Crystalline bilayer formation in homoleptic low-spin Fe(II) compounds with alkyl chain substituents

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Experimental

Synthesis of *N*-(di(pyridin-2-yl)methyl)alkyl-1-amine ligands (LC_4-C_{16})

Synthesis of ligands LC_4-LC_{16} was achieved via a modified literature procedure.[1]

***N*-(Di(pyridin-2-yl)methyl)butan-1-amine (LC_4)**: Di(2-pyridyl) ketone (1.0136 g, 5.5 mmol), acetic acid (5 drops) and butylamine (1.6090 g, 22.0 mmol) were dissolved in 30 mL of MeOH and refluxed with stirring for 24 hours. The solution was cooled to room temperature and the methanol was evaporated under reduced pressure. The orange residue was dissolved in 50 mL of diethyl ether and washed with 3 x 50 mL of deionised water. The organic layer was then concentrated under reduced pressure and the orange-yellow residue dissolved in 50 mL of dichloromethane, which was washed with 2 x 50 mL water. The organic phase was dried over anhydrous magnesium sulphate and the solution filtered. The dichloromethane was evaporated, affording a yellow-orange residue as the pure imine. The imine precursor was dissolved in 30 mL of methanol then cooled to 0°C. To this solution was added 2.5 eq. of $NaBH_4$ and the reaction stirred for 2.5 hours. The methanol was evaporated and the orange residue was dissolved in 50 mL of diethyl ether and washed with 3 x 50 mL deionised water. The organic layer was then concentrated under reduced pressure and the residue dissolved in 50 mL of CH_2Cl_2. The solution was then washed with 2 x 50 mL of water and 50 mL of aq. NaCl (10% w/v). The organic phase was dried over anhydrous magnesium sulphate, filtered and the solvent evaporated, affording pure LC_4. Yield = 1.018 g, 75.9%. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 8.55 (ddd, *J* = 1.0, 1.8, 5.0 Hz, 2H), 7.56 (td, *J* = 1.7, 7.7 Hz, 2H), 7.42 (d, *J* = 8.0 Hz, 2H), 7.12 (ddd, *J* = 1.0, 4.8, 7.5 Hz, 2H), 5.09 (s, 1H), 2.60 (t, *J* = 7.2 Hz, 2H), 1.55 (quin, *J* = 7.2, 7.7 Hz, 2H), 1.35 (sext, *J* = 7.2, 7.7, 2H), 0.88 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 161.6, 149.1, 136.5, 122.6, 122.3, 69.5, 47.8, 32.3, 20.4, 13.9. MS (ESI$^+$) (MeOH): *m/z* calcd for $C_{15}H_{19}N_3$ $[M]^+$, 241.34; found, 264.15 $[M + Na]^+$, 169.08 $[M - C_4H_9NH]^+$.

***N*-(Di(pyridin-2-yl)methyl)hexan-1-amine (LC_6)**: Preparation of LC_6 was done via the same procedure as $L1C_4$, using hexylamine (0.5565 g, 5.5 mmol). Yield = 1.356 g, 91.5%. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 8.55 (ddd, *J* = 0.8, 2.0, 4.8 Hz, 2H), 7.60 (td, *J* = 1.8, 7.7 Hz, 2H), 7.41 (d, *J* = 7.8 Hz, 2H), 7.12 (ddd, *J* = 1.0, 4.9, 7.5 Hz, 2H), 5.09 (s, 1H), 2.97 (br, 1H), 2.60 (t, *J* = 7.3 Hz, 2H), 1.56 (quin, *J* = 6.9, 7.2 Hz, 2H), 1.29 (m, *J* = 7.6, 6H), 0.86 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 161.7, 149.2, 136.5, 122.4, 122.1, 69.6, 48.1, 31.8, 30.2, 27.0, 22.6, 14.0.

MS (ESI$^+$) (MeOH): *m/z* calcd for $C_{17}H_{23}N_3$ [*M*]$^+$, 269.39; found, 292.18 [*M* + Na]$^+$, 169.08 [*M* - $C_6H_{13}NH$]$^+$.

***N*-(Di(pyridin-2-yl)methyl)octan-1-amine (LC_8)**: Preparation of LC_8 was done via the same procedure as LC_6, using octylamine (0.7108 g, 5.5 mmol). Yield = 1.008 g, 61.6%. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 8.56 (d, *J* = 4.1 Hz, 2H), 7.62 (t, *J* = 7.7 Hz, 2H), 7.42 (d, *J* = 7.9 Hz, 2H), 7.13 (t, *J* = 6.1 Hz, 2H), 5.1 (s, 1H), 2.82 (br, 1H), 2.60 (t, *J* = 7.4 Hz, 2H), 1.58 (quin, *J* = 6.7, 7.2 Hz, 2H), 1.25 (m, 10H), 0.87 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 161.3, 149.3, 136.7, 122.4, 122.2, 69.4, 48.0, 31.9, 30.1, 29.5, 29.3, 27.4, 22.7, 14.1. MS (ESI$^+$) (MeOH): m/z calcd for $C_{19}H_{27}N_3$ [*M*]$^+$, 297.45; found, 320.21 [*M* + Na]$^+$, 298.23 [*M* + H]$^+$, 169.08 [*M* - $C_8H_{17}NH$]$^+$.

***N*-(Di(pyridin-2-yl)methyl)decan-1-amine (LC_{10})**: Preparation of LC_{10} was done via the same procedure as LC_6, using decylamine (1.0136 g, 5.5 mmol). Yield = 1.253 g, 70.0%. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 8.55 (ddd, *J* = 1.0, 1.8, 5.1 Hz, 2H), 7.61 (td, *J* = 1.8, 7.7 Hz, 2H), 7.42 (d, *J* = 7.9 Hz, 2H), 7.13 (ddd, *J* = 1.1, 4.8, 7.5 Hz, 2H), 5.11 (s, 1H), 2.62 (t, *J* = 7.3 Hz, 2H), 1.58 (quin, *J* = 7.1, 7.5 Hz, 2H), 1.24 (m, 14H), 0.86 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 161.3, 149.3, 136.6, 122.4, 122.2, 69.3, 48.0, 31.9, 30.1, 29.6, 29.5, 29.3, 29.3, 27.3, 22.7, 14.1. MS (ESI$^+$) (MeOH): *m/z* calcd for $C_{21}H_{31}N_3$ [*M*]$^+$, 325.50; found, 348.3 [*M* + Na]$^+$, 326.24 [*M* + H]$^+$, 169.08 [*M* - $C_{10}H_{21}NH$]$^+$.

***N*-(Di(pyridin-2-yl)methyl)dodecan-1-amine (LC_{12})**: Preparation of LC_{12} was done via the same procedure as LC_6, using dodecylamine (1.0194 g, 5.5 mmol). Yield = 1.478 g, 76.0%. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 8.60 (ddd, *J* = 0.7, 1.8, 4.9 Hz, 2H), 7.65 (td, *J* = 1.8, 7.6 Hz, 2H), 7.46 (d, *J* = 7.9 Hz, 2H), 7.17 (ddd, *J* = 1.0, 4.9, 7.5 Hz, 2H), 5.15 (s, 1H), 2.63 (t, *J* = 7.3 Hz, 2H), 1.60 (quin, *J* = 7.2, 7.4 Hz, 2H), 1.24 (m, 18H), 0.88 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 161.7, 149.2, 136.6, 122.3, 122.1, 69.6, 48.1, 31.9, 30.3, 29.7, 29.7, 29.6, 29.6, 29.4, 27.4, 22.7, 14.1. MS (ESI$^+$) (MeOH): *m/z* calcd for $C_{23}H_{35}N_3$ [*M*]$^+$, 353.55; found, 376.28 [*M* + Na]$^+$, 354.30 [*M* + H]$^+$, 184.10 [*M* - $C_{12}H_{25}$]$^+$.

***N*-(Di(pyridin-2-yl)methyl)tetradecan-1-amine (LC_{14}):** Preparation of LC_{14} was done via the same procedure as LC_6, using tetradecylamine (1.1737 g, 5.5 mmol). Yield = 1.049 g, 50.0%. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 8.56 (ddd, *J* = 0.8, 1.8, 5.0 Hz, 2H), 7.61 (td, *J* = 1.8, 7.7 Hz, 2H), 7.42 (d, *J* = 7.9 Hz, 2H), 7.13 (ddd, *J* = 1.0, 4.8, 7.5 Hz, 2H), 5.10 (s, 1H), 2.60 (t, *J* = 7.2 Hz, 2H), 1.57 (quin, *J* = 6.8, 7.8 Hz, 2H), 1.24 (m, 22H), 0.88 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 161.3, 149.3, 136.7, 122.4, 122.2, 69.4, 48.0, 31.9, 30.2, 30.1, 29.5, 29.3, 29.6, 27.4, 22.7, 14.1. MS (ESI$^+$) (MeOH): *m/z* calcd for $C_{25}H_{39}N_3$ [*M*]$^+$, 381.61; found, 381.80 [*M*]$^+$.

***N*-(Di(pyridin-2-yl)methyl)hexadecan-1-amine (LC_{16})**: Preparation of LC_{16} was done via the same procedure as LC_6, using hexadecylamine (1.3280 g, 5.5 mmol). Yield = 1.0081 g, 45%. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 8.55 (ddd, *J* = 0.8, 1.9, 4.8 Hz, 2H), 7.60 (td, *J* = 1.9, 7.7 Hz, 2H), 7.41 (d, *J* = 7.9 Hz, 2H), 7.12 (dd, *J* = 1.0, 4.9, 7.5 Hz, 2H), 5.07 (s, 1H), 2.60 (t, *J* = 7.3 Hz, 2H), 1.55 (quin, *J* = 6.9, 7.4 Hz, 2H), 1.25 (m, 26H), 0.88 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 161.8, 149.2, 136.5, 122.3, 122.0, 69.6, 48.1, 31.9, 30.3, 29.7, 29.6, 29.6, 29.5, 29.3, 27.4, 22.7, 14.0. MS (ESI$^+$) (MeOH): *m/z* calcd for $C_{27}H_{43}N_3$ $[M]^+$, 409.66; found, 409.04 $[M]^+$.

Synthesis of $1C_4$-C_{16}

$[Fe^{II}(LC_4)_2](BF_4)_2$ ($1C_4$): $Fe(BF_4)_2{\cdot}6H_2O$ (33.8 mg, 0.1 mmol) and LC_4 (48.2 mg, 0.2 mmol) were dissolved in 8 mL of methanol and stirred for 30 minutes. The resulting orange solution was filtered and the methanol was allowed to slowly evaporate, affording orange X-ray quality single crystals of the compound **$1C_4$**. Yield = 53.4 mg, 75%. MS (ESI$^+$) (MeOH): *m/z* calcd for $C_{30}H_{38}B_2F_8FeN_6$ $[M]^+$, 712.13; found, 538.30 $[M - 2BF_4]^+$, 316.10 $[M - LC_4 - 2BF_4 + F]^+$. Elemental analysis (air-dried crystals) found: C, 50.52; H, 5.54; N, 11.69. Calc. for $C_{32}H_{38}B_2F_8FeN_6$ (solvate free): C, 50.60; H, 5.38; N, 11.80 %. FTIR (ν_{max} / cm^{-1}): 3251w, 3180vw, 2964w, 2927w, 2865w, 1612w, 1562vw, 1466m, 1444m, 1378w, 1341w, 1282w, 1213vw, 1163w, 1033vs, 983s, 939m, 874vw, 842vw, 788w, 771s, 755m, 699w, 649w.

$[Fe^{II}(LC_6)_2](CF_3SO_3)_2$ ($1C_6$): $FeCl_2{\cdot}4H_2O$ (19.9 mg, 0.1 mmol), $NaCF_3SO_3$ (34.4 mg, 0.2 mmol) and LC_6 (53.8 mg, 0.2 mmol) were dissolved in 8 mL of ethanol and stirred for 30 minutes. The resulting dark orange solution was filtered and the ethanol was allowed to slowly evaporate, affording X-ray quality, orange single crystals of the compound **$1C_6$**. Yield = 63.4 mg, 71%. MS (ESI$^+$) (MeOH): *m/z* calcd for $C_{36}H_{46}F_6FeN_6O_6S_2$ $[M]^+$, 892.76; found, 540.20 $[2LC_6 + H]^+$, 297.12 $[M - 2CF_3SO_3]^{2+}$. Elemental analysis (air-dried crystals) found: C, 48.26; H, 4.98; N, 9.51. Calc. for $C_{36}H_{46}F_6FeN_6O_6S_2$ (solvate free): C, 47.95; H, 5.25; N, 9.32 %. FTIR (ν_{max} / cm^{-1}): 3480br w, 3238w, 3187w, 3074vw, 2926m, 2852w, 1606w, 1480w sh, 1470m, 1447m, 1282s, 1263vs, 1252vs sh, 1223s, 1149vs, 1063w, 1031 vs, 974vw, 939vw, 792w, 777m, 763s, 753m, 727vw, 656w.

$[Fe^{II}(LC_8)_2](CF_3SO_3)_2$ ($1C_8$): **$1C_8$** was prepared via the same method as **$1C_6$**, using $FeCl_2{\cdot}4H_2O$ (19.9 mg, 0.1 mmol), $NaCF_3SO_3$ (34.4 mg, 0.2 mmol) and LC_8 (59.40 mg, 0.2 mmol). Single crystals were determined to be anhydrous when in the presence of remnant ethanol. Bulk samples of air-dried crystals isolated as the monohydrate. Yield = 67.7 mg, 70%. MS (ESI$^+$)

(MeOH): *m/z* calcd for $C_{40}H_{54}F_6FeN_6O_6S_2$ $[M]^+$, 948.86; found, 971.30 $[M + Na]^+$, 799.40 $[M - CF_3SO_3]^+$, 325.22 $[M - 2CF_3SO_3]^{2+}$. Elemental analysis (air-dried crystals) found: C, 49.72; H, 5.67; N, 8.54. Calc. for $C_{40}H_{56}F_6FeN_6O_7S_2$ (monohydrate): C, 49.69; H, 5.84; N 8.69 %. FTIR (ν_{max} / cm^{-1}): 3480br w, 3238w, 3185w br, 3074vw, 2926m, 2852w, 1606w, 1556vw, 1528vw, 1480w sh, 1470m, 1447m, 1282s, 1263vs, 1252vs sh, 1223s, 1149vs, 1063w, 1031 vs, 974vw, 939vw, 792w, 777m, 763s, 753m, 727vw, 656w.

$[Fe^{II}(LC_{10})_2](CF_3SO_3)_2$ ($1C_{10}$): **$1C_{10}$** was prepared via the same method as **$1C_6$**, using $FeCl_2{\cdot}4H_2O$ (19.9 mg, 0.1 mmol), $NaCF_3SO_3$ (34.4 mg, 0.2 mmol) and LC_{10} (65.00 mg, 0.2 mmol). The resulting dark orange solution was filtered and the ethanol was allowed to slowly evaporate, affording X-ray quality, orange single crystals of compound **$1C_{10}$** which were determined to be anhydrous when in the presence of remnant ethanol. Bulk samples of air-dried crystals were characterised as monohydrated and were used for further characterisation. Yield = 61.4 mg, 60%. MS (ESI^+) (MeOH): *m/z* calcd for $C_{44}H_{62}F_6FeN_6O_6S_2$ $[M]^+$, 1004.97; found, 1027.40 $[M + Na]^+$, 855.40 $[M - CF_3SO_3]^+$, 353.22 $[M - 2CF_3SO_3]^{2+}$. Elemental analysis (air-dried crystals) found, C, 51.85; H, 5.82; N, 8.04. Calc. for $C_{44}H_{64}F_6FeN_6O_7S_2$ (monohydrate): C, 51.66; H, 6.31; N, 8.22 %. FTIR (ν_{max} / cm^{-1}): 3480br w, 3238w, 3187w, 3074vw, 2926m, 2852w, 1606w, 1480w sh, 1470m, 1447m, 1282s, 1263vs, 1252vs sh, 1223s, 1149vs, 1063w, 1031 vs, 974vw, 939vw, 792w, 777m, 763s, 753m, 727vw, 656w.

$[Fe^{II}(LC_{12})_2](CF_3SO_3)_2$ ($1C_{12}$): **$1C_{12}$** was prepared via the same method as **$1C_6$**, using $FeCl_2{\cdot}4H_2O$ (19.9 mg, 0.1 mmol), $NaCF_3SO_3$ (34.4 mg, 0.2 mmol) and LC_{12} (70.60 mg, 0.2 mmol). The resulting dark orange solution was filtered and the ethanol was allowed to slowly evaporate, affording X-ray quality, orange single crystals of compound **$1C_{12}$** which were determined to be anhydrous when in the presence of remnant ethanol. Bulk samples of air-dried crystals were characterised via elemental analysis, which matched the anhydrous single crystal formula and were used for further characterisation. Yield = 65.8 mg, 62%. MS (ESI^+) (MeOH): *m/z* calcd for $C_{48}H_{70}F_6FeN_6O_6S_2$ $[M]^+$, 1061.08; found, 911.50 $[M - CF_3SO_3 + H]^+$, 354.30 $[LC_{12} + H]^+$. Elemental analysis (air-dried crystals) found, C, 54.42; H, 6.42; N, 7.81. Calc. for $C_{48}H_{70}F_6FeN_6O_6S_2$ (solvate-free): C, 54.33; H, 6.65; N, 7.92 %. FTIR (ν_{max} / cm^{-1}): 3480br w, 3238w, 3187w, 3074vw, 2926m, 2852w, 1606w, 1480w sh, 1470m, 1447m, 1282s, 1263vs, 1252vs sh, 1223s, 1149vs, 1063w, 1031 vs, 974vw, 939vw, 792w, 777m, 763s, 753m, 727vw, 656w.

$[Fe^{II}(LC_{14})_2](BF_4)_2 \cdot 0.5H_2O \cdot 0.5MeOH$ ($1C_{14}$): **$1C_{14}$** was prepared via the same method as **$1C_4$**, using $Fe(BF_4)_2 \cdot 6H_2O$ (33.8 mg, 0.1 mmol) and LC_{14} (76.2 mg, 0.2 mmol). The resulting dark orange solution was filtered and the methanol was allowed to slowly evaporate, affording X-ray quality, orange single crystals of compound **$1C_{14}$** which were determined to be solvated by 0.5 water and 0.5 MeOH molecules per formula unit. Bulk samples of air-dried crystals were characterised as representative of the single crystal formula and were used for further characterisation. Powder samples, for use in the PXRD studies, of **$1C_{14}$** were obtained by performing the reaction at concentrations 10 times higher than stated above. The powders precipitated after 10 min stirring and were collected via vacuum filtration before being dried under vacuum for 5 hours. The elemental analysis of the powder reflected that of the bulk crystal sample and was used for powder X-ray diffraction studies. Yield = 71.6 mg, 70.4%. MS (ESI^+) (MeOH): *m/z* calcd for $C_{50}H_{78}B_2F_8FeN_6$ $[M]^+$, 992.67; found, 905.7 $[M - BF_4]^+$, 409.30 $[M - 2BF_4]^{2+}$. Elemental analysis (air-dried crystals) found: C, 59.74; H, 7.66; N, 8.19; (powder) found: C, 60.10; H, 7.99; N, 8.28 Calc. for $C_{50.5}H_{81}B_2F_8FeN_6O$ (includes 0.5 H_2O and 0.5 MeOH solvates): C, 59.60; H, 8.02; N 8.26 %. FTIR (ν_{max} / cm^{-1}): 3624w, 3542w, 3251w, 3180vw, 3168w, 2964w, 2927vs, 2865s, 1612w, 1562vw, 1466m, 1444m, 1378w, 1341w, 1282w, 1213vw, 1163w, 1033vs, 983s, 939m, 874vw, 842vw, 788w, 771s, 755m, 699w, 649w.

$[Fe^{II}(LC_{16})_2](CF_3SO_3)_2 \cdot H_2O$ ($1C_{16}$): **$1C_{16}$** was prepared via the same method as **$1C_6$**, using $FeCl_2 \cdot 4H_2O$ (19.9 mg, 0.1 mmol), $NaCF_3SO_3$ (81.8 mg, 0.2 mmol) and LC_{12} (70.60 mg, 0.2 mmol. The resulting dark orange solution was filtered and the ethanol was allowed to slowly evaporate, affording X-ray quality, orange single crystals of compound **$1C_{16}$** which were anhydrous according to X-ray diffraction studies (see below). However, bulk samples of air-dried crystals were characterised as monohydrated and were used for further characterisation. Yield = 53.1 mg, 51%. MS (ESI^+) (MeOH): *m/z* calcd for $C_{56}H_{86}F_6FeN_6O_6S_2$ $[M]^+$, 1173.30; found, 1195.70 $[M + Na]^+$, 1023.60 $[M - CF_3SO_3]^+$, 410.40 $[M - 2CF_3SO_3]^{2+}$. Elemental analysis (air-dried crystals) found: C, 56.47; H, 7.50; N, 7.09. Calc. for $C_{56}H_{88}F_6FeN_6O_7S_2$ (monohydrate): C, 56.46; H, 7.45; N 7.05 %. FTIR (ν_{max} / cm^{-1}): 3480br w, 3238w, 3187w, 3074vw, 2926m, 2852w, 1606w, 1480w sh, 1470m, 1447m, 1282s, 1263vs, 1252vs sh, 1223s, 1149vs, 1063w, 1031 vs, 974vw, 939vw, 792w, 777m, 763s, 753m, 727vw, 656w.

Single Crystal X-ray Diffraction

Table S1 Single crystal X-ray diffraction details and parameters for compounds **$1C_4$**-**$1C_8$**.

Parameters	**$1C_4$**	**$1C_6$**	**$1C_8$**
Formula	$C_{30}H_{38}B_2F_8FeN_6$	$C_{36}H_{46}F_6FeN_6O_6S_2$	$C_{40}H_{54}F_6FeN_6O_6S_2$
M_r	712.16	892.77	948.88
Cryst syst	monoclinic	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/c$	$P2_1/c$
a / Å	9.6481(3)	20.8837(3)	23.8910(6)
b / Å	18.3359(4)	10.45420(10)	10.3579(2)
c / Å	18.2408(5)	19.3400(3)	19.4682(5)
α / °	90.000	90.000	90.000
β / °	95.377(3)	108.114(2)	110.978(3)
γ / °	90.000	90.000	90.000
V / Å^3	3212.72(15)	4013.09(10)	4498.30(2)
T / K	100	100	100
Z	4	4	4
ρ_{calcd} / g.cm^{-3}	1.4722	1.4775	1.4010
λ / Å	0.71073	0.71073	1.54178
No. of indep reflns	7315	9179	8188
No. reflns with $I > 2\sigma(I)$	5769	7983	6741
No. of params	444	516	552
No. of restraints	0	0	0
Final R1[a], wR2[b], ($I > 2\sigma(I)$)	0.0459, 0.1019	0.0383, 0.0945	0.0667, 0.1808
R1[a], wR2[b] (all data)	0.0661, 0.1102	0.0460, 0.0990	0.0781, 0.1932
Goodness of fit	1.0449	1.0220	1.0393
Largest residuals / e Å^{-3}	0.9091	1.3350	0.8888

[a] $R1 = \Sigma[|F_0| - |F_c|]/\Sigma[|F_0|$, [b] $wR2 = [\Sigma w(F_0^2 - F_c^2)/\Sigma wF_0^4)]^{1/2}$

Table S2 Single crystal X-ray diffraction details and parameters for compounds **$1C_{10}$**-**$1C_{16}$**.

