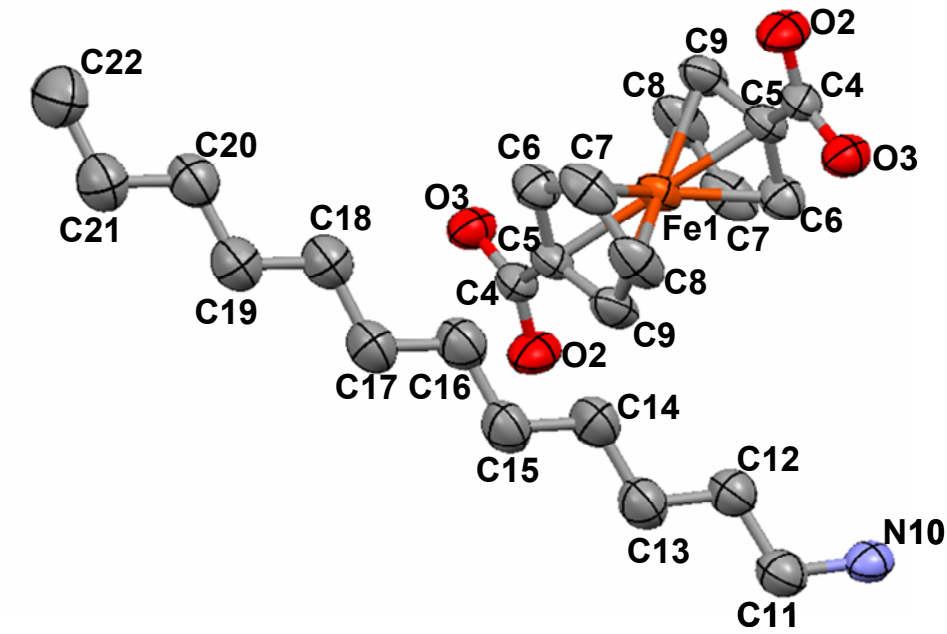
Compound: 1_9



Hydrogen bonding parameters

1_9				
N10—H10A···O3^{i}	0.89	1.90	2.770 (3)	164.2
N10—H10B···O3^{ii}	0.89	1.87	2.724 (3)	159.6
N10—H10C···O2^{iii}	0.89	1.82	2.694 (3)	166.9
Symmetry codes: (i) -x+1, -y+1, -z+1; (ii) x+1, y, z; (iii) x, y, z.				