Parameters	**$1C_{10}$**	**$1C_{12}$**	**$1C_{14}$**	**$1C_{16}$**
Formula	$C_{44}H_{62}F_6FeN_6O_6S_2$	$C_{48}H_{70}F_6FeN_6O_6S_2$	$C_{50.5}H_{80.5}B_2F_8FeN_6O$	$C_{56}H_{86}F_6FeN_6O_6S_2$
M_r	1004.96	1061.10	1017.68	1173.27
Cryst syst	monoclinic	monoclinic	triclinic	monoclinic
Space group	$P2_1/c$	$P2_1/c$	$\bar{P}_1$	$C2/c$
a / Å	25.8831(6)	27.5740(7)	10.5737(2)	60.5410(2)
b / Å	10.2810(2)	10.1229(2)	17.0941(3)	10.3428(5)
c / Å	19.4228(4)	19.4863(3)	29.4514(4)	19.2128(10)
α / deg	90.000	90.000	88.860(1)	90.000
β / deg	111.103(2)	104.208(2)	86.862(1)	98.330(4)
γ / deg	90.000	90.000	89.547(2)	90.000
V / Å^3	4821.860(19)	5272.81(19)	5314.12(16)	11903.40(10)
T / K	100	100	100	100
Z	4	4	4	8
ρ_{calcd} / g.cm^{-3}	1.384	1.3366	1.2720	1.3090
λ / Å	0.71073	1.54178	0.71073	1.54178
No. of indep reflns	11060	9879	24353	10876
No. reflns with $I > 2\sigma$(I)	9357	7089	19406	8122
No. of params	588	669	1261	723
No. of restraints	0	0	0	0
Final R1[a], wR2[b], ($I > 2\sigma$(I))	0.0584, 0.1373	0.0570, 0.1438	0.0715, 0.1634	0.0898, 0.2274
R1[a], wR2[b] (all data)	0.0712, 0.1438	0.0829, 0.1627	0.0917, 0.1729	0.1123, 0.2477
Goodness of fit	1.0924	1.0043	1.0970	1.0490
Largest residuals / e Å^{-3}	1.3400	0.5981	2.1890	0.8340

[a] $R1 = \Sigma[|F_0| - |F_c|]/\Sigma[|F_0|$, [b] $wR2 = [\Sigma w(F_0^2 - F_c^2)/\Sigma wF_0^4)]^{1/2}$

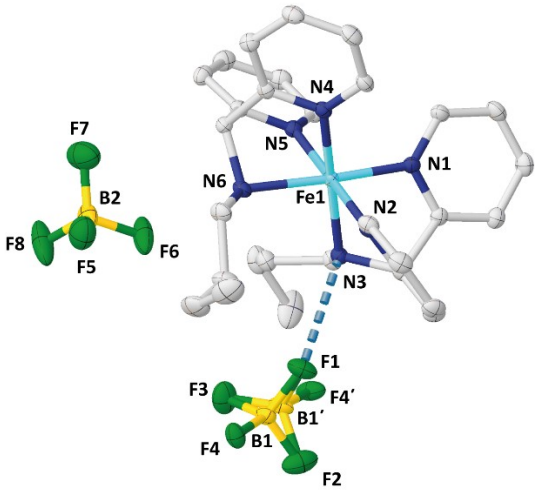


Figure S1 Asymmetric unit of **1C$_4$** at 100 K. Disorder on the BF_4 anion was modelled with a part A:B chemical occupancy ratio of 0.72:0.28. Hydrogen atoms omitted for clarity. Legend: iron, turquoise; nitrogen, blue; carbon, grey; boron, yellow; fluorine, green.

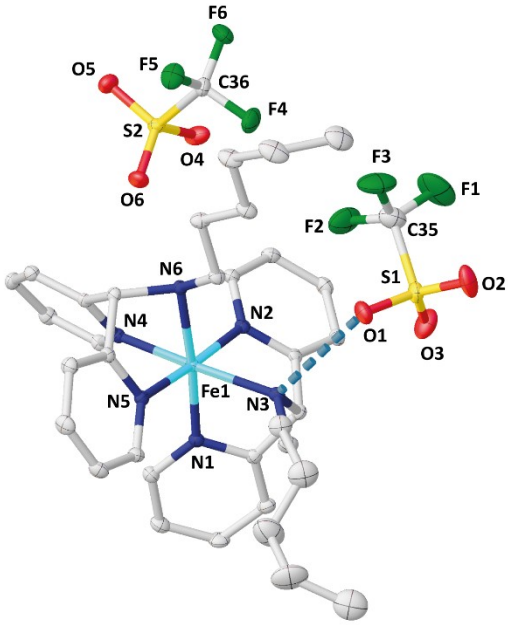


Figure S2 Asymmetric unit of **1C$_6$** at 100 K with selected atom labels. Hydrogen atoms omitted for clarity. Legend: iron, turquoise; nitrogen, blue; carbon, grey; sulphur, yellow; oxygen, red.

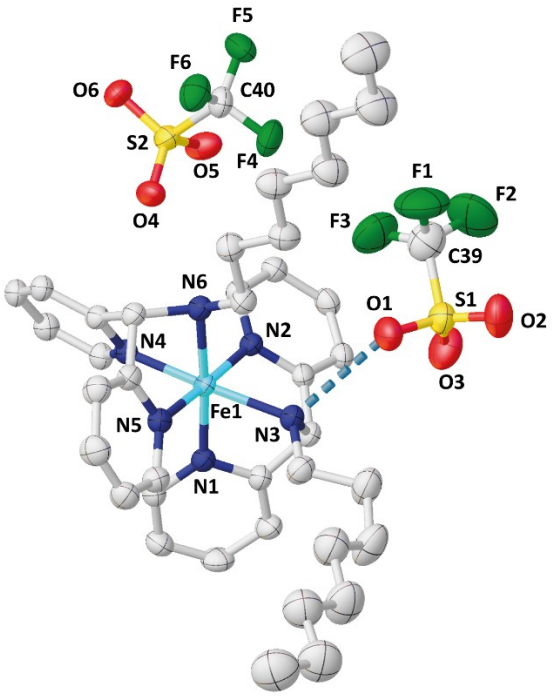


Figure S3 Asymmetric unit of **1C$_8$** at 100 K with selected atom labels. Hydrogen atoms omitted for clarity. Legend: iron, turquoise; nitrogen, blue; carbon, grey; sulphur, yellow; oxygen, red.

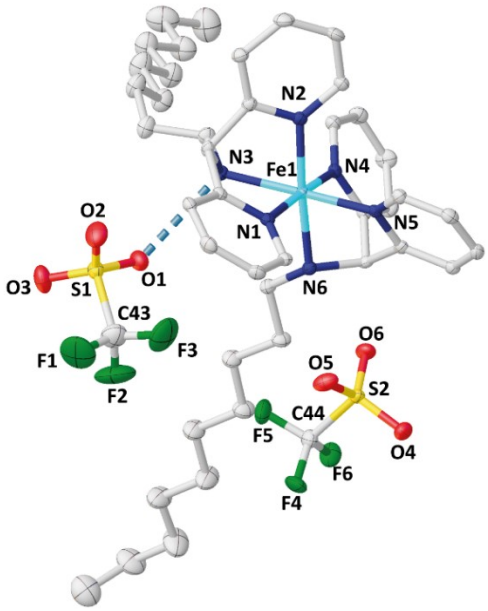


Figure S4 Asymmetric unit of **1C$_{10}$** at 100 K with selected atom labels. Hydrogen atoms omitted for clarity. Legend: iron, turquoise; nitrogen, blue; carbon, grey; sulphur, yellow; oxygen, red.

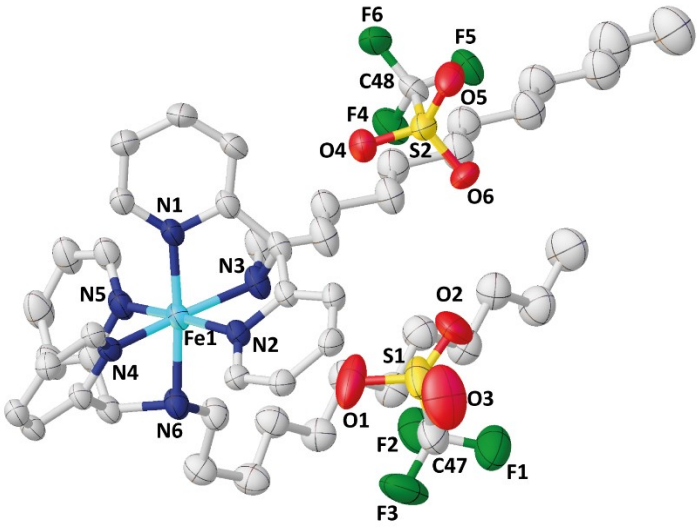


Figure S5 Asymmetric unit of **1C$_{12}$** at 100 K with selected atom labels. Hydrogen atoms omitted for clarity. Legend: iron, turquoise; nitrogen, blue; carbon, grey; sulphur, yellow; oxygen, red.

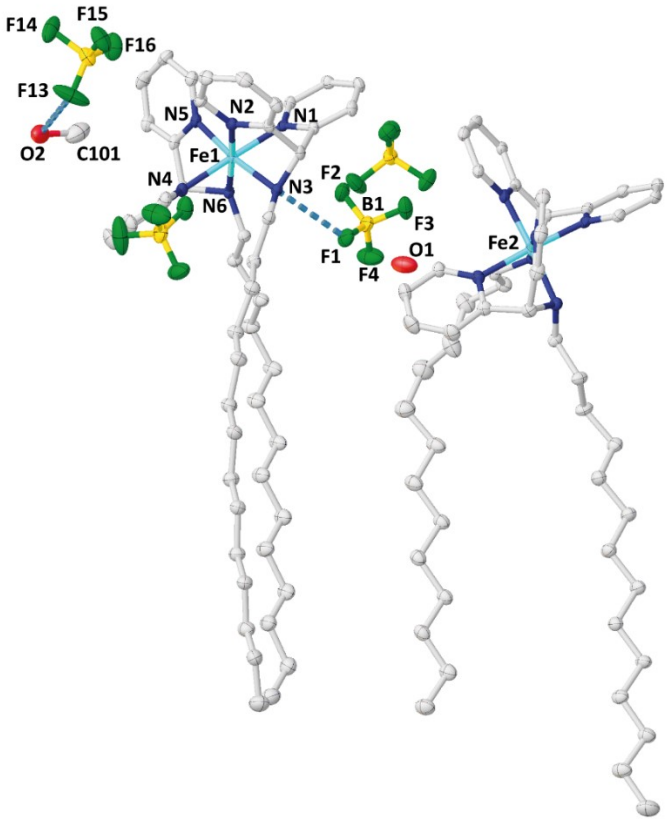


Figure S6 Asymmetric unit of **1C$_{14}$** at 100 K with selected atom labels. Only part 1 shown. Hydrogen atoms omitted for clarity. Legend: iron, turquoise; nitrogen, blue; carbon, grey; sulphur, yellow; oxygen, red.

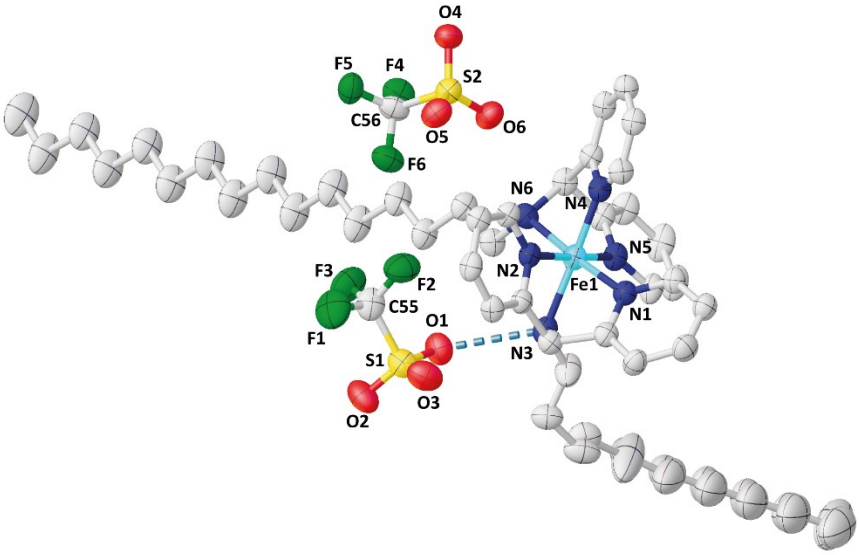


Figure S7 Asymmetric unit of **1C$_{16}$** at 100 K with selected atom labels. Only part 1 shown. Hydrogen atoms omitted for clarity. Legend: iron, turquoise; nitrogen, blue; carbon, grey; sulphur, yellow; oxygen, red.

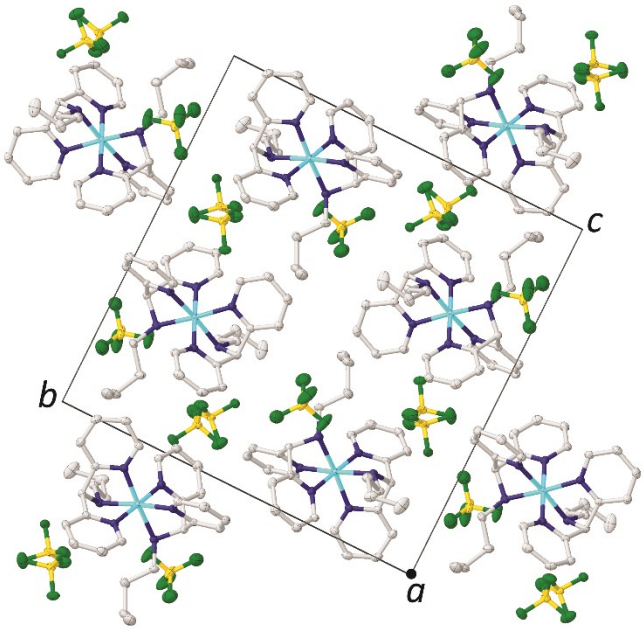


Figure S8 Unit cell of **1C$_4$** at 100 K as viewed along the *a* axis.

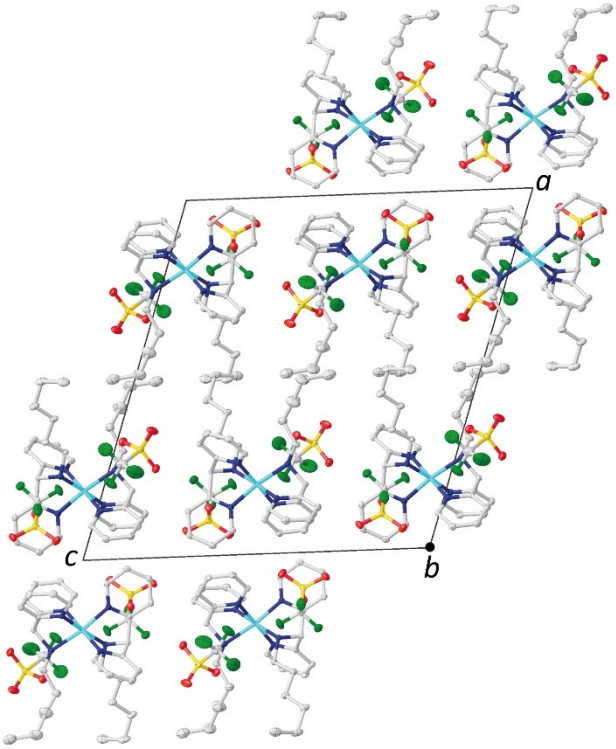


Figure S9 Unit cell of **1C$_6$** at 100 K as viewed along the *b* axis.

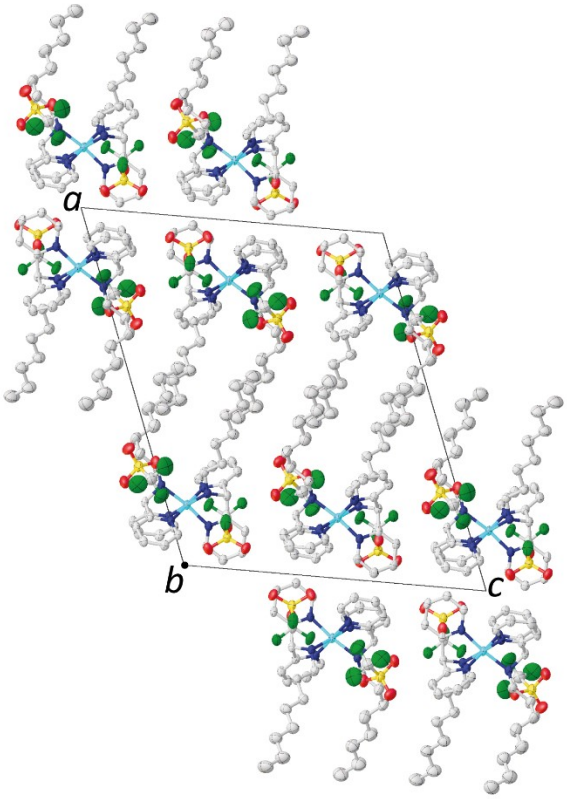


Figure S10 Unit cell of **1C$_8$** at 100 K as viewed along the *b* axis.

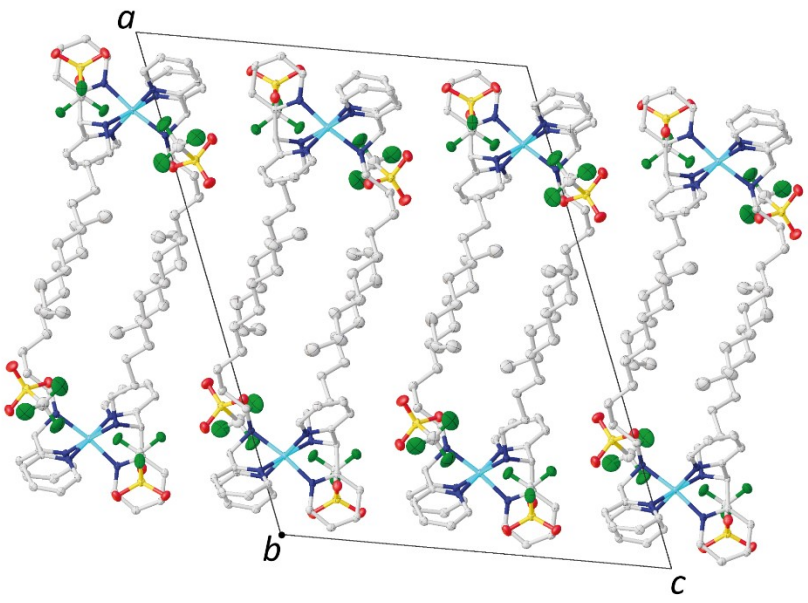


Figure S11 Unit cell of **1C$_{10}$** at 100 K as viewed along the *b* axis.

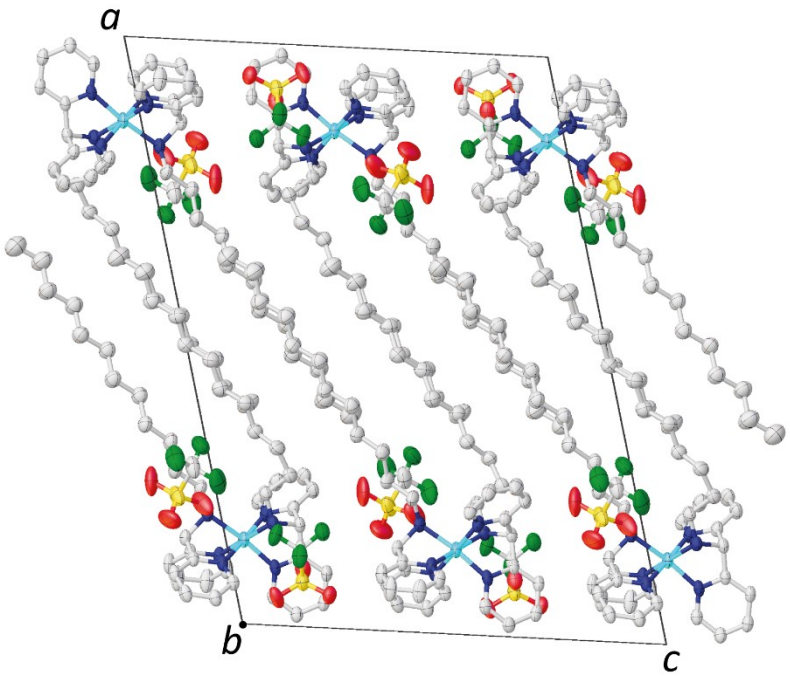


Figure S12 Unit cell of **1C$_{12}$** at 100 K as viewed along the *b* axis.

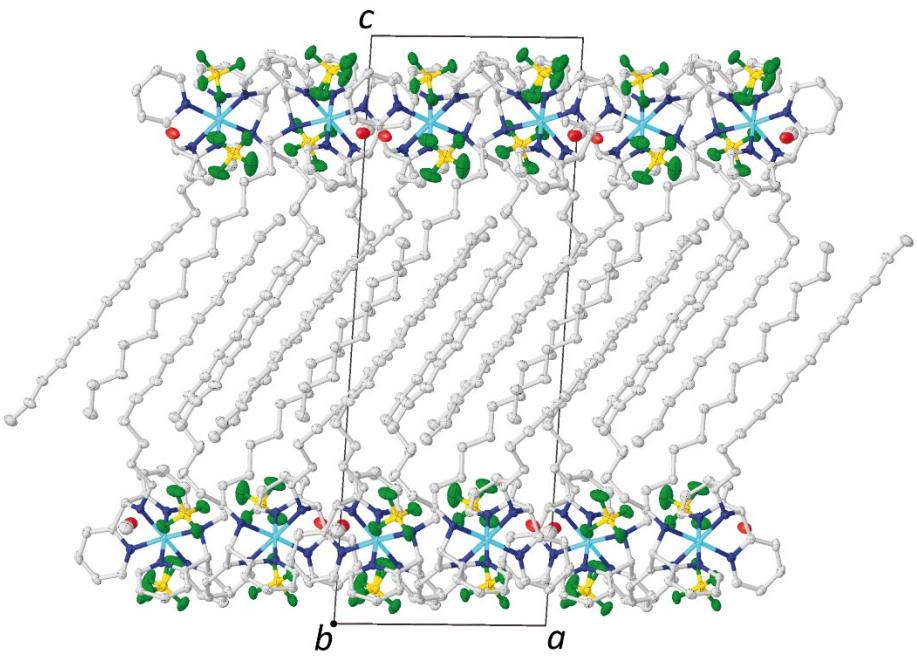


Figure S13 Unit cell of **1C$_{14}$** at 100 K as viewed along the *b* axis.

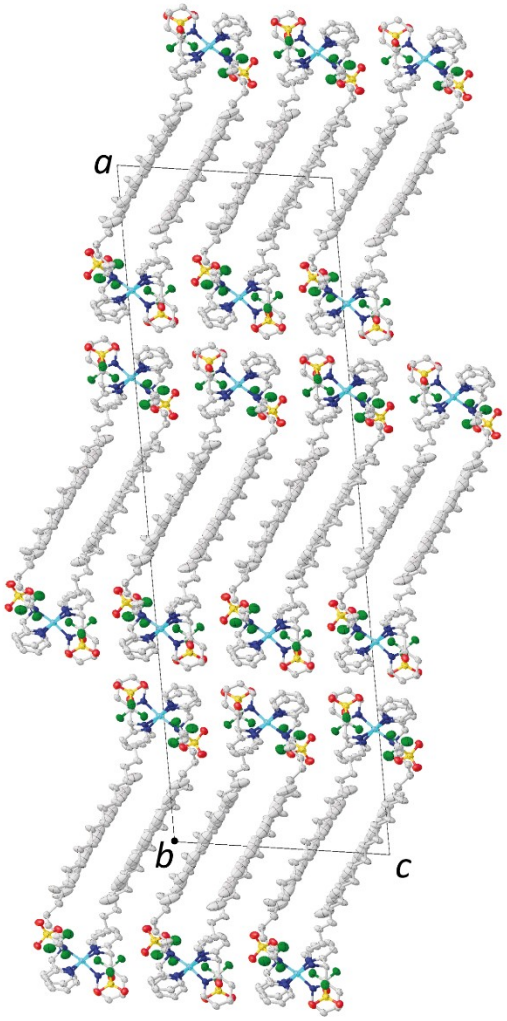


Figure S14 Unit cell of **1C$_{16}$** at 100 K as viewed along the *b* axis.

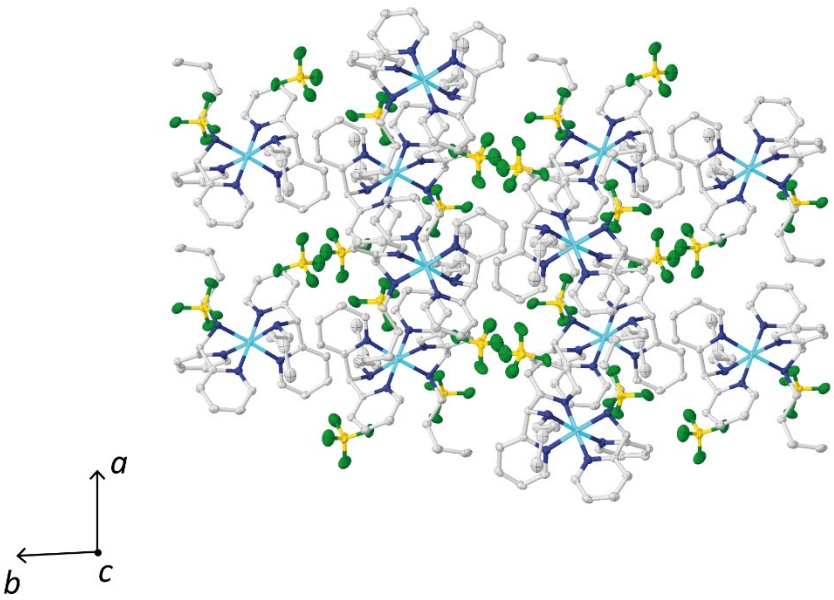


Figure S15 Packing of **1C$_4$** at 100 K as viewed down the *c* axis.

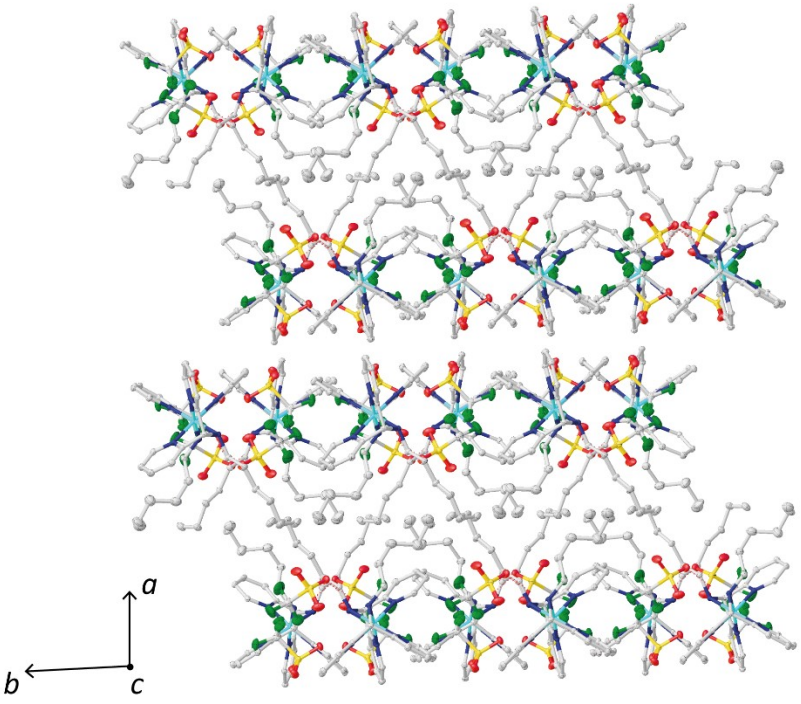


Figure S16 Packing of **1C$_6$** at 100 K as viewed down the *c* axis.

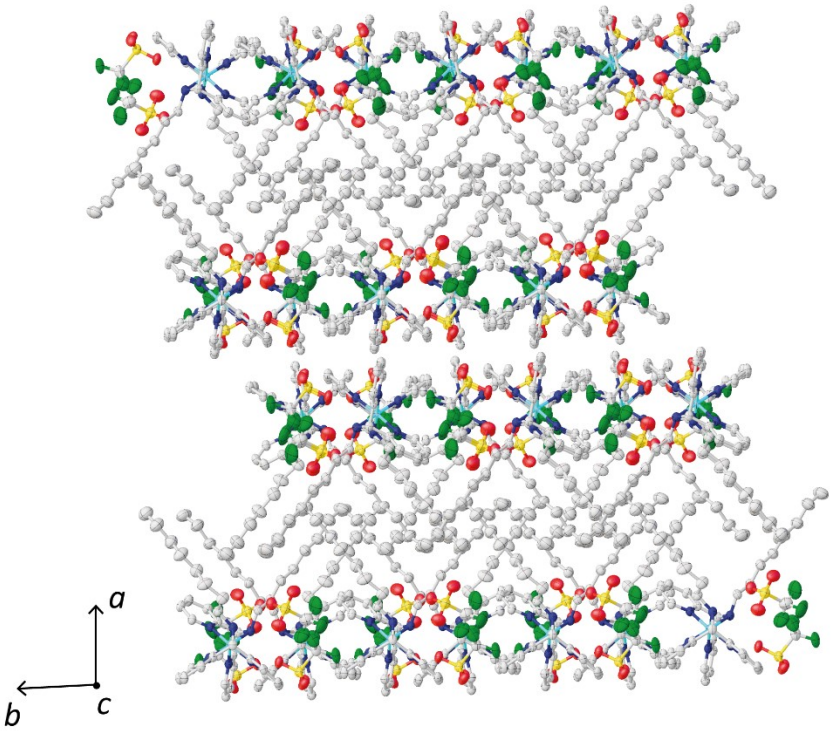


Figure S17 Packing of **1C$_8$** at 100 K as viewed down the *c* axis.

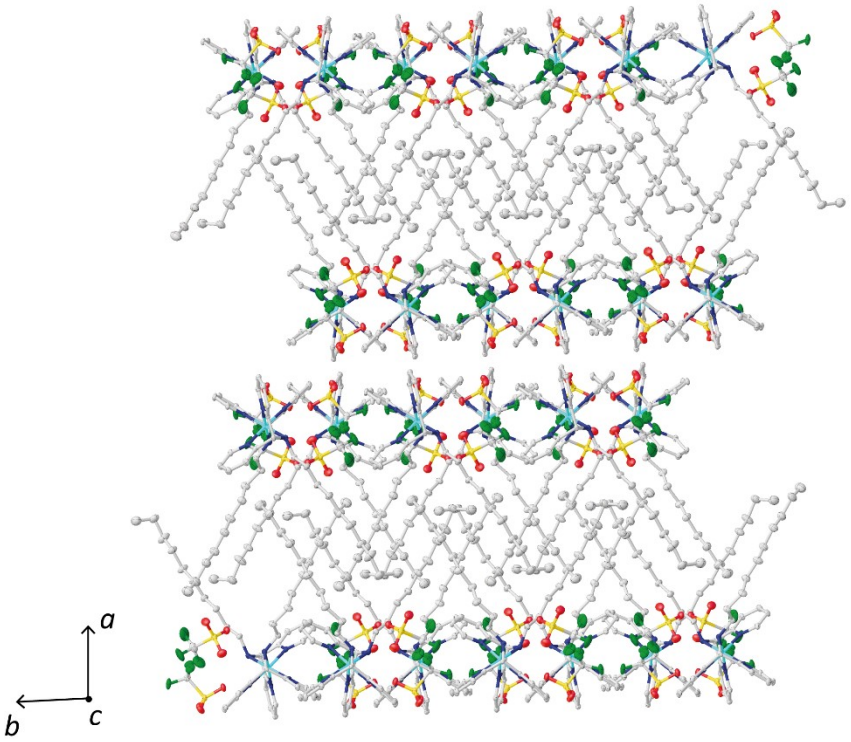


Figure S18 Packing of **1C$_{10}$** at 100 K as viewed down the *c* axis.

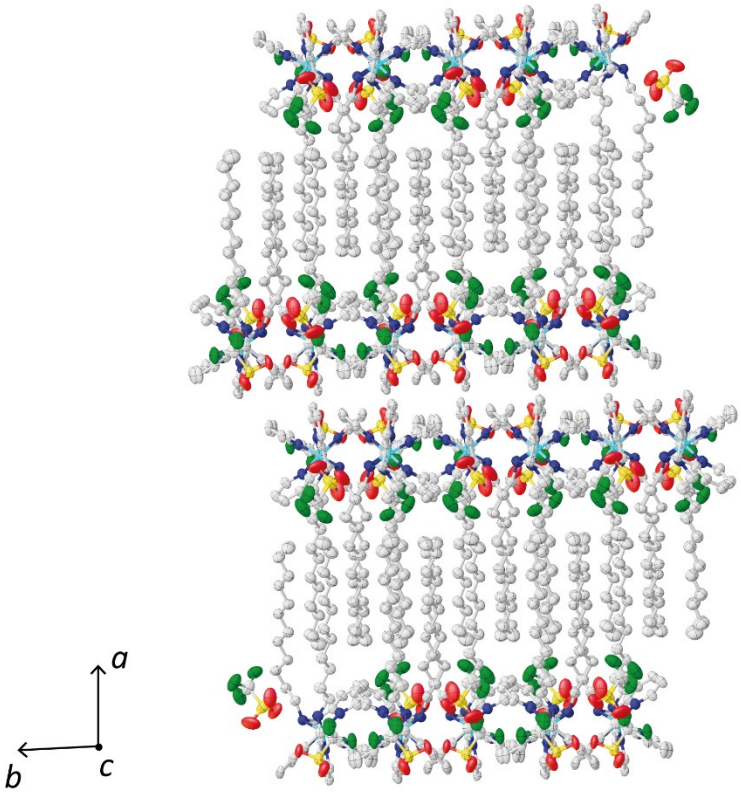


Figure S19 Packing of **1C$_{12}$** at 100 K as viewed down the *c* axis.

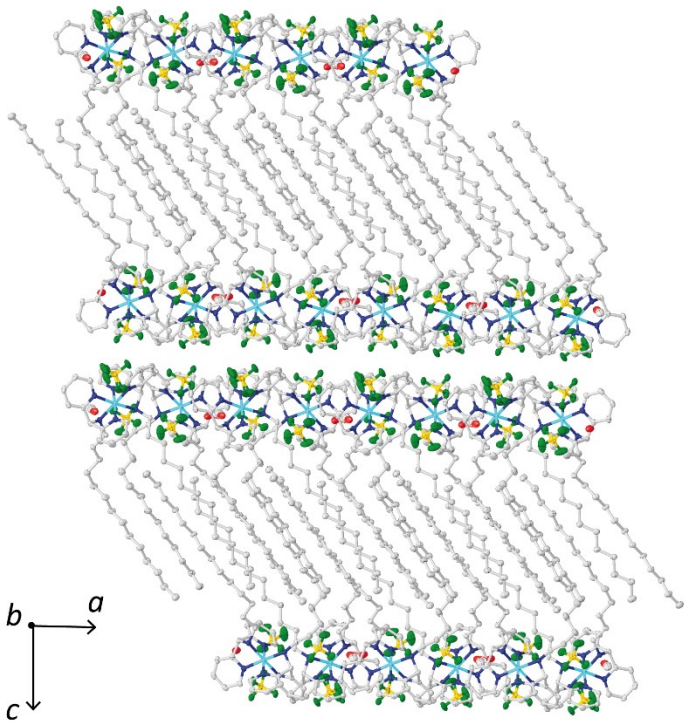


Figure S20 Packing of **1C$_{14}$** at 100 K as viewed down the *b* axis.

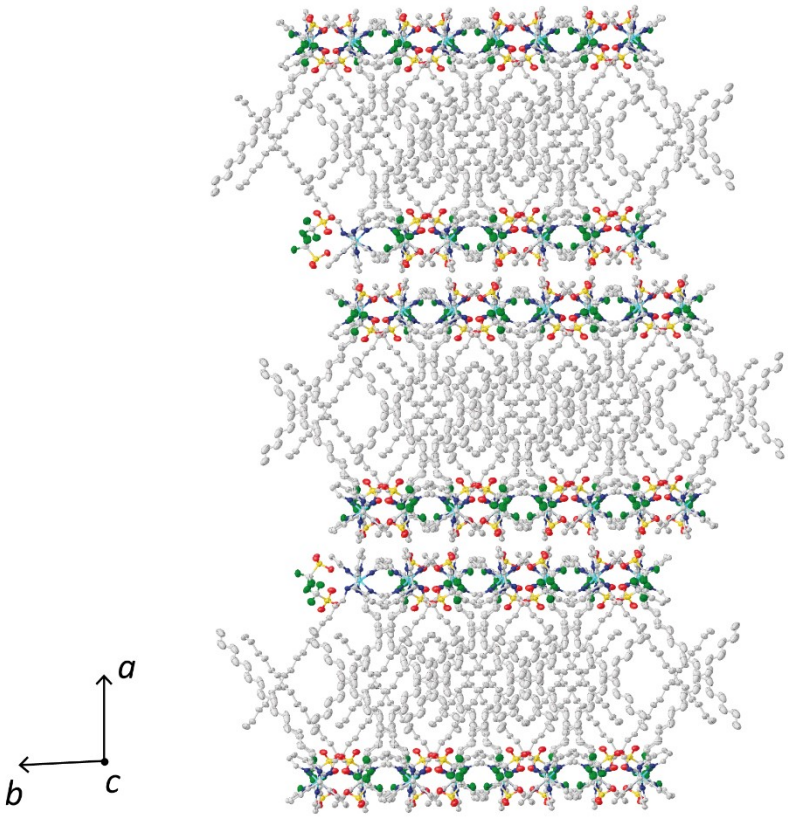


Figure S21 Packing of **1C$_{16}$** at 100 K as viewed down the *c* axis.

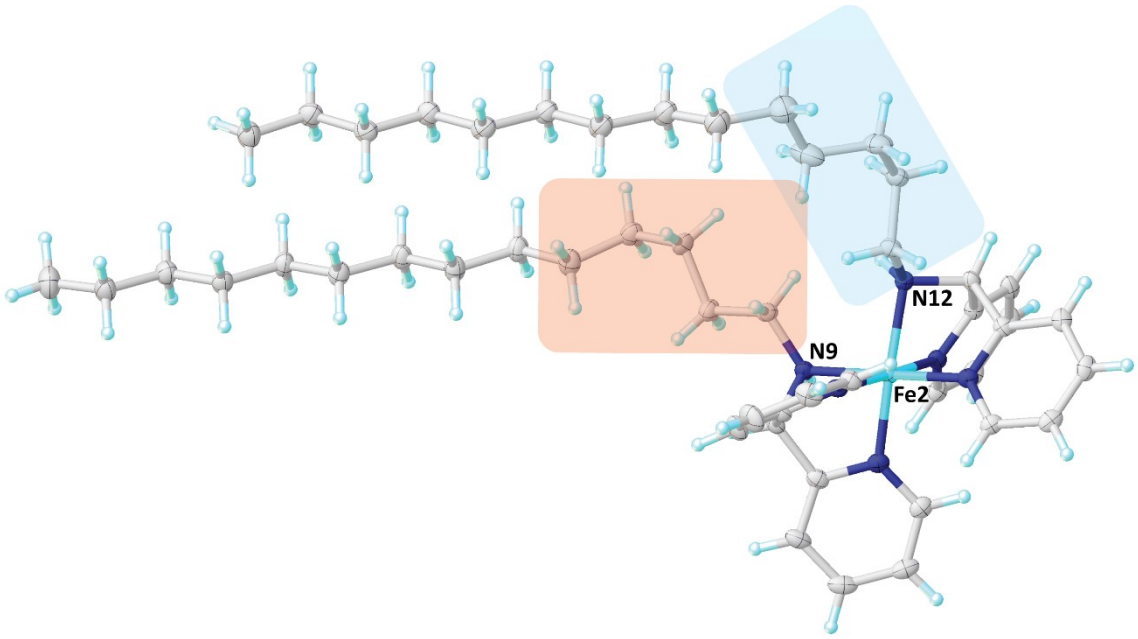


Figure S22 One of the dications of **1C$_{14}$** at 100 K with boxes highlighting the non-uniform *anti*/*gauche* arrangements of the alkyl chain tails in order to extend the chains in a parallel direction.

Variable temperature magnetic susceptibility studies

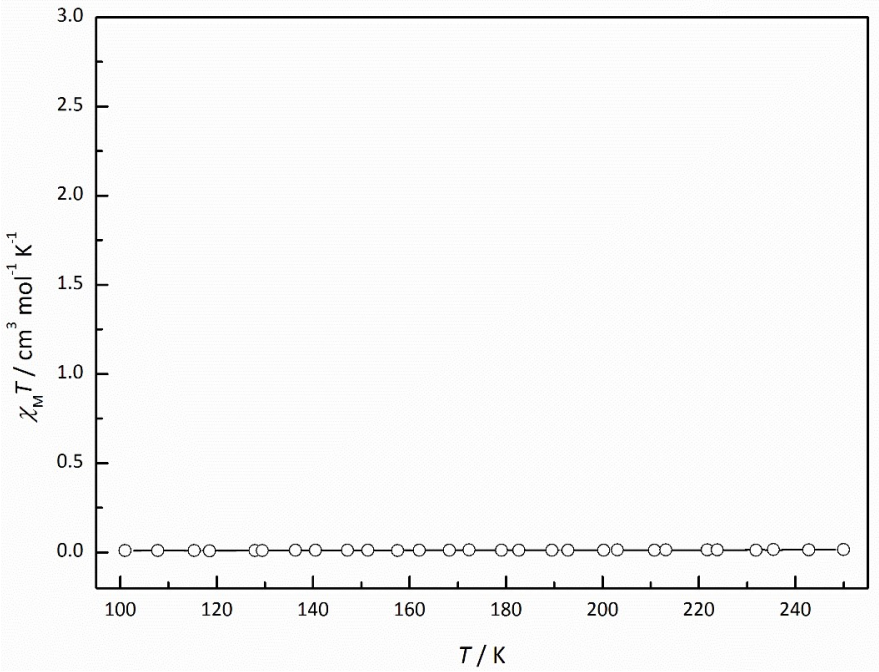


Figure S23 $\chi_M T$ vs. T data for **1C$_4$**.

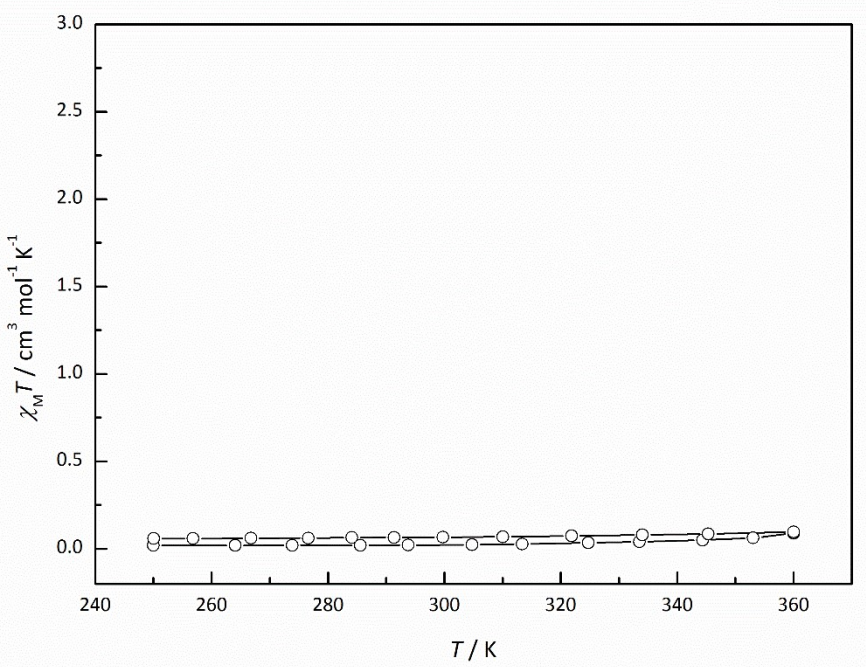


Figure S24 $\chi_M T$ vs. T data for **1C$_6$**.

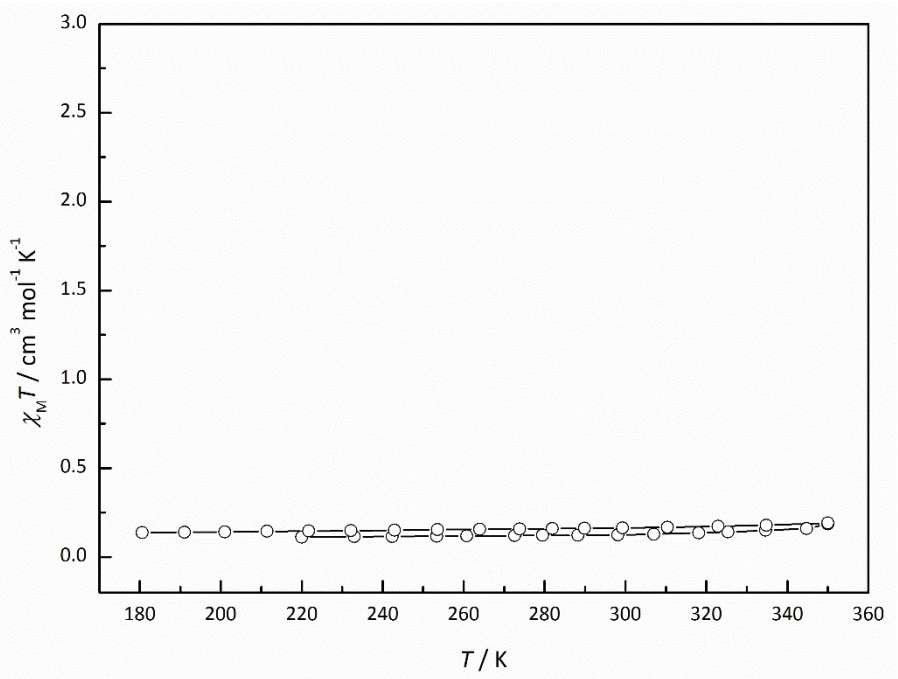


Figure S25 $\chi_M T$ vs. T data for **1C$_8$**.