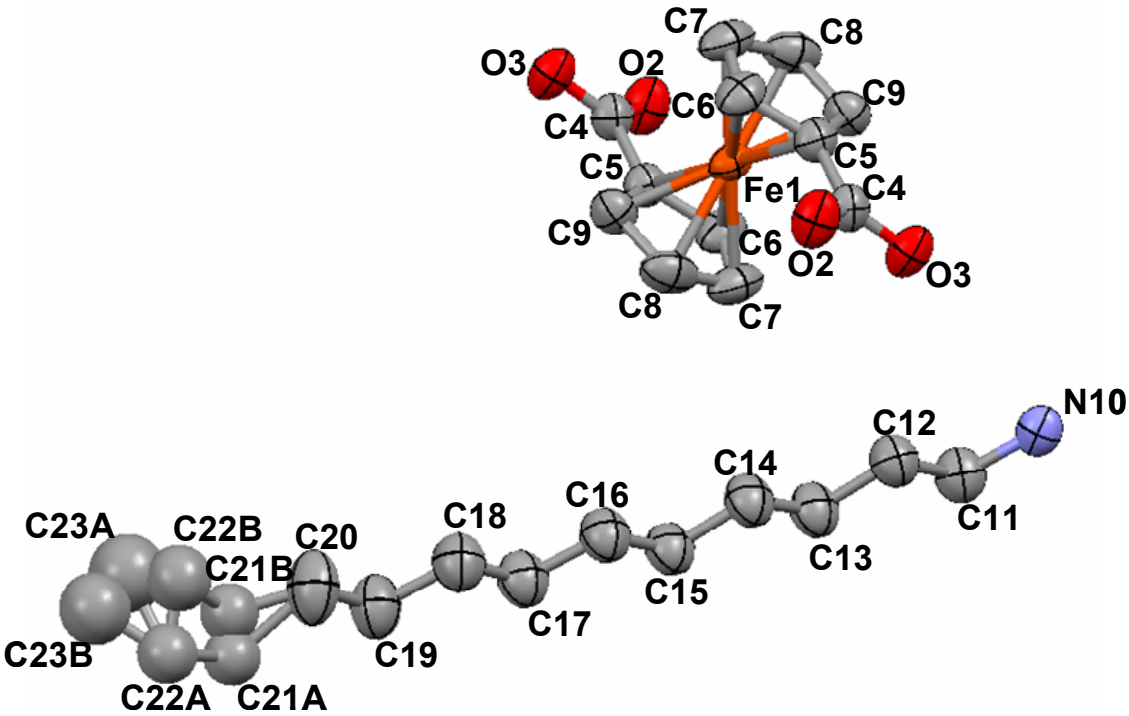
Compound: 1_{11}



Hydrogen bonding parameters

1_{11}				
N10—H10A···O3^{i}	0.89	1.91	2.775 (3)	164.6
N10—H10B···O3^{ii}	0.89	1.87	2.724 (3)	159.5
N10—H10C···O2^{iii}	0.89	1.82	2.697(3)	166.6
Symmetry codes: (i) -x, -y+1, -z; (ii) x-1, y-1, z; (iii) x, y-1, z				

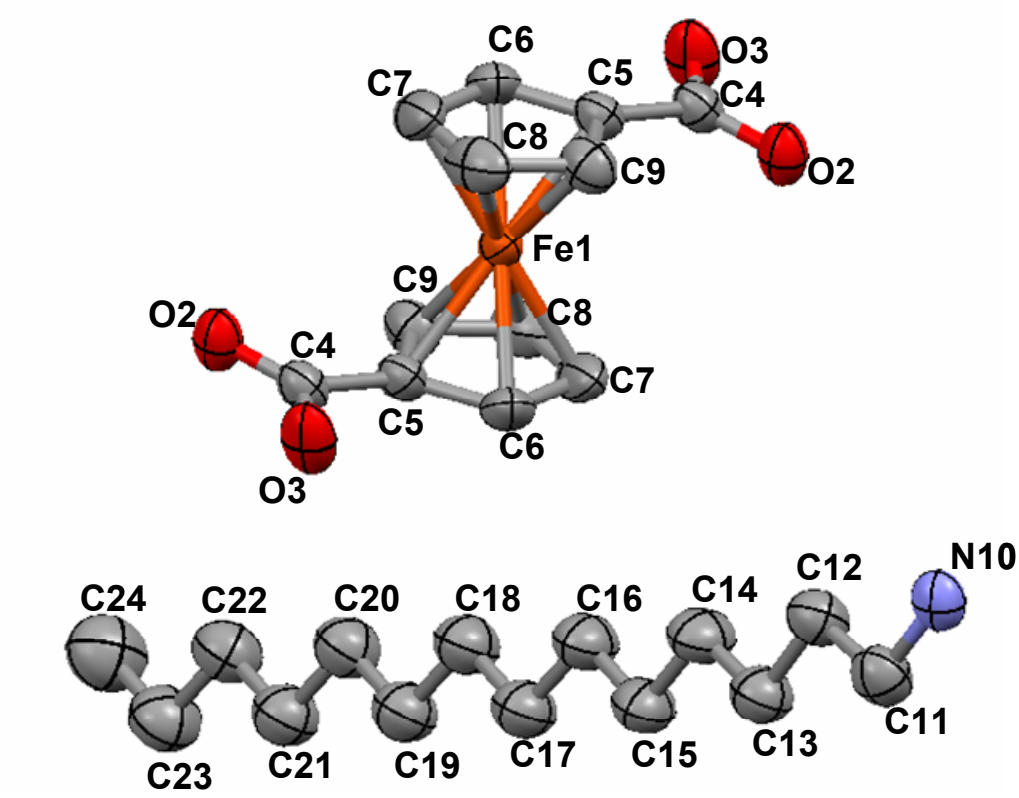
Compound: 1_{12}



Hydrogen bonding parameters

1_{12}				
N10—H10A···O3^{i}	0.89	1.91	2.778 (3)	162.8
N10—H10B···O3^{ii}	0.89	1.88	2.731 (3)	160.5
N10—H10C···O2^{iii}	0.89	1.85	2.722 (3)	167.9
Symmetry codes: (i) -x+1, -y+1, -z; (ii) x-1, y-1, z; (iii) x, y-1, z				