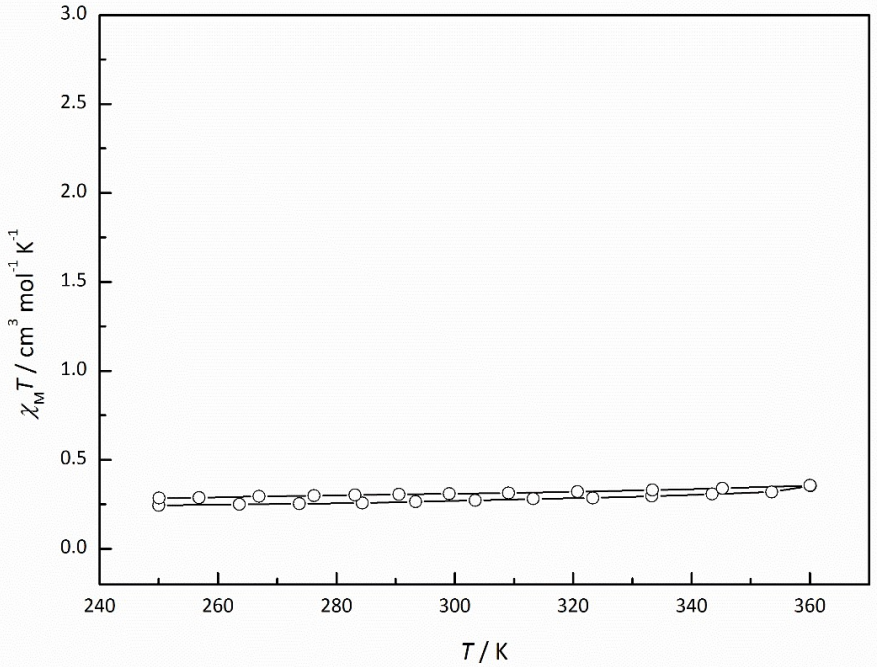


Figure S26 $\chi_M T$ vs. T data for **1C$_{10}$**.

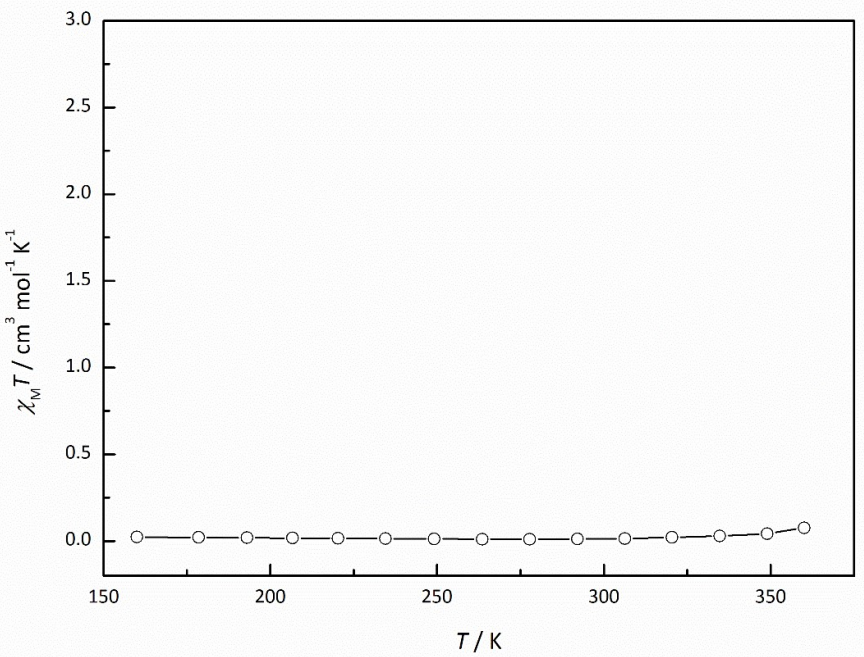


Figure S27 $\chi_M T$ vs. T data for **1C$_{12}$**.

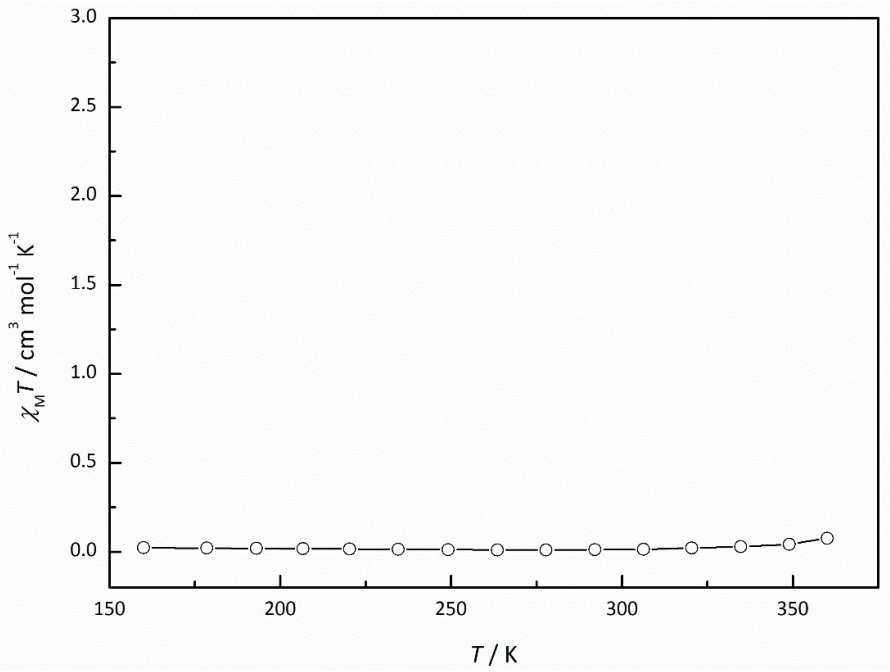


Figure S28 $\chi_M T$ vs. T data for **1C$_{14}$**.

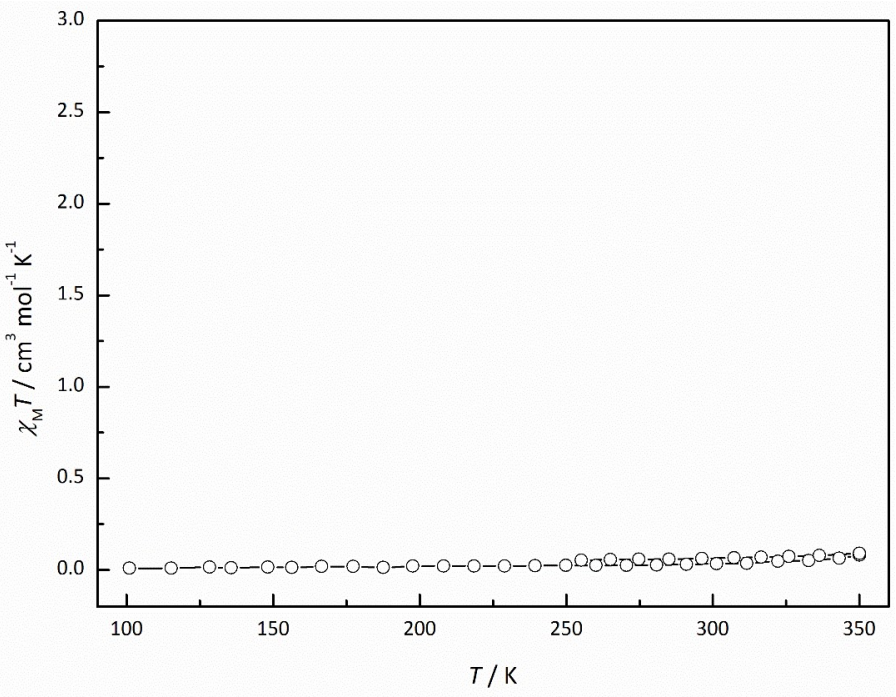


Figure S29 $\chi_M T$ vs. T data for **1C$_{16}$**.

Differential scanning calorimetry

Table S3 Thermodynamic parameters from DSC measurements. Apart from for **1C$_{14}$**, all transitions occur in all three thermal cycles.

	T (K)	$\|\Delta H\|$ (kJ mol^{-1})[a]	$\|\Delta S\|$ (J mol^{-1} K^{-1})[b]	Mode	Cycle and Temperature Range
1C$_6$	389	10.58	27.22	Heating	Cycle 3 193 – 473 K
	376	8.86	23.58	Cooling	Cycle 3 193 – 473 K
1C$_8$	263	6.66	25.24	Cooling	Cycle 3 193 – 473 K
	268	5.49	20.47	Heating	Cycle 3 193 – 473 K
	433	2.15	4.96	Heating	Cycle 3 193 – 473 K
	415	2.36	5.69	Cooling	Cycle 3 193 – 473 K
1C$_{10}$	328	9.23	28.17	Heating	Cycle 3 193 – 473 K
	403	4.16	10.32	Heating	Cycle 3 193 – 473 K
	401	3.77	9.40	Cooling	Cycle 3 193 – 473 K
	303	7.70	25.43	Cooling	Cycle 3 193 – 473 K
1C$_{12}$	414	14.86	35.92	Heating	Cycle 3 193 – 473 K
	412	14.83	36.02	Cooling	Cycle 3 193 – 473 K
1C$_{16}$	407	29.23	71.82	Heating	Cycle 3 193 – 473 K
	410	28.80	70.17	Cooling	Cycle 3 193 – 473 K
	204	1.06	5.19	Cooling	Cycle 3 193 – 473 K
	210	1.20	5.70	Heating	Cycle 3 193 – 473 K

[a] Obtained from $\frac{dH}{dt} = C_p\frac{dT}{dt} + f(T,t)$, where $\frac{dH}{dt}$ is the total heat flow from linear heating rates, $C_p\frac{dT}{dt}$ is the reversing heat flow component of the total hear flow and $f(T,t)$ is the kinetic component of the total heat flow. [b] Obtained from $\Delta H/T$.

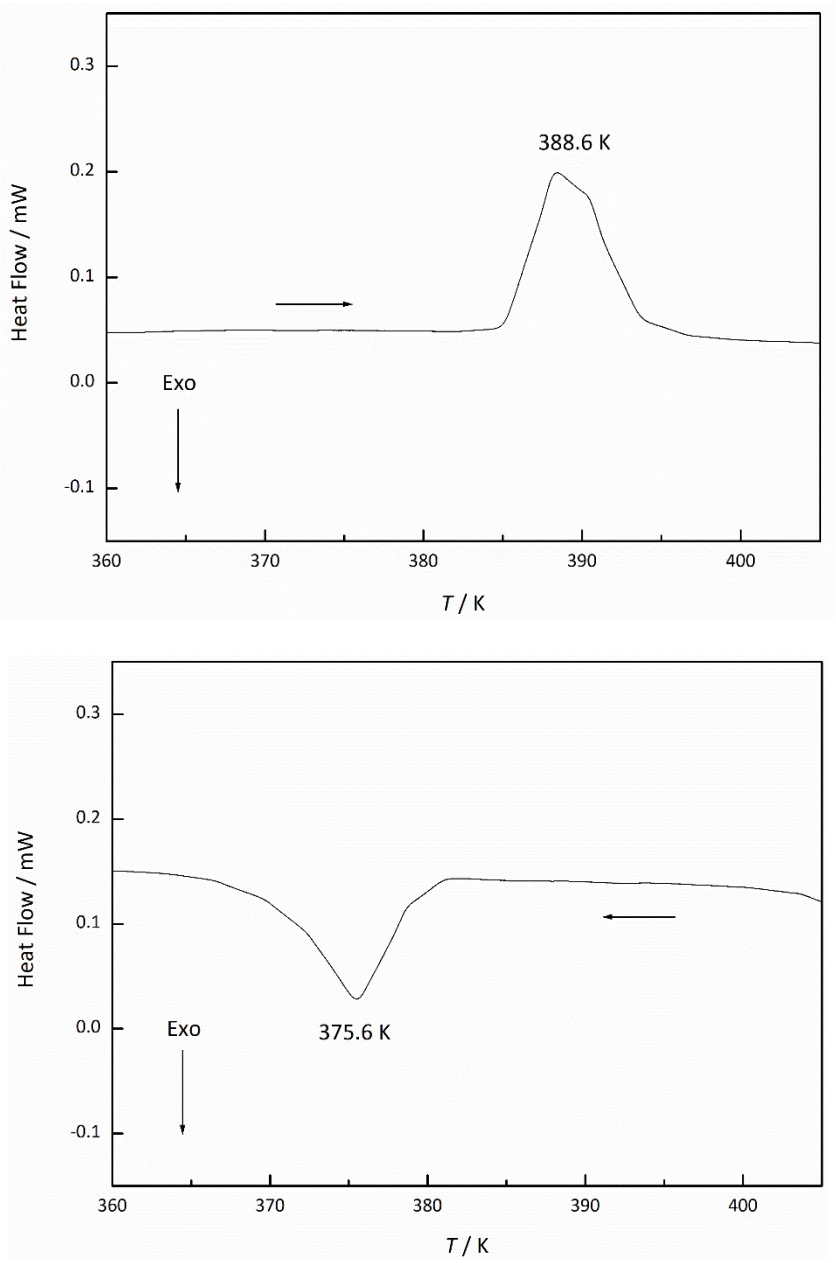


Figure S30 Modulated DSC thermograms of **1C$_6$** in heating (top) and cooling modes (bottom).

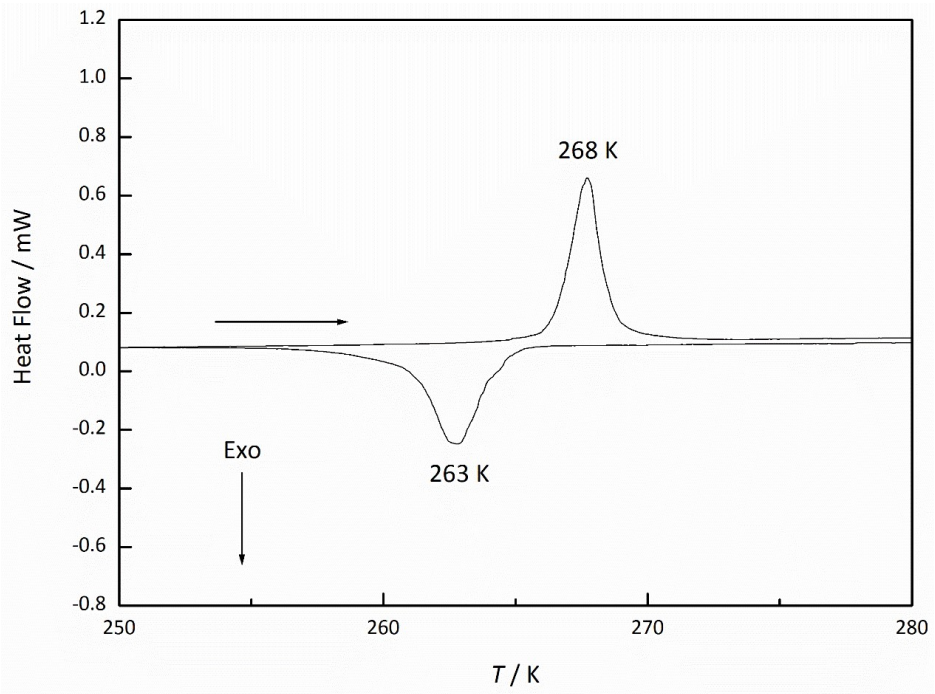


Figure S31 DSC thermogram of **1C$_8$** from cycle 3.

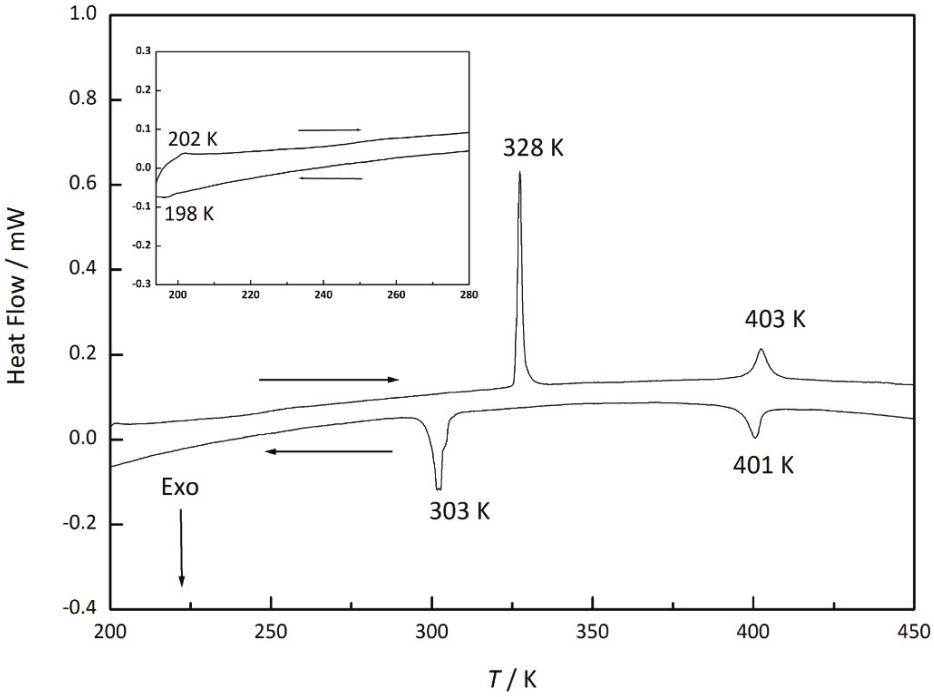


Figure S32 DSC thermogram of **1C$_{10}$** during cycle 3. Inset graph shows small hysteretic peaks at low temperature from the same cycle.

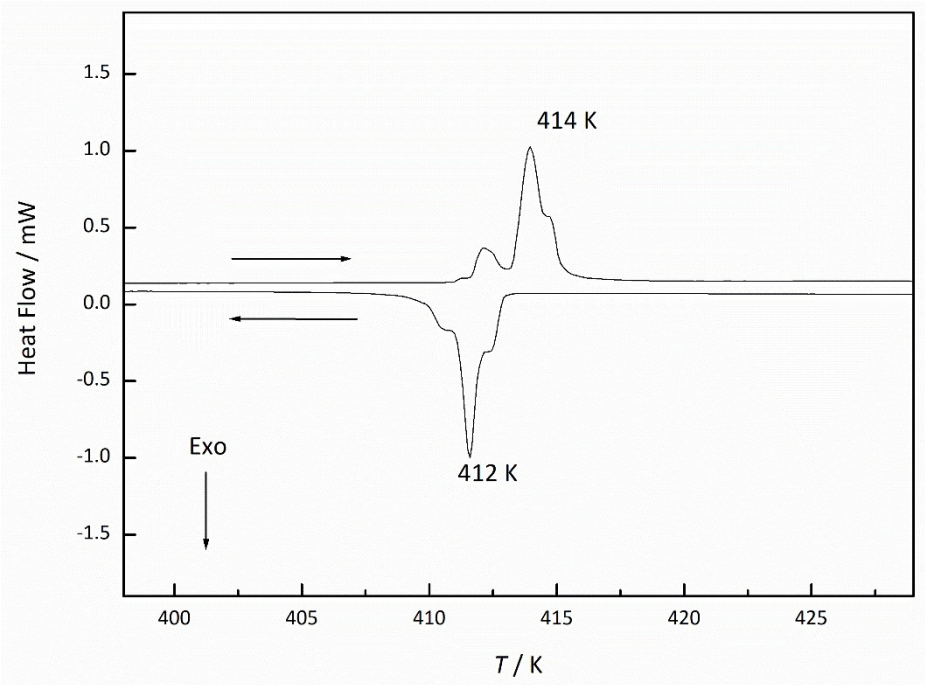


Figure S33 Cyclic DSC thermogram of **1C$_{12}$** from cycle 2.

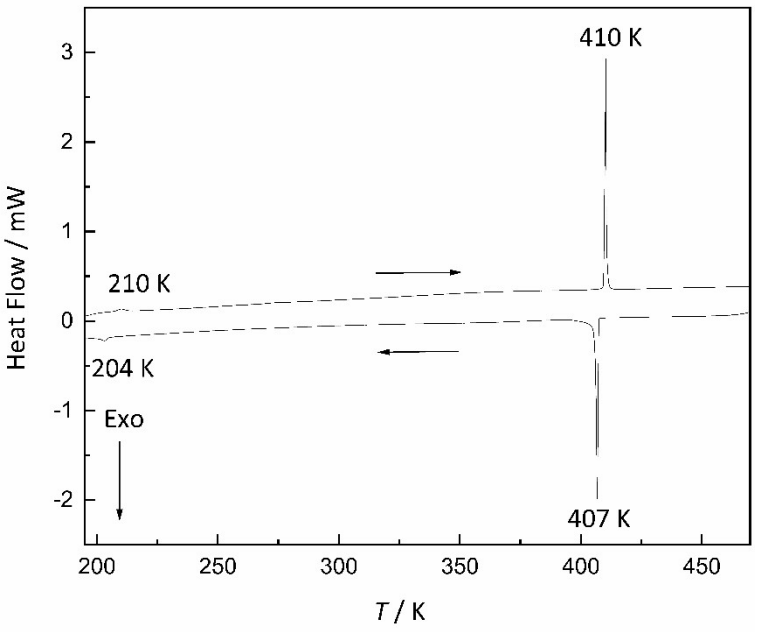


Figure S34 Cyclic DSC thermogram of **1C$_{16}$** from cycle 2.

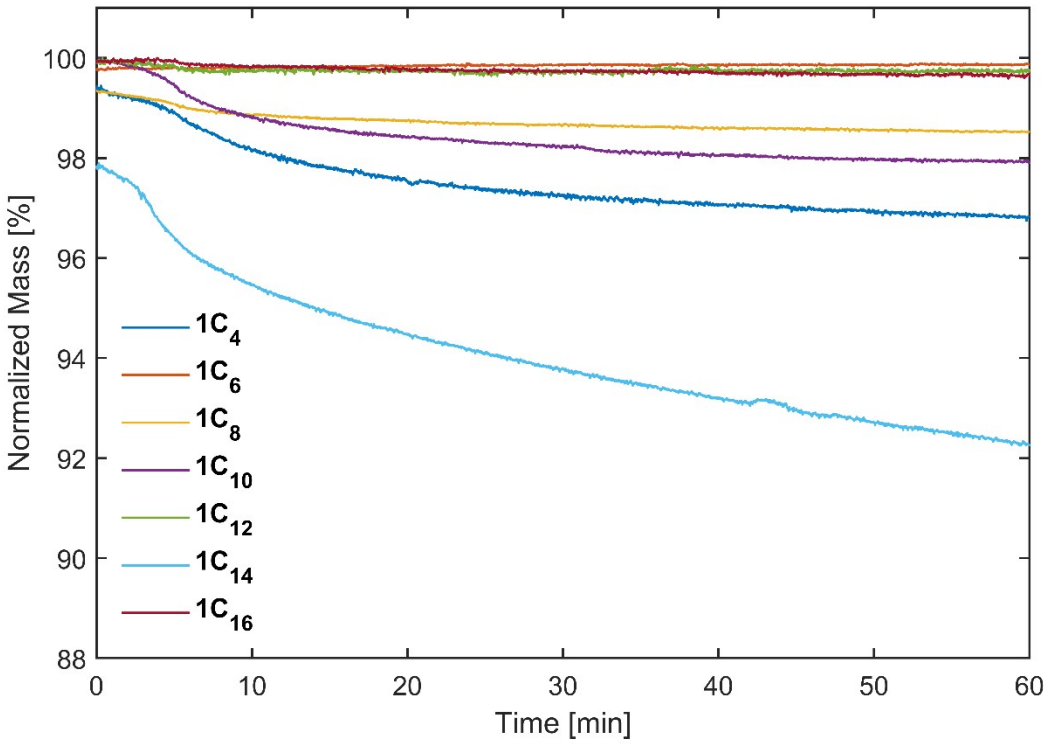


Figure S35 Isothermal TGA graphs for **$1C_4$**-**$1C_{16}$** at 423 K.

Table S4 Summary table of relative mass loss after 60 min at 423 K for **$1C_4$**-**$1C_{16}$**.

Compound	Relative mass loss after 60 min at 423 K [%]
$1C_4$	3.2
$1C_6$	0.1
$1C_8$	1.5
$1C_{10}$	2.1
$1C_{12}$	0.3
$1C_{14}$	7.7
$1C_{16}$	0.3

^{1}H NMR of $1C_4$-$1C_{16}$ in DMSO-d6

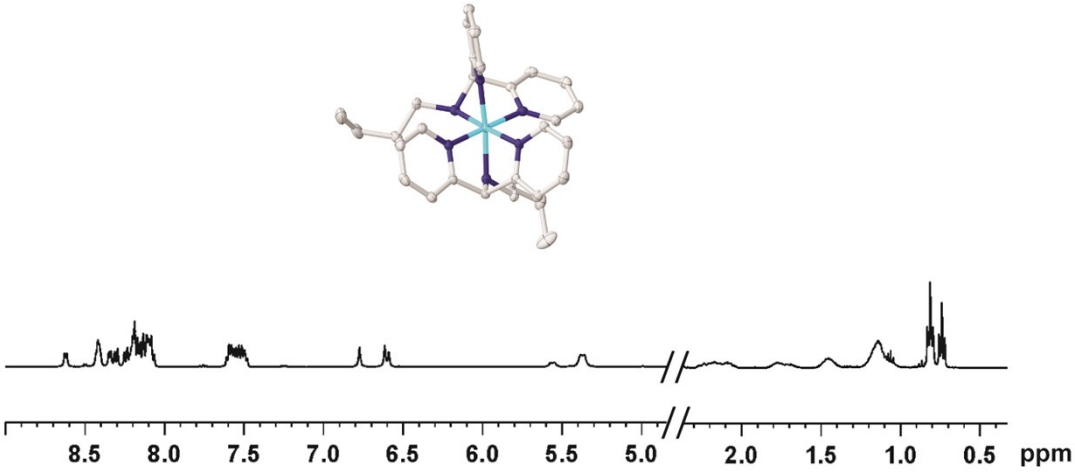


Figure S36 ^{1}H NMR spectrum of **$1C_4$** (9.4 mg cm^{-3}) at 303 K in DMSO-d6 with TMS internal reference.

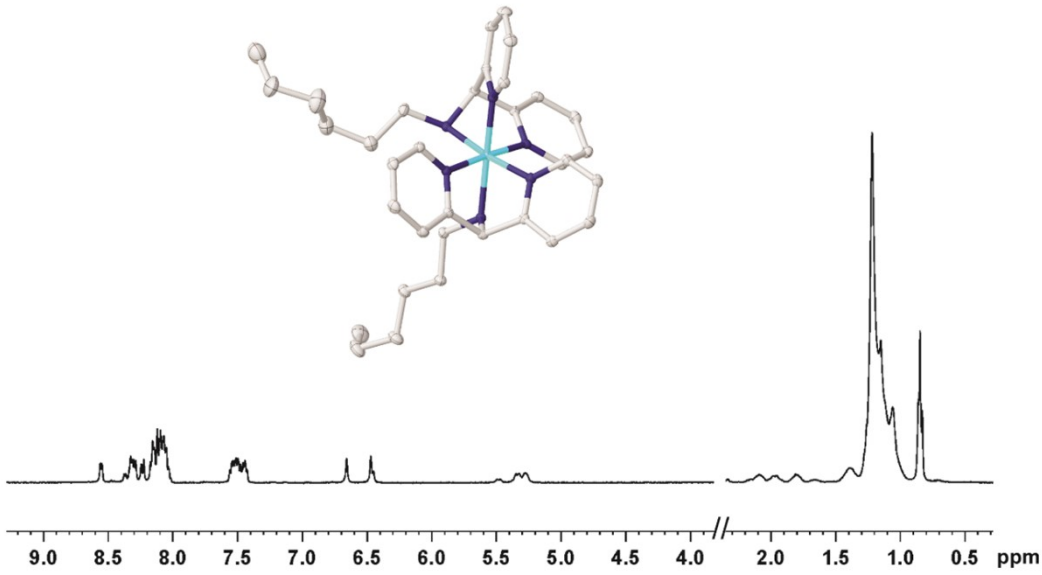


Figure S37 ^{1}H NMR spectrum of **$1C_6$** (10.2 mg cm^{-3}) at 303 K in DMSO-d6 with TMS internal reference.

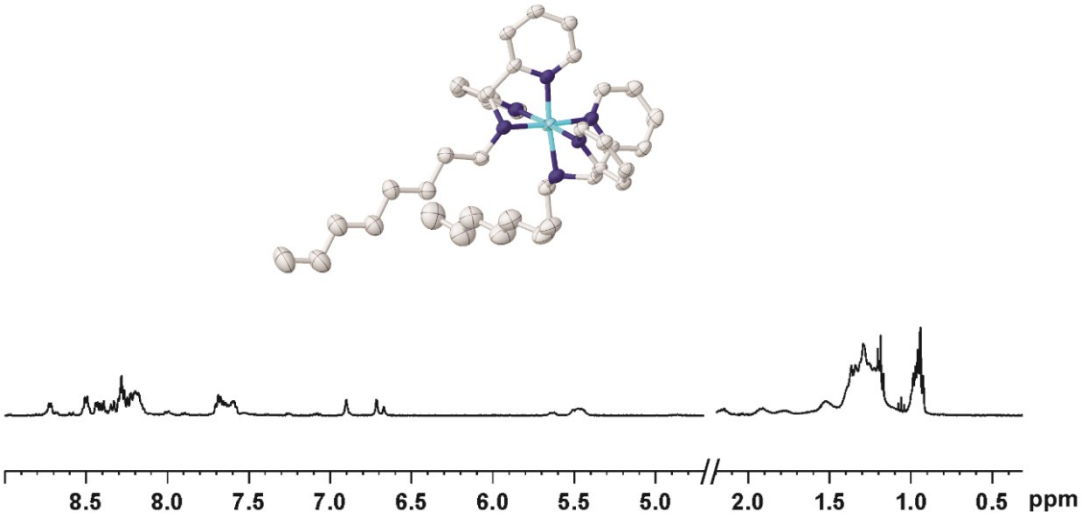


Figure S38 ^{1}H NMR spectrum of **1C$_8$** (10.2 mg cm^{-3}) at 303 K in DMSO-d6 with TMS internal reference.

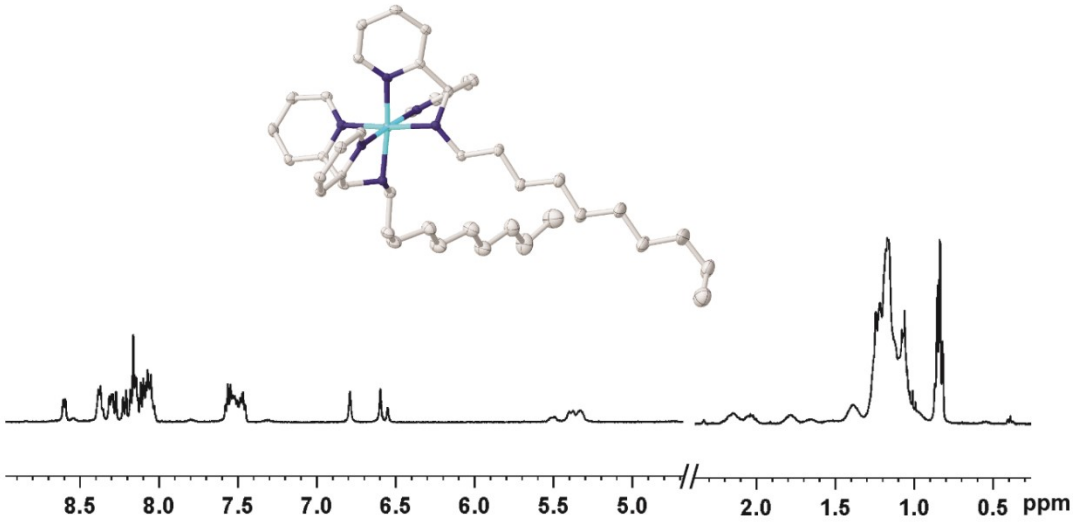


Figure S39 ^{1}H NMR spectrum of **1C$_{10}$** (10.6 mg cm^{-3}) at 303 K in DMSO-d6 with TMS internal reference.

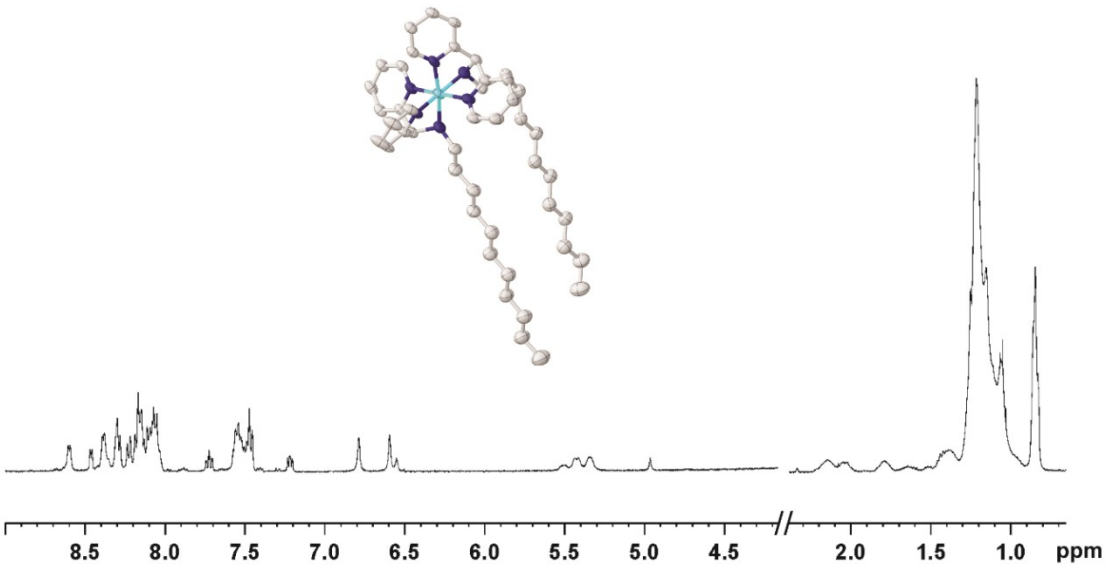


Figure S40 ^{1}H NMR spectrum of **1C$_{12}$** (11.2 mg cm^{-3}) at 303 K in DMSO-d6 with TMS internal reference.

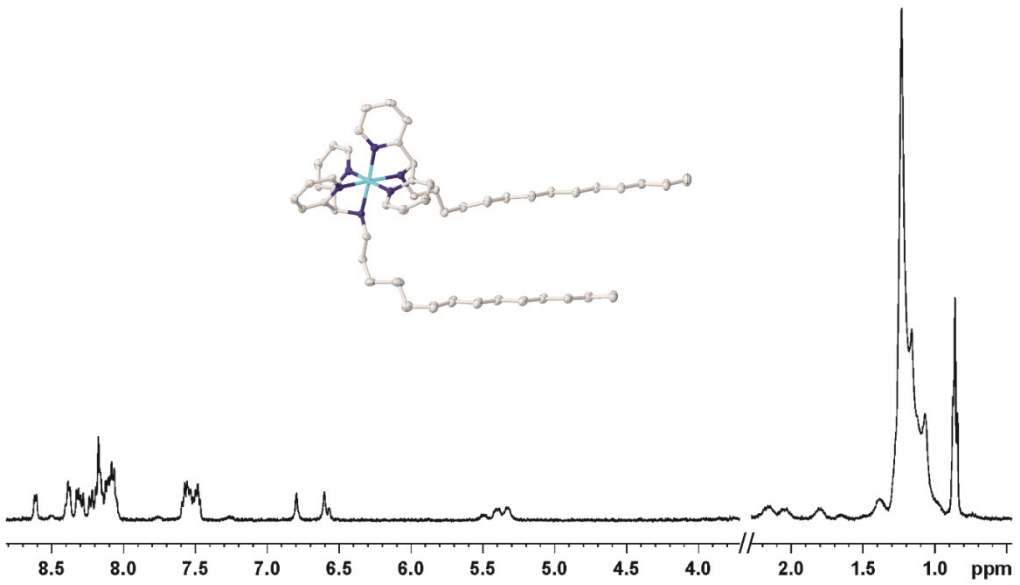


Figure S41 ^{1}H NMR spectrum of **1C$_{14}$** (10.2 mg cm^{-3}) at 303 K in DMSO-d6 with TMS internal reference.

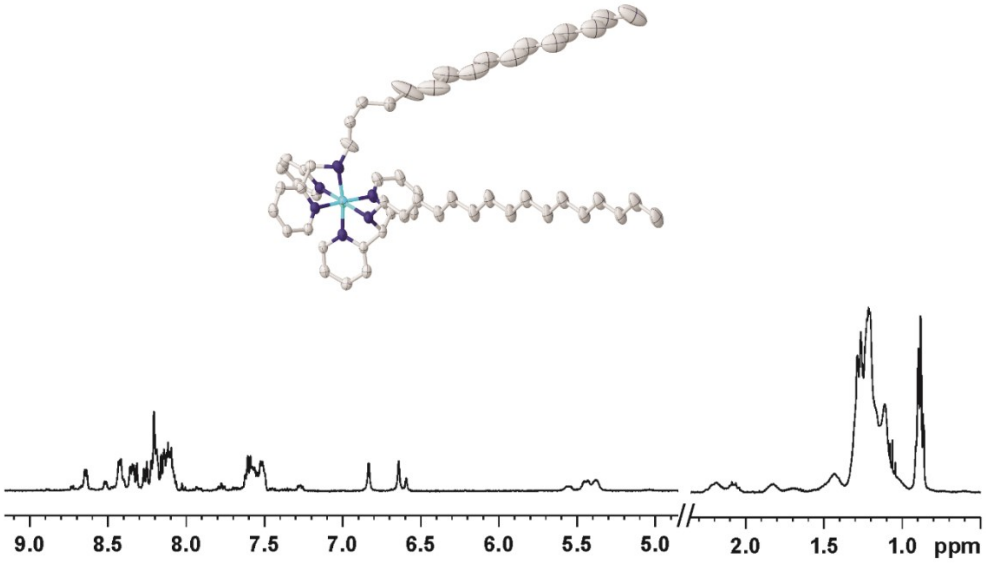


Figure S42 ^{1}H NMR spectrum of **1C$_{16}$** (10.6 mg cm^{-3}) at 303 K in DMSO-d6 with TMS internal reference.

^{1}H NMR of $1C_4$-$1C_{16}$ in acetonitrile-d3

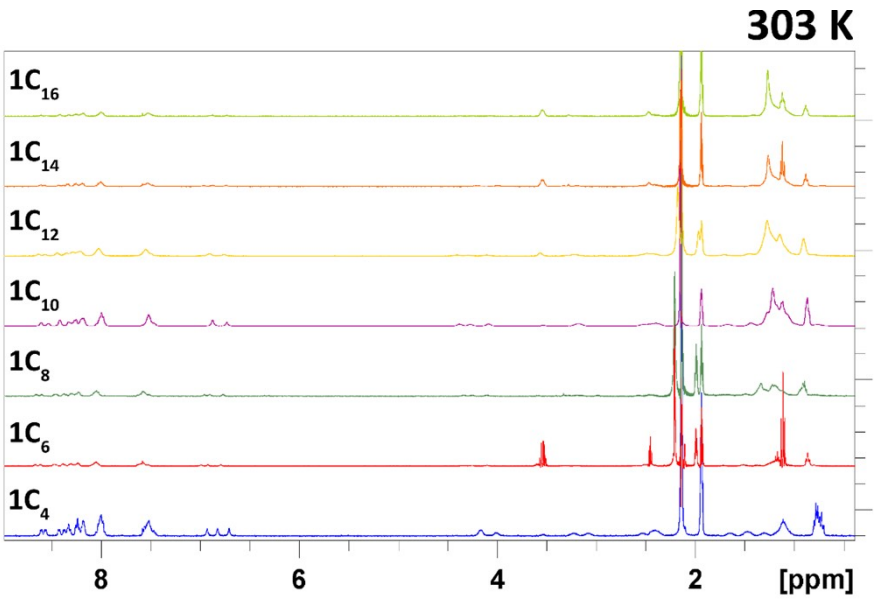


Figure S43 ^{1}H NMR spectrum of **$1C_4$-$1C_{16}$** at 303 K in acetonitrile-d3 with TMS internal reference. Concentrations of **$1C_4$-$1C_{16}$** (in order) were 10.1, 9.4, 10.1, 18.4, 14.2, 12.2 and 9.8 mg cm^{-3}.

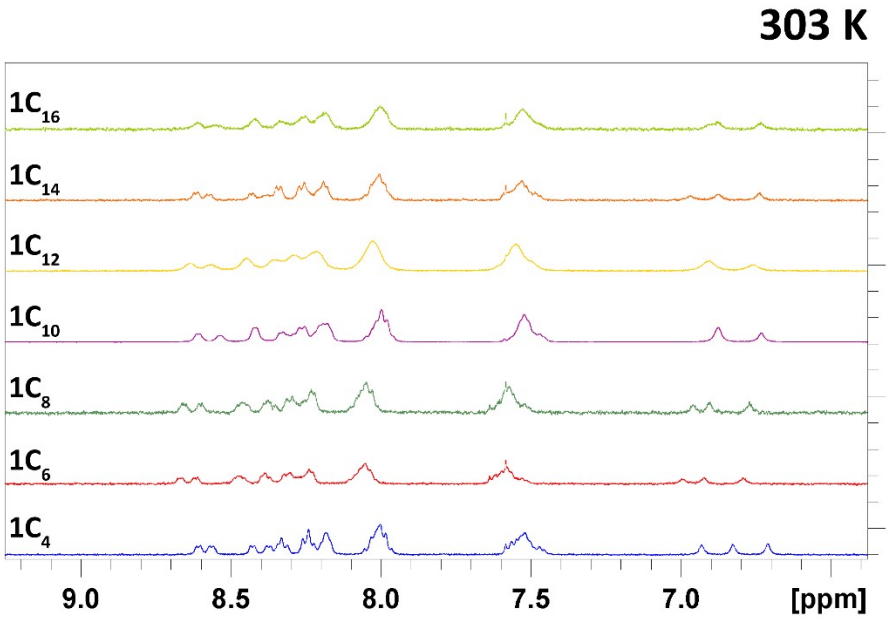


Figure S44 Partial (aromatic region) ^{1}H NMR spectrum of **$1C_4$-$1C_{16}$** at 303 K in acetonitrile-d3 with TMS internal reference. Concentrations of **$1C_4$-$1C_{16}$** (in order) were 10.1, 9.4, 10.1, 18.4, 14.2, 12.2 and 9.8 mg cm^{-3}.

^{1}H NMR of $1C_4$-$1C_{16}$ acetone-d6

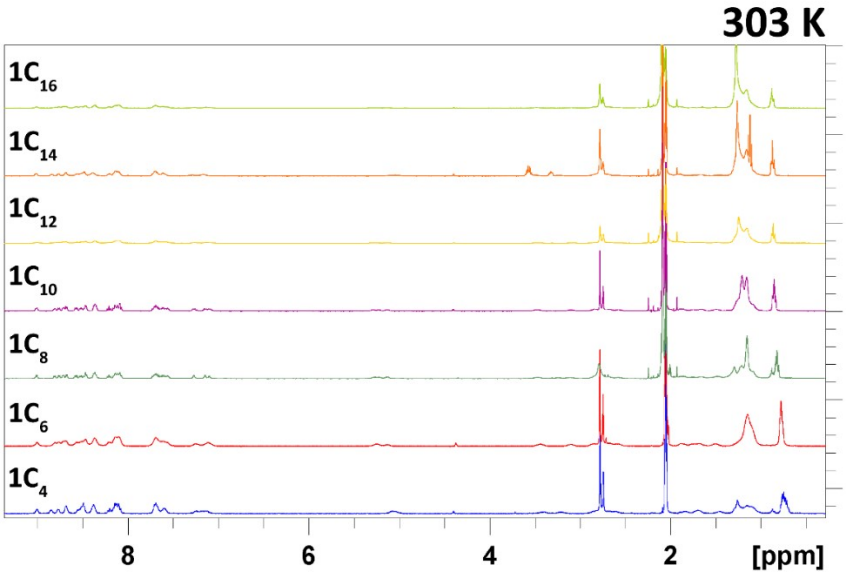


Figure S45 ^{1}H NMR spectrum of **$1C_4$-$1C_{16}$** at 303 K in acetone-d6 with TMS internal reference. Concentrations of **$1C_4$-$1C_{16}$** (in order) were 6.4, 9.4, 14.4, 10.6, 10.4, 8.8 and 11.2 mg cm^{-3}.

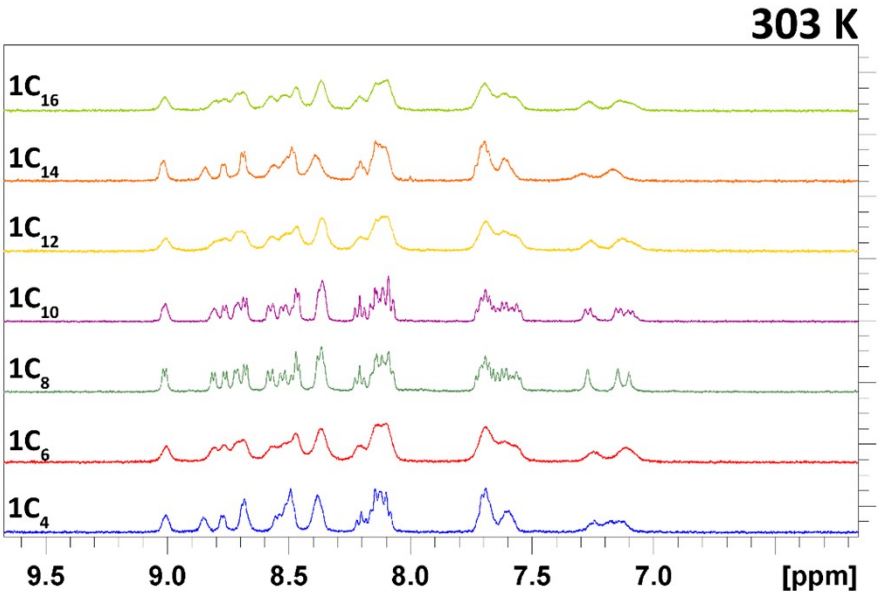


Figure S46 Partial (aromatic region) ^{1}H NMR spectrum of **$1C_4$-$1C_{16}$** at 303 K in acetone-d6 with TMS internal reference. Concentrations of **$1C_4$-$1C_{16}$** (in order) were 6.4, 9.4, 14.4, 10.6, 10.4, 8.8 and 11.2 mg cm^{-3}.