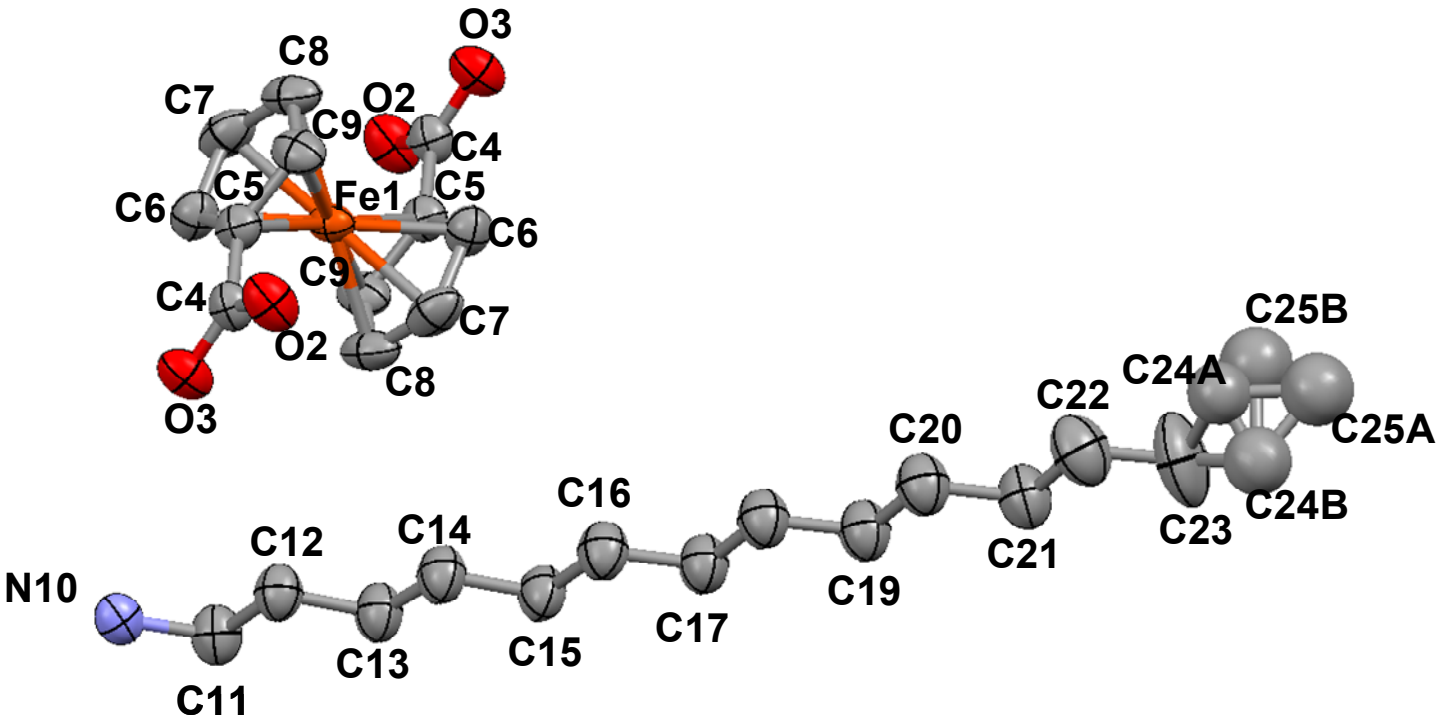
Compound: 1_{13}



Hydrogen bonding parameters

1_{13}				
N10—H10C···O2^{i}	0.89	1.92	2.779 (3)	162.8
N10—H10B···O2^{ii}	0.89	1.87	2.729 (3)	160.7
N10—H10A···O3^{iii}	0.89	1.82	2.697 (3)	169.5
Symmetry codes: (i) -x+1, -y, -z; (ii) x+1, y-1, z; (iii) x, y-1, z.				

ompound: 1_{14}



Hydrogen bonding parameters

F.2A$_{14}$				
N10—H10A···O3^{i}	0.89	1.92	2.777 (3)	161.3
N10—H10B···O2^{ii}	0.89	1.84	2.725 (3)	170.2
N10—H10C···O3^{iii}	0.89	1.88	2.737 (3)	161.3
Symmetry codes: (i) $x+1, y, z$; (ii) $-x+1, -y, -z+1$; (iii) $-x+2, -y, -z+1$.				