^{1}H NMR of $1C_4$-$1C_{16}$ in DMSO-d6 (Evans Method)

$$\chi_M = \frac{\chi_0 \, m_r^{para}}{m_r^{solvent}} + 3000\frac{\Delta v}{4\pi \, v_0 \, C} \quad (1)$$

Where χ_0 is the molar susceptibility of the solvent, m_r^{para} is the molecular mass of the metal species, $m_r^{solvent}$ is the molecular mass of the solvent, Δv is the relative shift of the TMS signals in Hertz, v_0 is the spectrometer frequency in Hertz and C is the concentration of metal species in solution in mol dm^{-3}

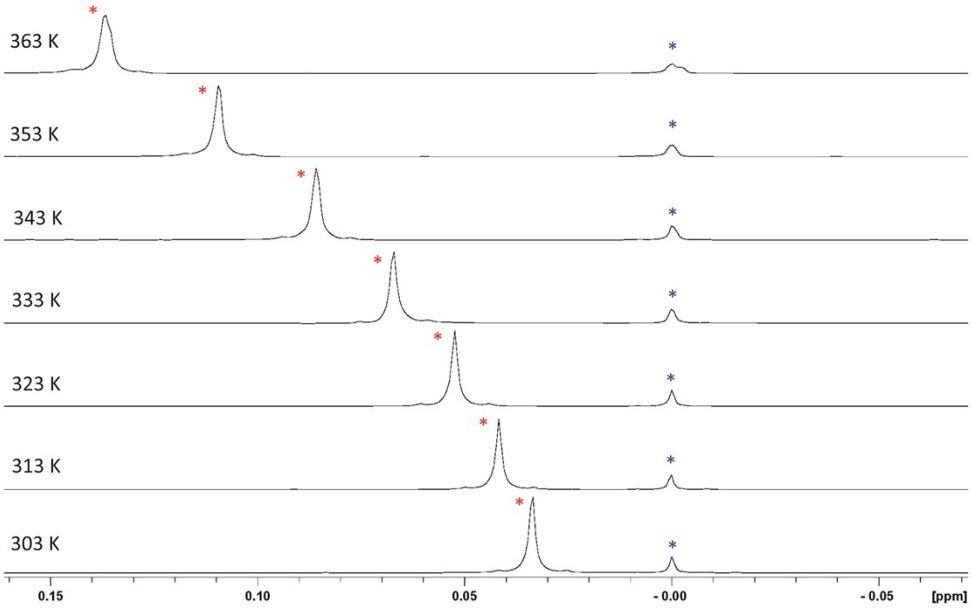


Figure S47 ^{1}H NMR overlay spectrum of **$1C_4$** (10.2 mg cm^{-3}) showing only the TMS peaks from sample solution (red asterisk) and control solution (blue asterisk) from the Evans method measured between 303-363 K in DMSO-d6 with TMS internal reference.

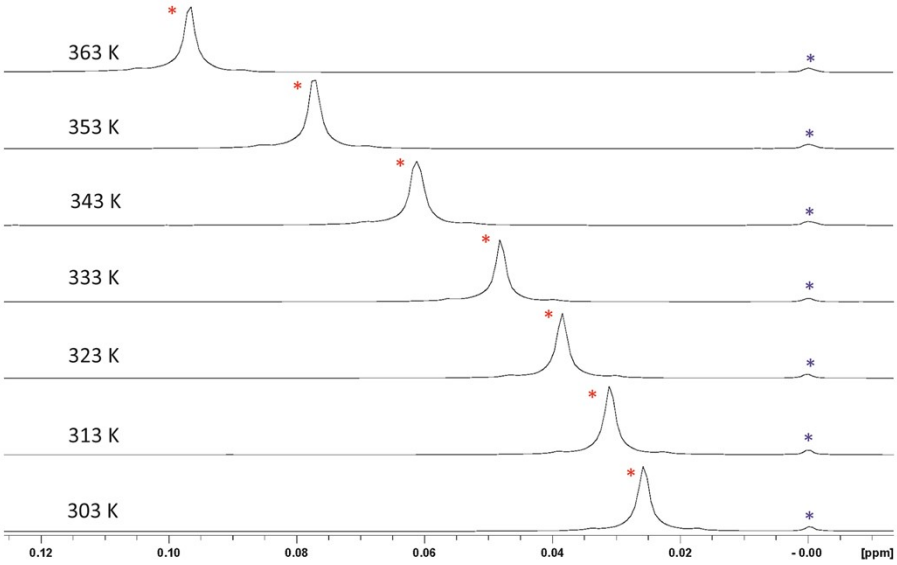


Figure S48 ^{1}H NMR overlay spectrum of **1C$_6$** (10.2 mg cm^{-3}) showing only the TMS peaks from sample solution (red asterisk) and control solution (blue asterisk) from the Evans method measured between 303-363 K in DMSO-d6 with TMS internal reference.

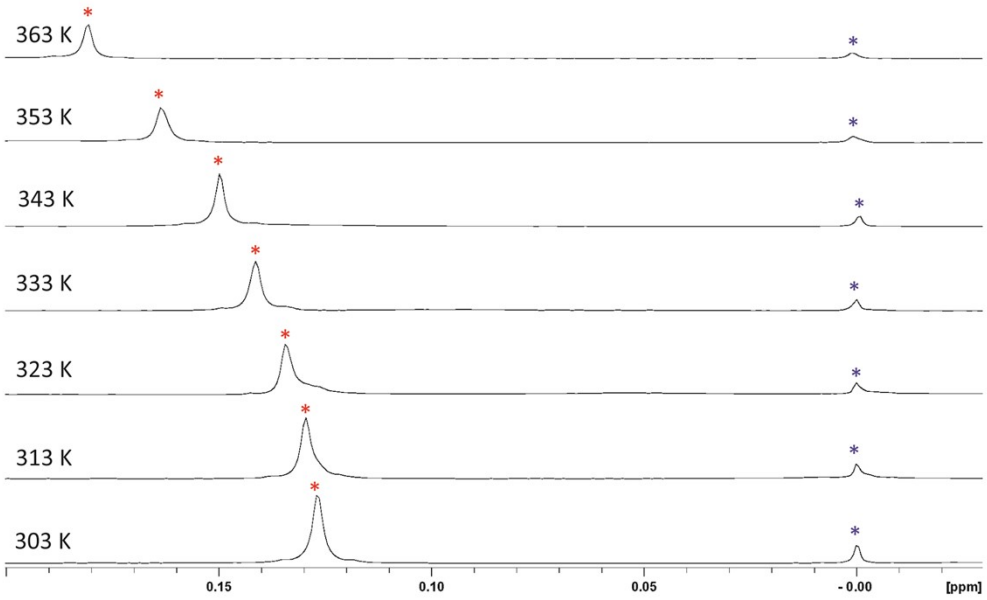


Figure S49 ^{1}H NMR overlay spectrum of **1C$_8$** (10.2 mg cm^{-3}) showing only the TMS peaks from sample solution (red asterisk) and control solution (blue asterisk) from the Evans method measured between 303-363 K in DMSO-d6 with TMS internal reference.

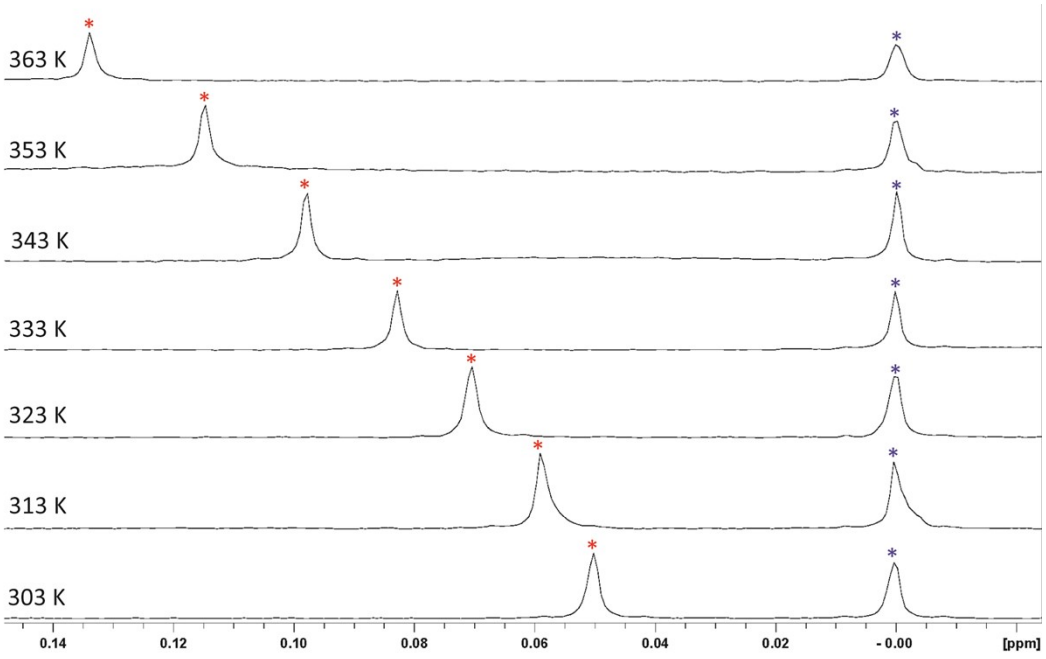


Figure S50 ^{1}H NMR overlay spectrum of **1C$_{10}$** (10.6 mg cm^{-3}) showing only the TMS peaks from sample solution (red asterisk) and control solution (blue asterisk) from the Evans method measured between 303-363 K in DMSO-d6 with TMS internal reference.

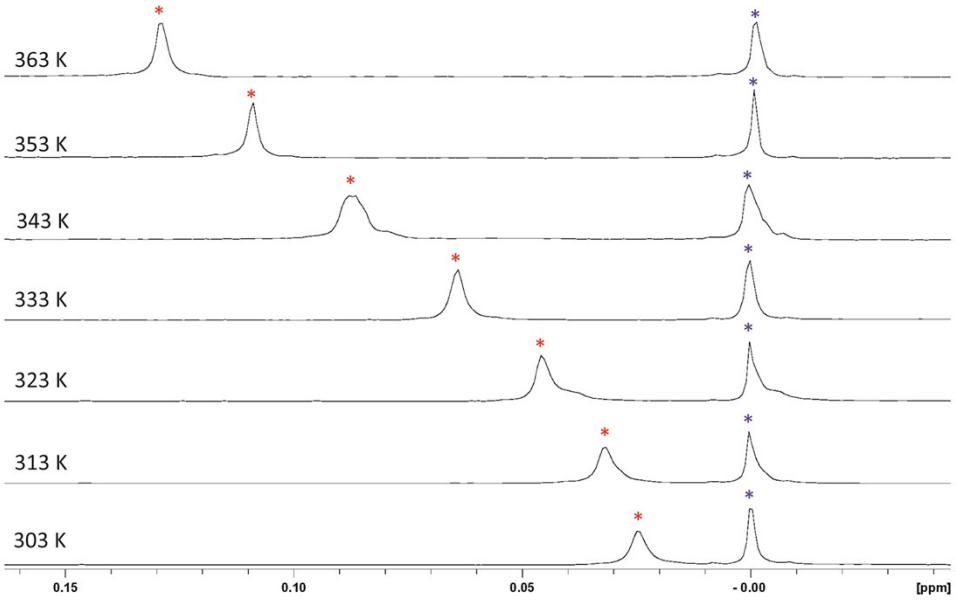


Figure S51 ^{1}H NMR overlay spectrum of **1C$_{12}$** (11.2 mg cm^{-3}) showing only the TMS peaks from sample solution (red asterisk) and control solution (blue asterisk) from the Evans method measured between 303-363 K in DMSO-d6 with TMS internal reference.

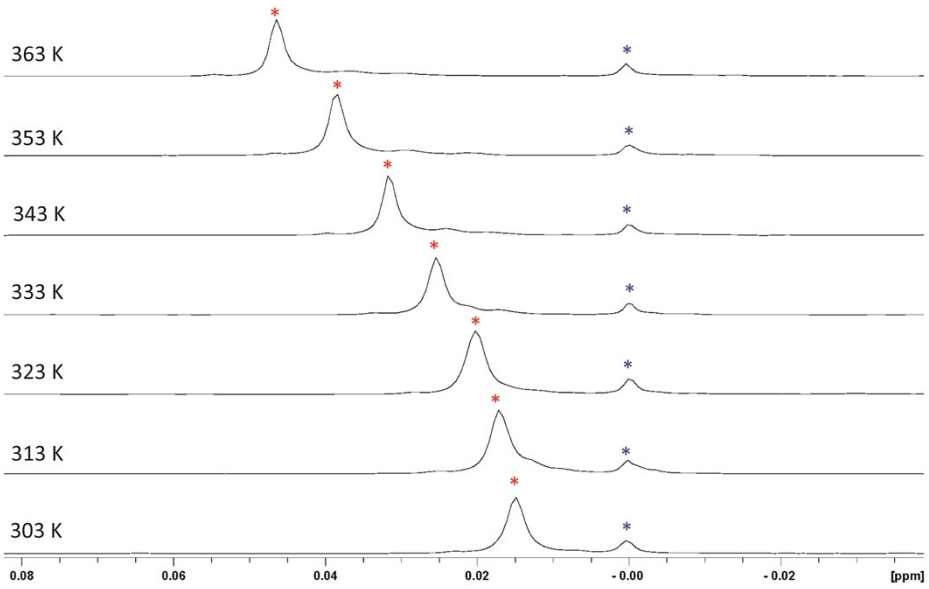


Figure S52 1H NMR overlay spectrum of **1C$_{14}$** (10.2 mg cm^{-3}) showing only the TMS peaks from sample solution (red asterisk) and control solution (blue asterisk) from the Evans method measured between 303-363 K in DMSO-d6 with TMS internal reference.

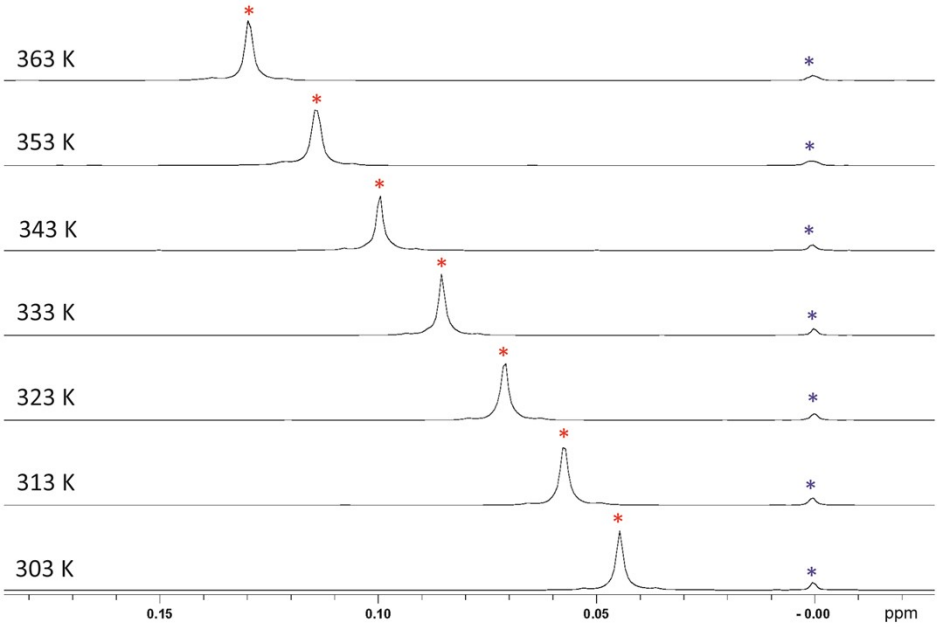


Figure S53 ^{1}H NMR overlay spectrum of **1C$_{16}$** (10.6 mg cm^{-3}) showing only the TMS peaks from sample solution (red asterisk) and control solution (blue asterisk) from the Evans method measured between 303-363 K in DMSO-d6 with TMS internal reference.

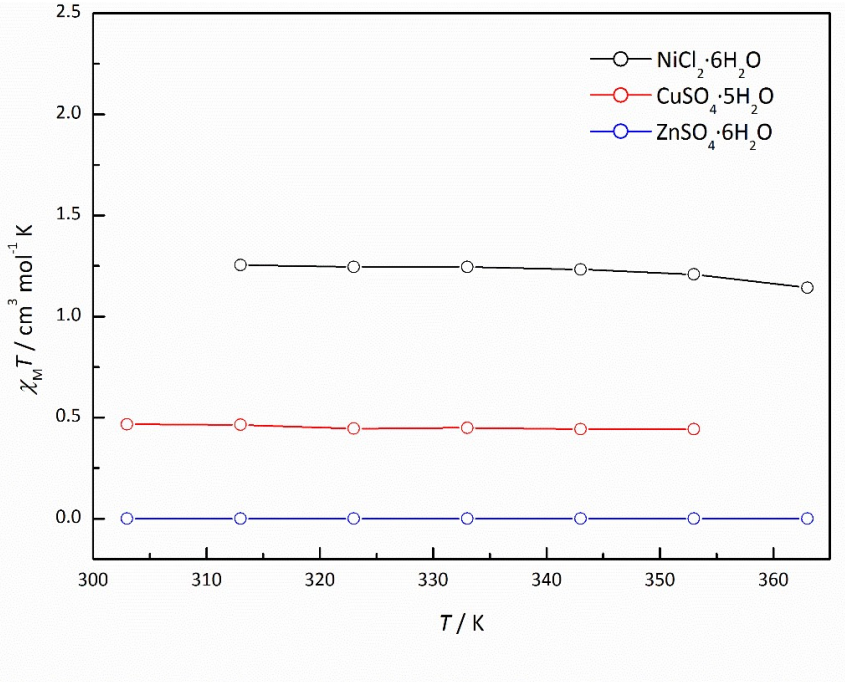
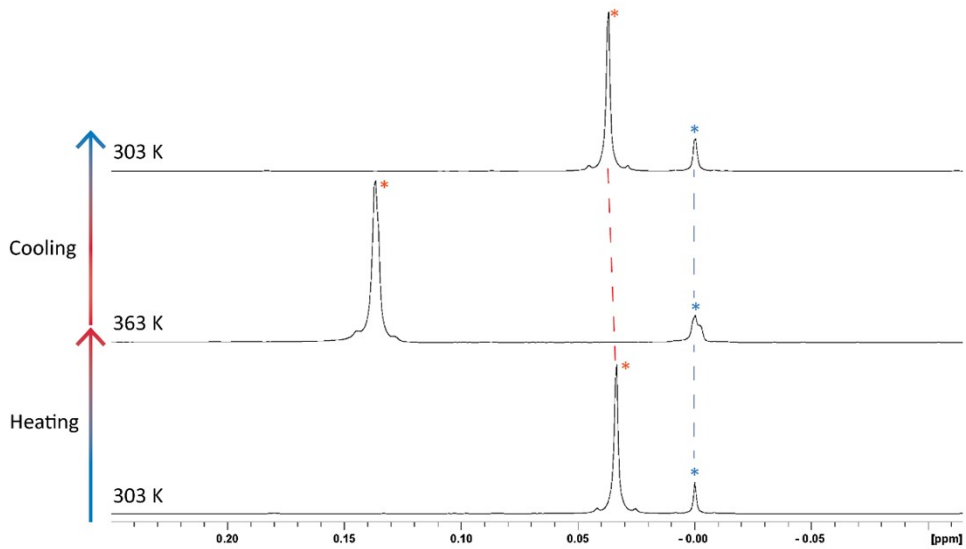


Figure S54 $\chi_M T$ vs. T plot for some transition metal standard solutions as determined by the Evans method. $NiCl_2 \cdot 6H_2O$ and $CuSO_4 \cdot 5H_2O$ were measured in D_2O at concentrations of 17.6 and 16.6 mg cm^{-3}, respectively. $ZnSO_4 \cdot 6H_2O$ was measured in DMSO-d6 at a concentration of



13.0 mg cm^{-3}.

Figure S55 Partial ^1H NMR overlay spectrum of **$1C_4$** (10.2 mg cm^{-3}) from the Evans method in DMSO-d6 with TMS internal reference. * mark the TMS peak from the paramagnetic solution of **$1C_4$** and * marks the TMS peak from the internal blank solution of DMSO-d6 and TMS.

Cooling from 363 K introduces water from condensation into the solution which affects the position of TMS. Applicable to **$1C_4$**-**$1C_{16}$**.

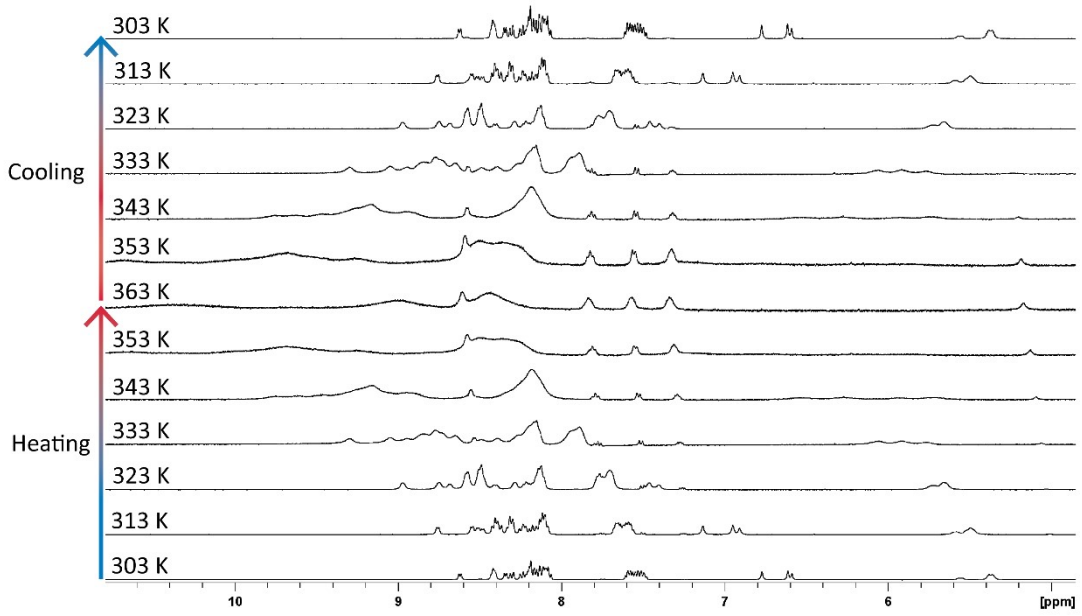


Figure S56 Partial ^{1}H NMR overlay spectrum of **1C$_4$** (10.2 mg cm^{-3}) via the Evans method in DMSO-d6 with TMS internal reference. Isotropic shift increases with temperature and is proportional to number of HS Fe(II) centres. Original spectrum at 303 K is reproduced after heating and cooling back to 303 K. Applicable to **1C$_4$**-**1C$_{16}$**.

Table S5 Various solvent parameters used in the ^{1}H NMR studies.

Solvent	[a]E_N^T	[b]*DN*	[c]*SB*	[d]β	[e]*P'*
DMSO-d6	0.444	29.8	0.647	0.76	7.2
acetonitrile-d3	0.460	14.1	0.286	0.31	5.8
acetone-d6	0.355	17.0	0.475	0.48	5.1

[a]Reichardt's E_N^T parameter is a widely-used indicator of solvent polarity.[2] [b]The Gutman donor number (*DN*) is a measure of Lewis basicity of a solvent.[3,4] [c]Catalan's *SB* parameter[5] describes the solvent's Brønsted basicity. [d]Kamlet and Taft's β is a measure of the hydrogen bond accepting character of the solvent.[6] [e]Solvent polarity index.[7]

UV-vis spectra

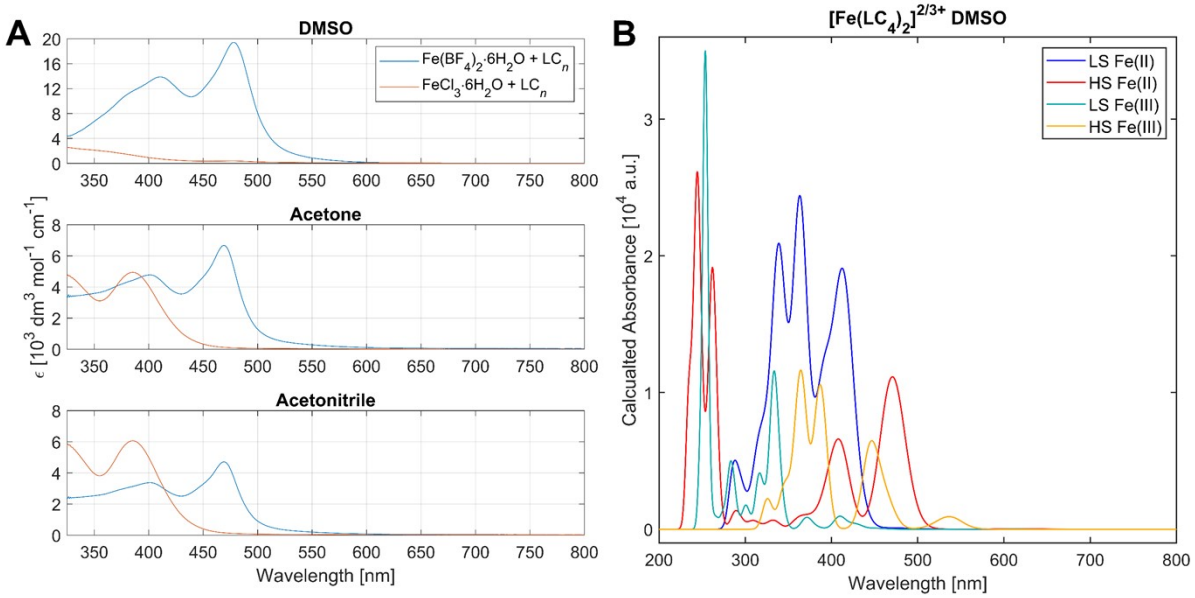


Figure S57 A) UV-vis spectra for the LC_n ligands (2 eq.) added to solutions of $Fe(BF_4)_2{\cdot}6H_2O$ and $FeCl_3{\cdot}6H_2O$ in dimethyl sulfoxide (top), acetone (middle) and acetonitrile (bottom). **B**) TD-DFT calculated UV-vis spectra for LS and HS $[Fe(LC_4)]^{2/3+}$ in DMSO. Gaussian line broadening of 1000 cm^{-1} was used for TD-DFT generated spectra.

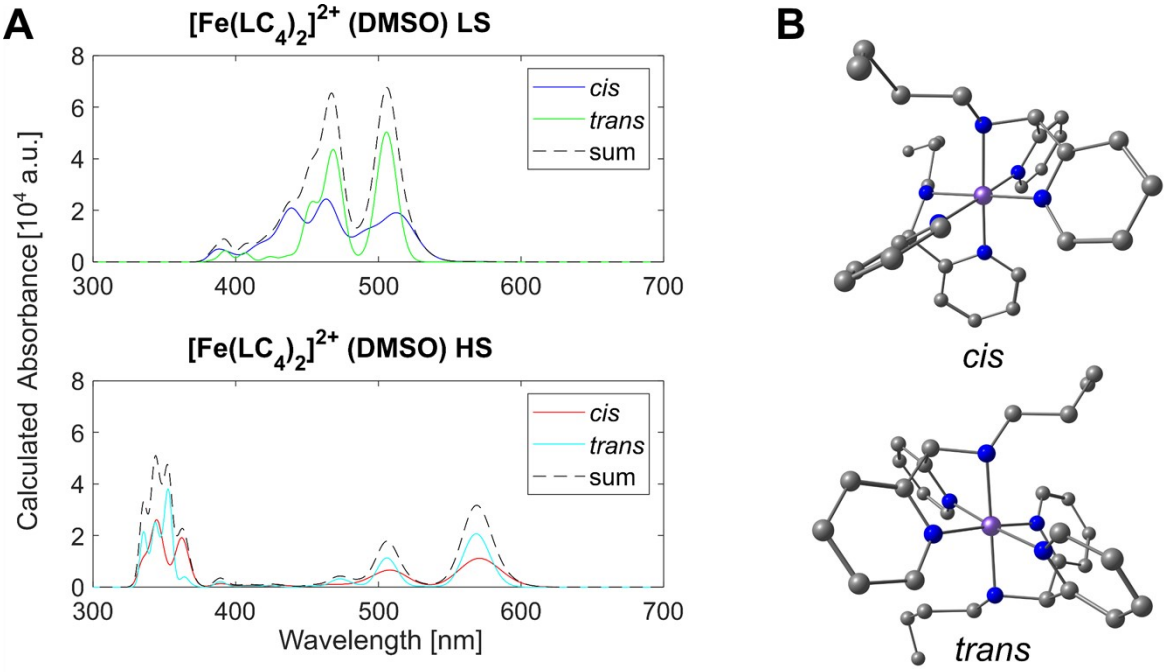


Figure S58 A) TD-DFT calculated UV-vis spectra for LS and HS $[Fe(LC_4)]^{2+}$ in DMSO with the LC_4 ligands in either the *cis* or *trans* conformation (coordinated secondary amine 90 or 180° from each other in the first coordination sphere). **B**) DFT optimized structures for the *cis* and *trans* adducts of $[Fe(LC_4)]^{2+}$. Gaussian line broadening of 1000 cm^{-1} was used for TD-DFT generated spectra.

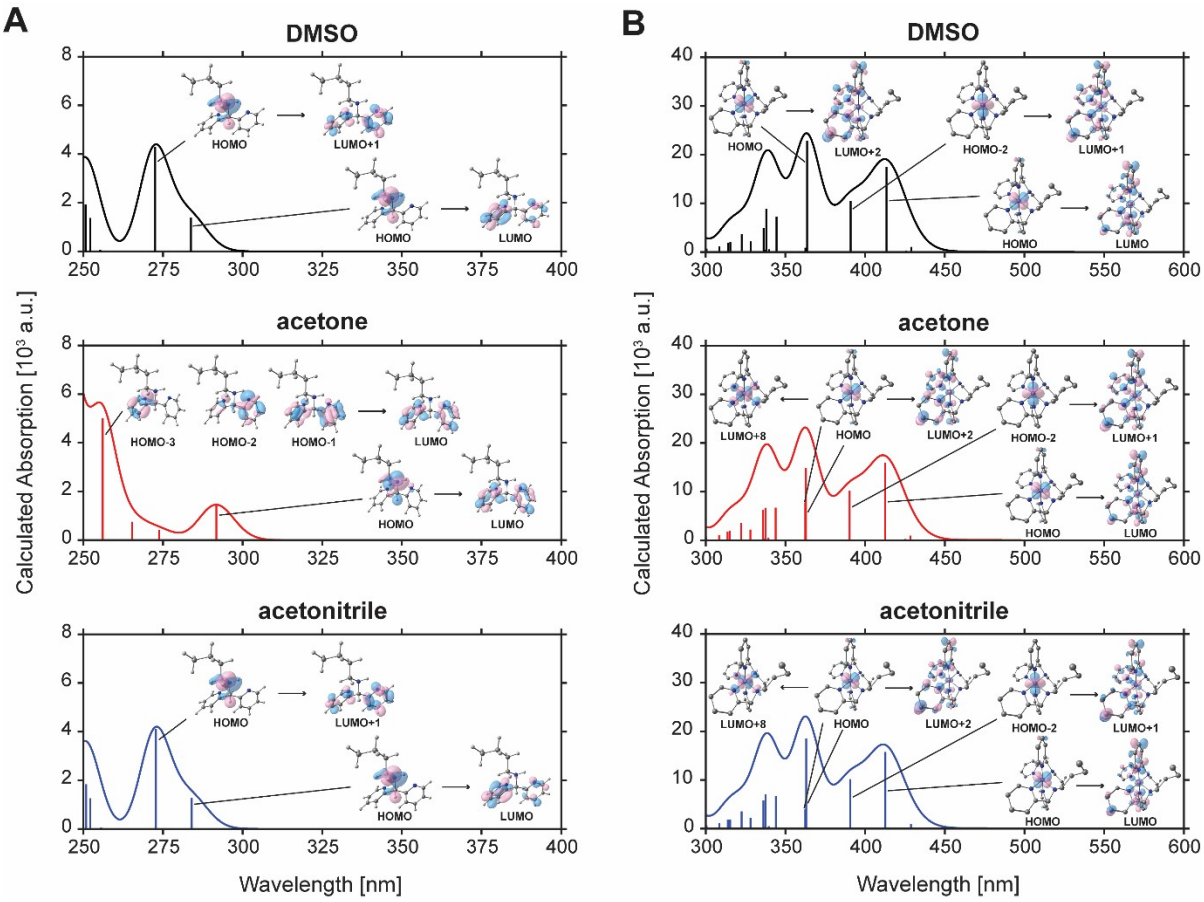


Figure S59 TD-DFT (B3LYP/ZORA/ZORA-def2-TZVP) calculated UV-vis spectra for **A** the LC_4 ligand and **B** the **$1C_4$** complex in various solvents from the BP86/def2-TZVP/D3BJ/CPCM(solvent) optimised geometries. A 1500 cm^{-1} Gaussian line broadening function was applied to the generated spectra. Molecular orbitals are plotted with an isosurface value of 0.05 a.u. Blue corresponds to positive electron density and pink corresponds to negative.

Infrared Spectroscopy

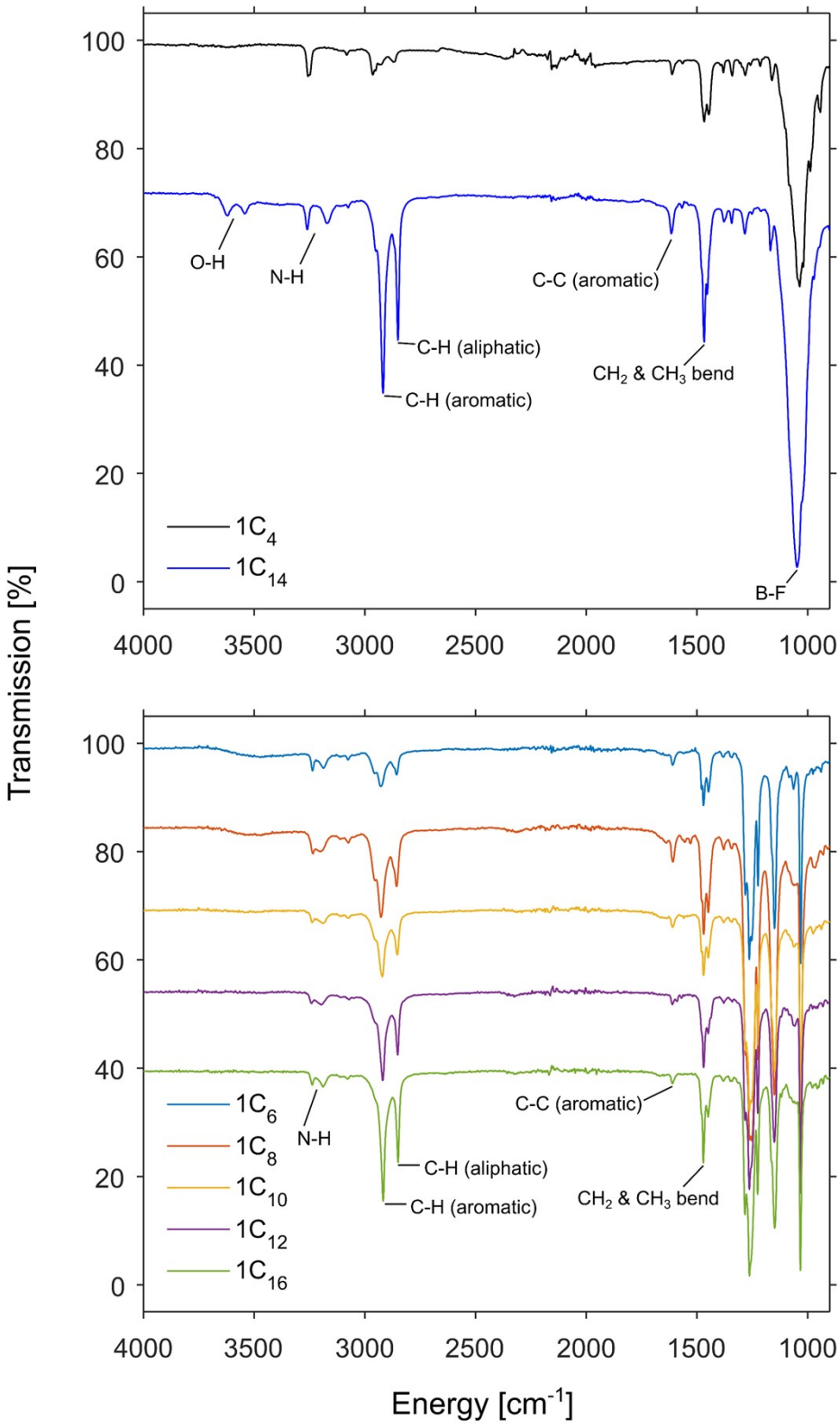


Figure S60 IR spectra for tetrafluoroborate salts **1C$_4$** and **1C$_{14}$** (top) and trifluoromethanesulfonate salts **1C$_6$**-**1C$_{12}$** and **1C$_{16}$** (bottom).

NMR studies on LC_4 to LC_{16}

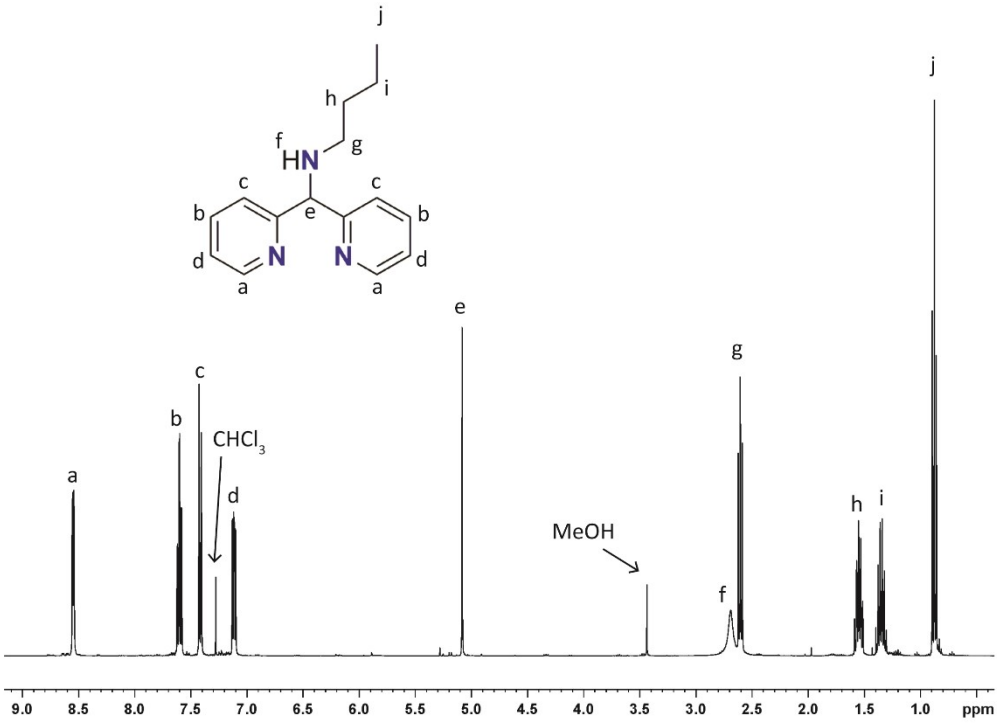
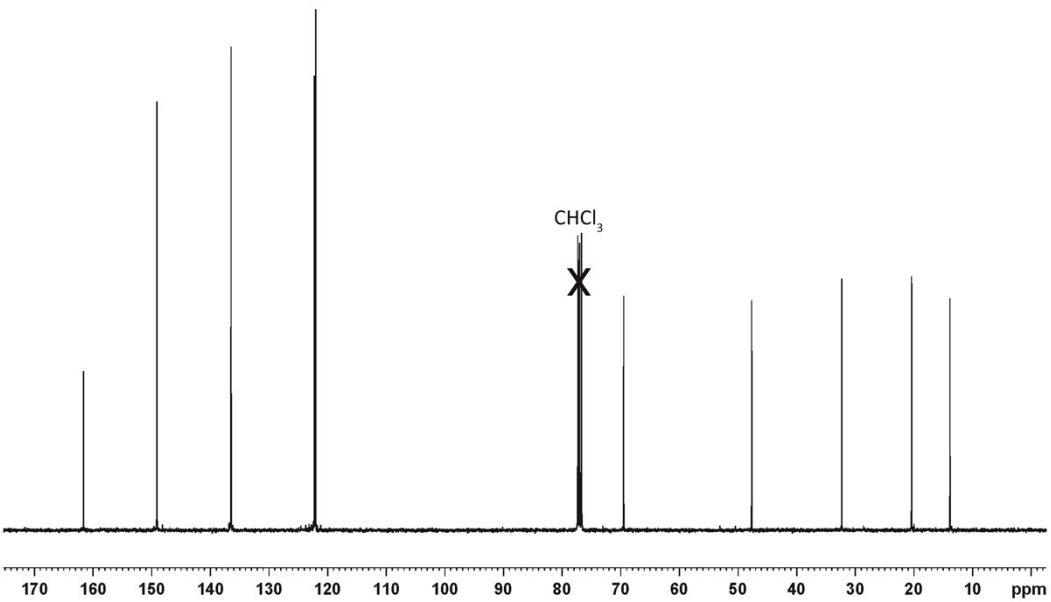


Figure S61 ^{1}H NMR spectrum of LC_4 in $CDCl_3$ with TMS internal reference.

Figure S62 ^{13}C NMR spectrum of LC_4 in $CDCl_3$ with TMS internal reference.



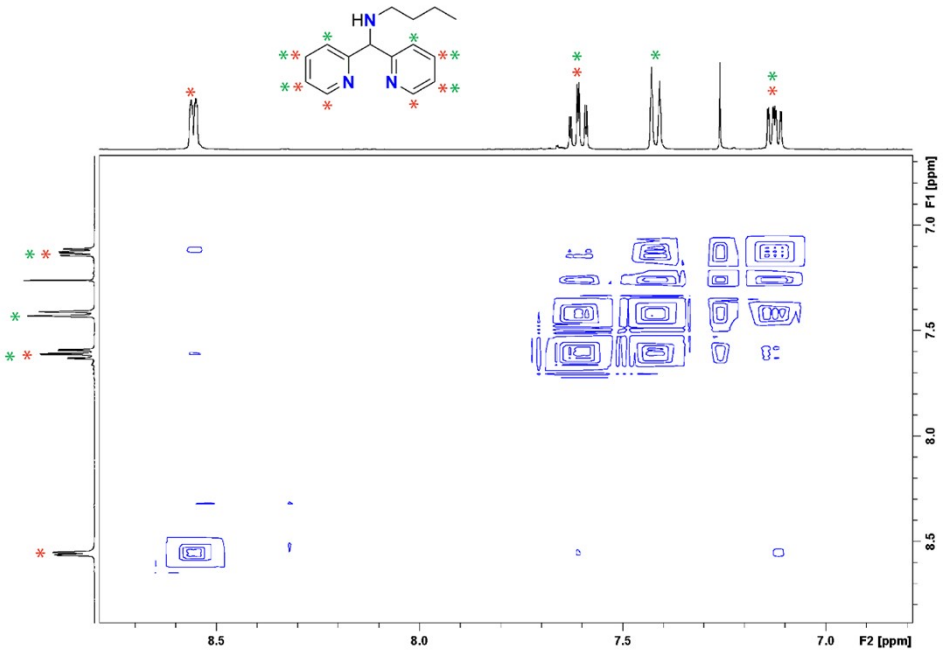


Figure S63 COSY NMR of LC_4 in $CDCl_3$. ^1H environments that are coupled through bond are marked with colour corresponding asterisks. COSY assignments for the LC_4 ligand are the same as those for the LC_6-LC_{16} ligands.

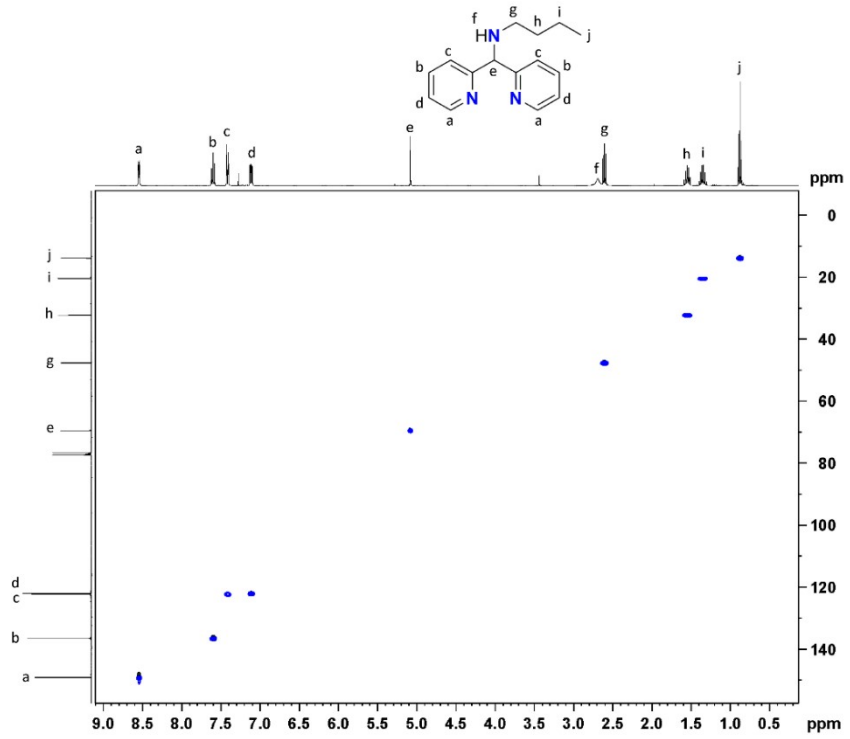


Figure S64 HSQC NMR of LC_4 in $CDCl_3$. HSQC assignments for the LC_4 ligand are the same as those for the LC_6-LC_{16} ligands.

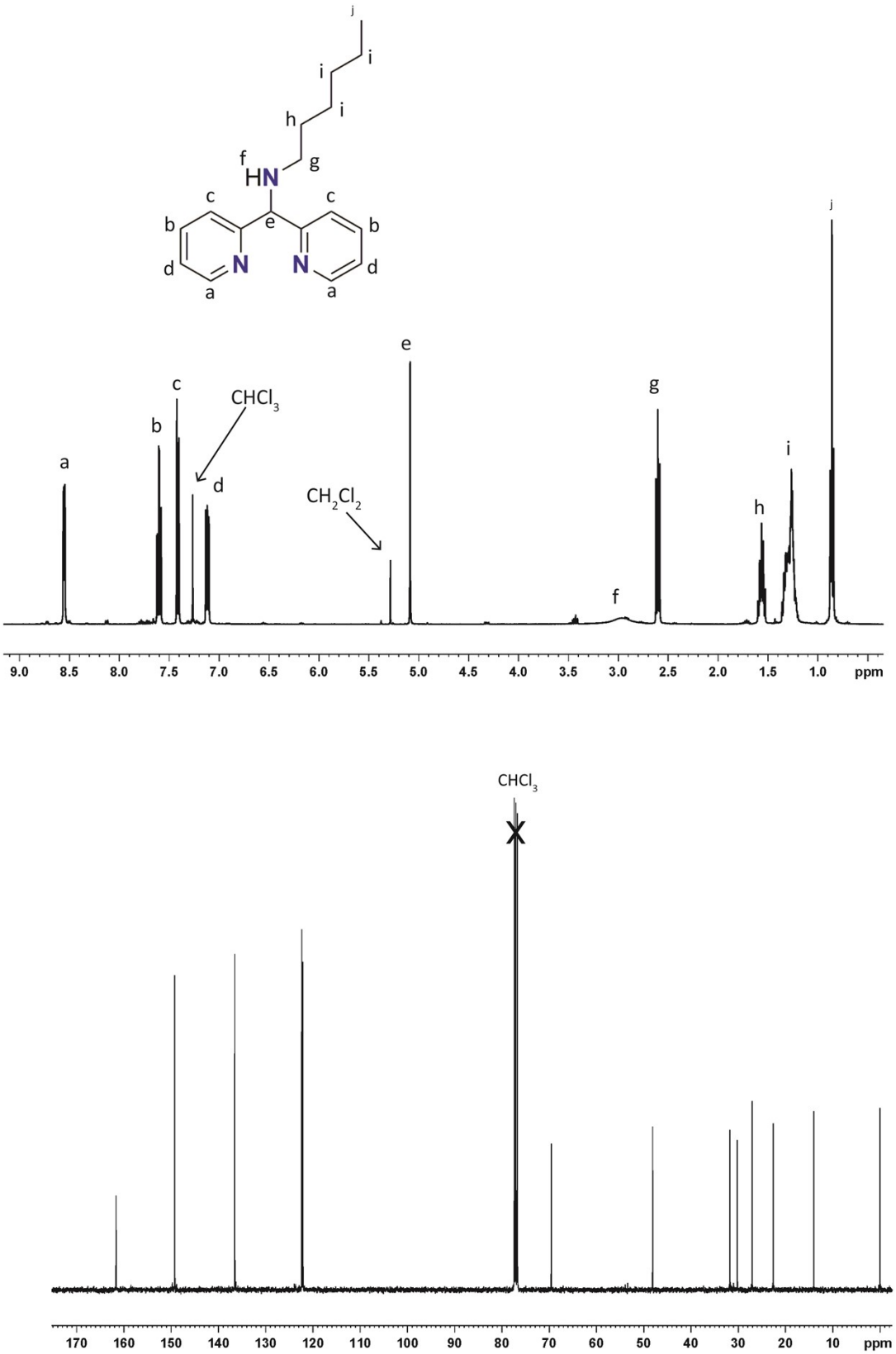


Figure S65 ^{1}H NMR spectrum of LC_6 in $CDCl_3$ with TMS internal reference.

Figure S66 ^{13}C NMR spectrum of LC_6 in $CDCl_3$ with TMS internal reference.

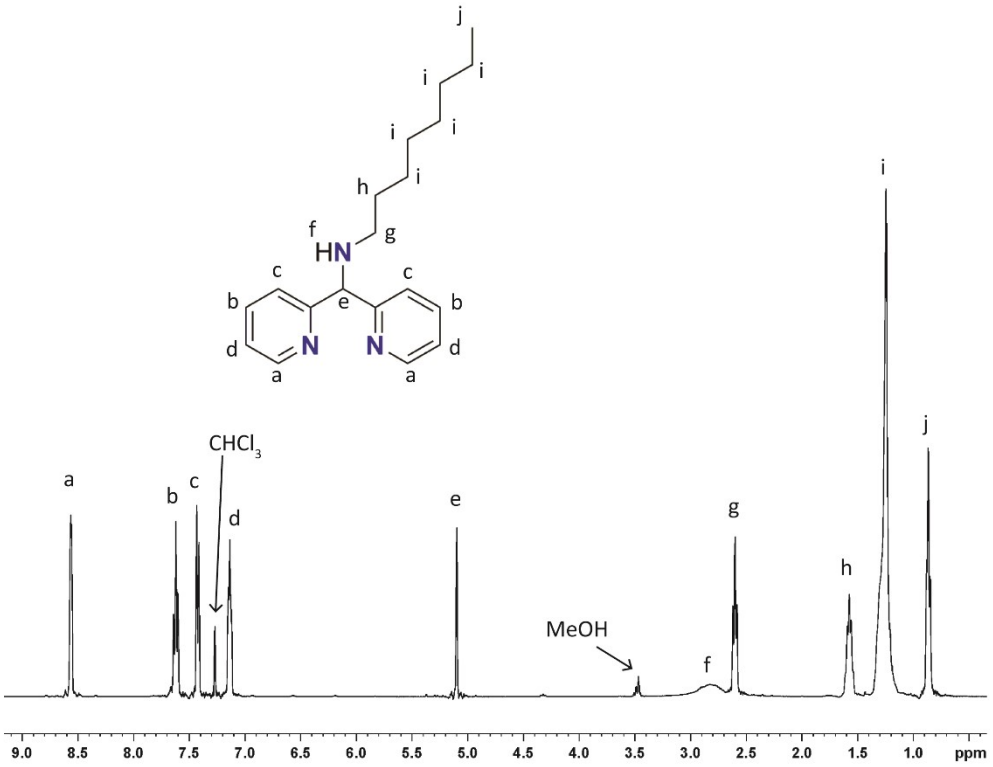


Figure S67 ^{1}H NMR spectrum of LC_8 in $CDCl_3$ with TMS internal reference.

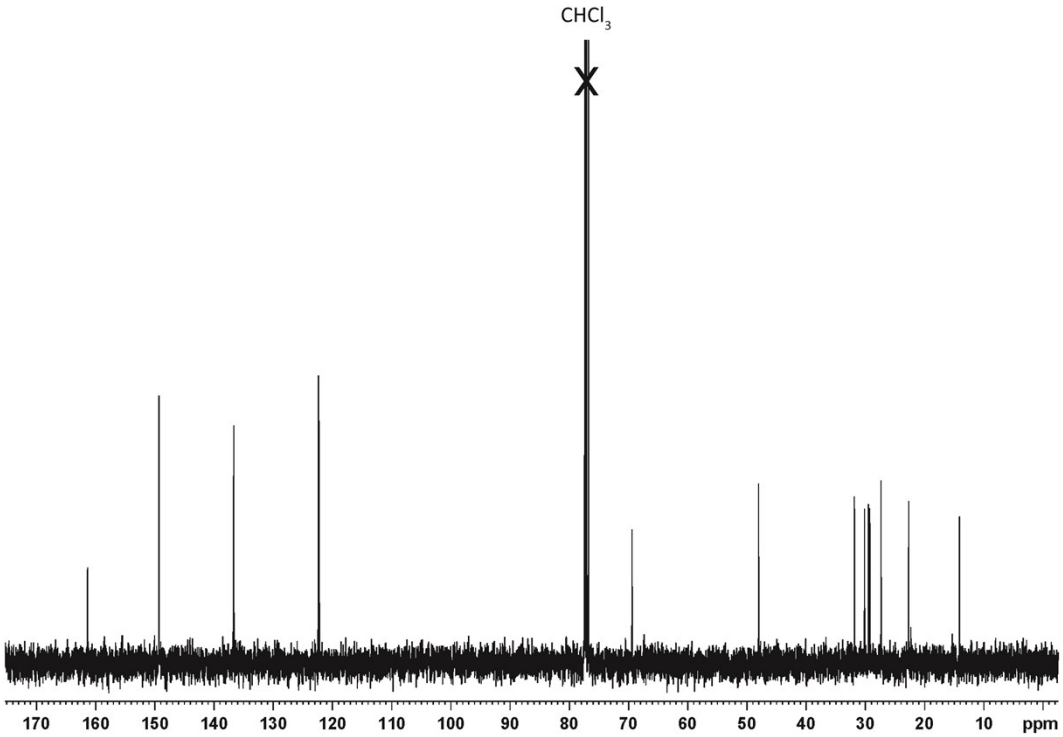


Figure S68 ^{13}C NMR spectrum of LC_8 in $CDCl_3$ with TMS internal reference.

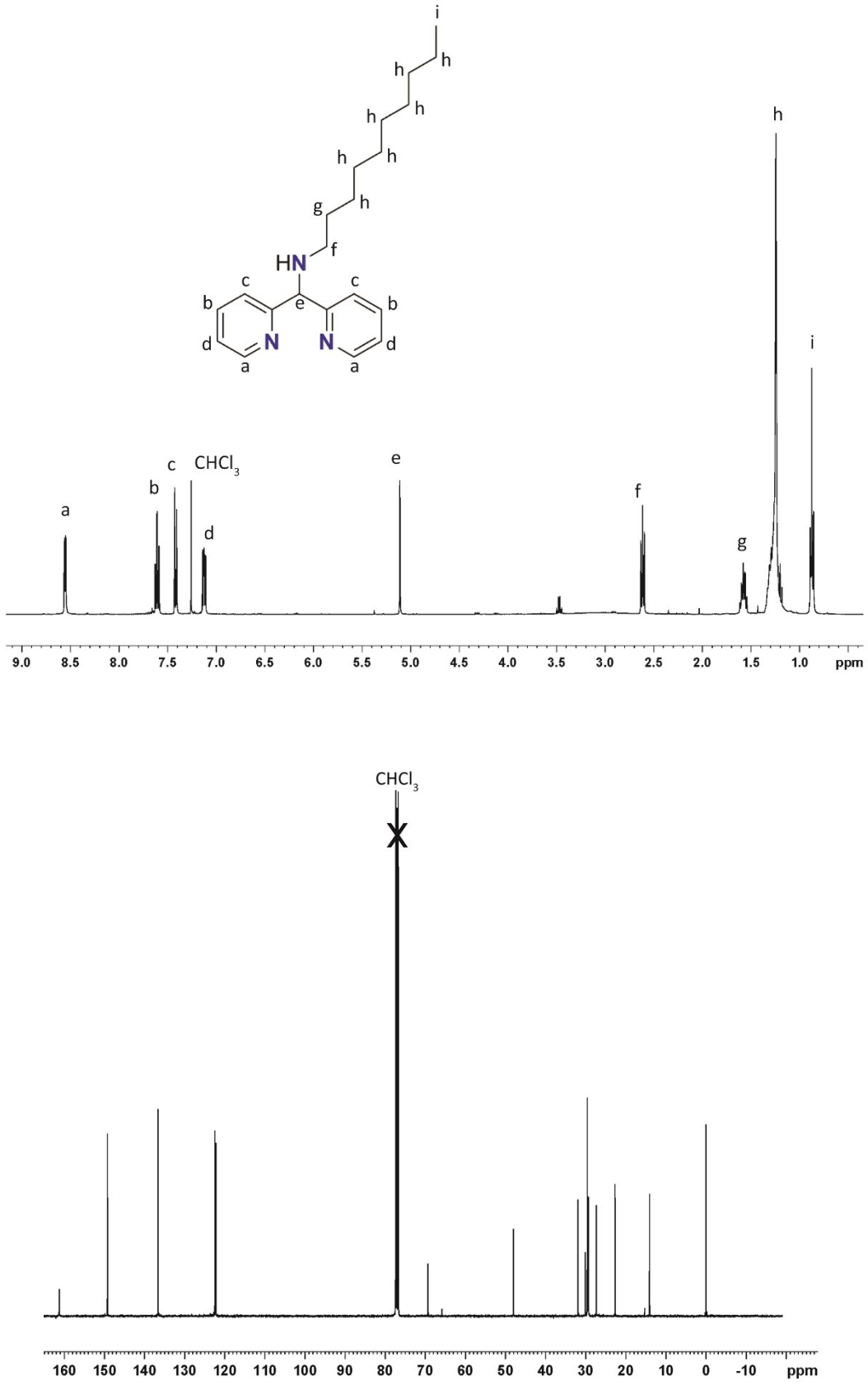
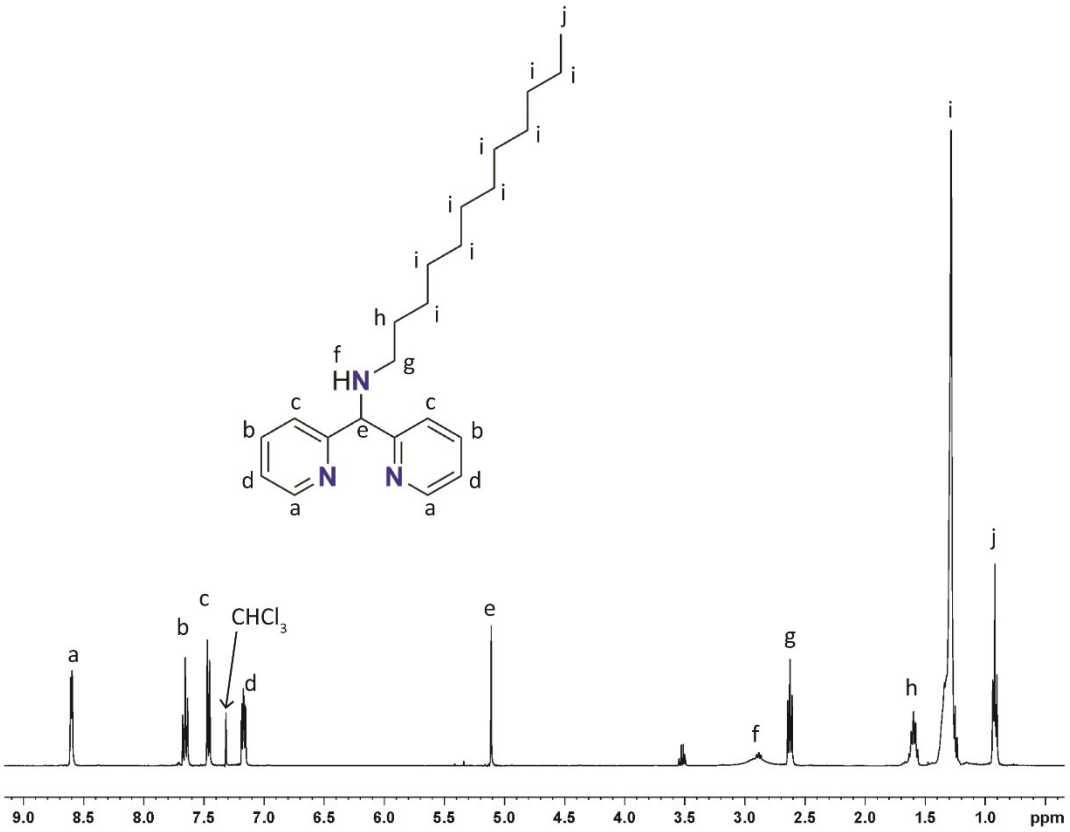


Figure S69 ^{1}H NMR spectrum of LC_{10} in $CDCl_3$ with TMS internal reference.

Figure S70 ^{13}C NMR spectrum of LC_{10} in $CDCl_3$ with TMS internal reference.



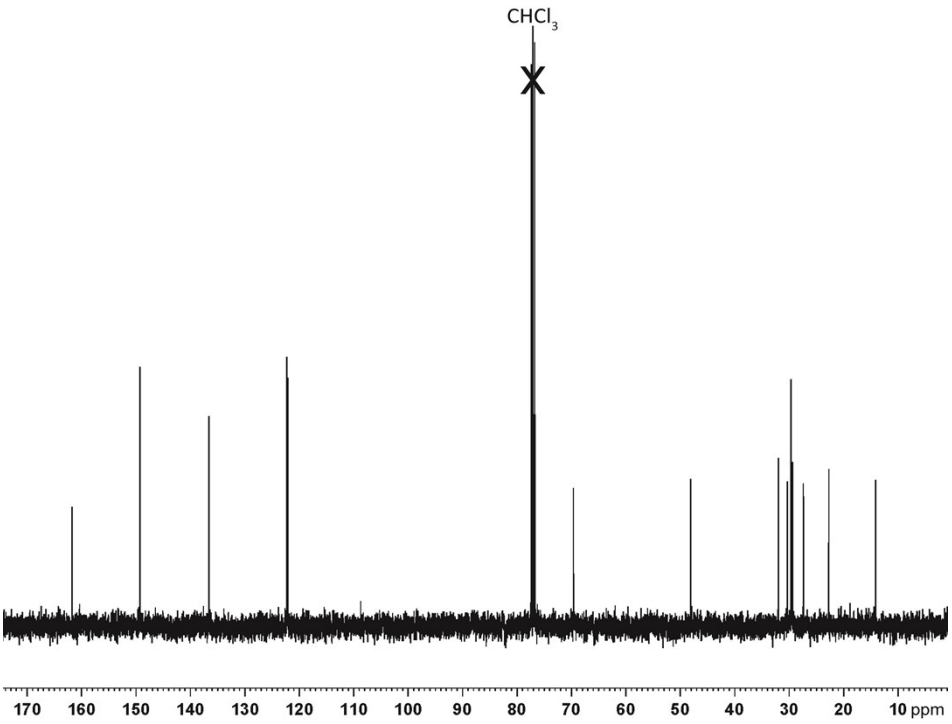


Figure S71 ^{1}H NMR spectrum of LC_{12} in $CDCl_3$ with TMS internal reference.

Figure S72 ^{13}C NMR spectrum of LC_{12} in $CDCl_3$ with TMS internal reference.

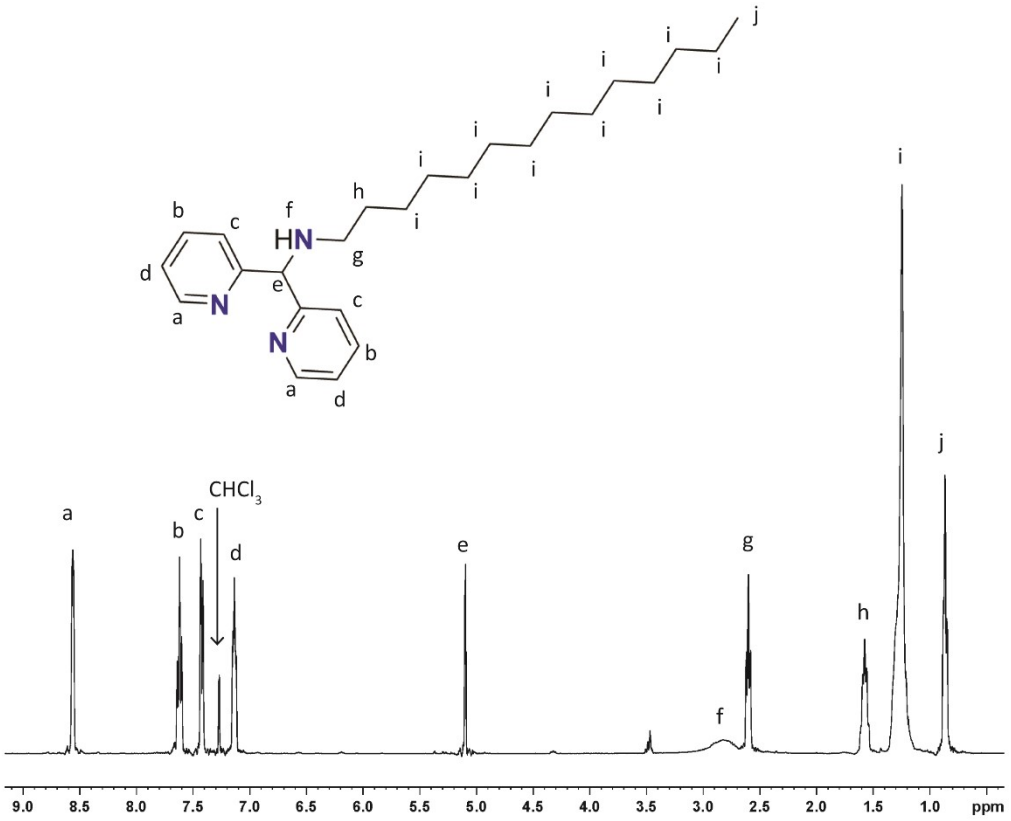


Figure S73 ^{1}H NMR spectrum of LC_{14} in $CDCl_3$ with TMS internal reference.

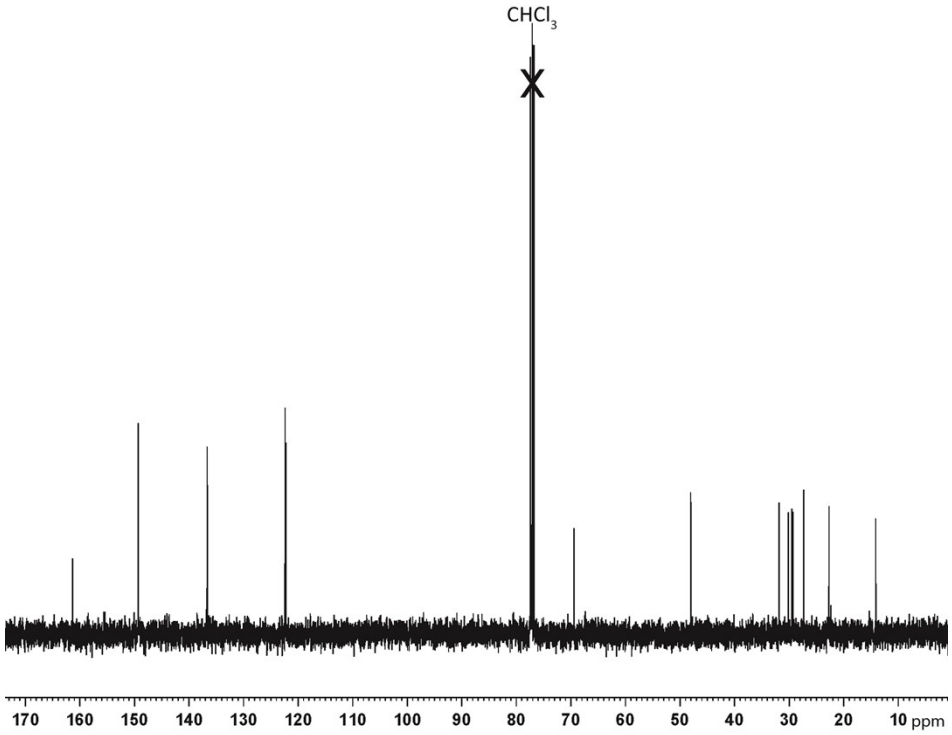


Figure S74 ^{13}C NMR spectrum of LC_{14} in $CDCl_3$ with TMS internal reference.

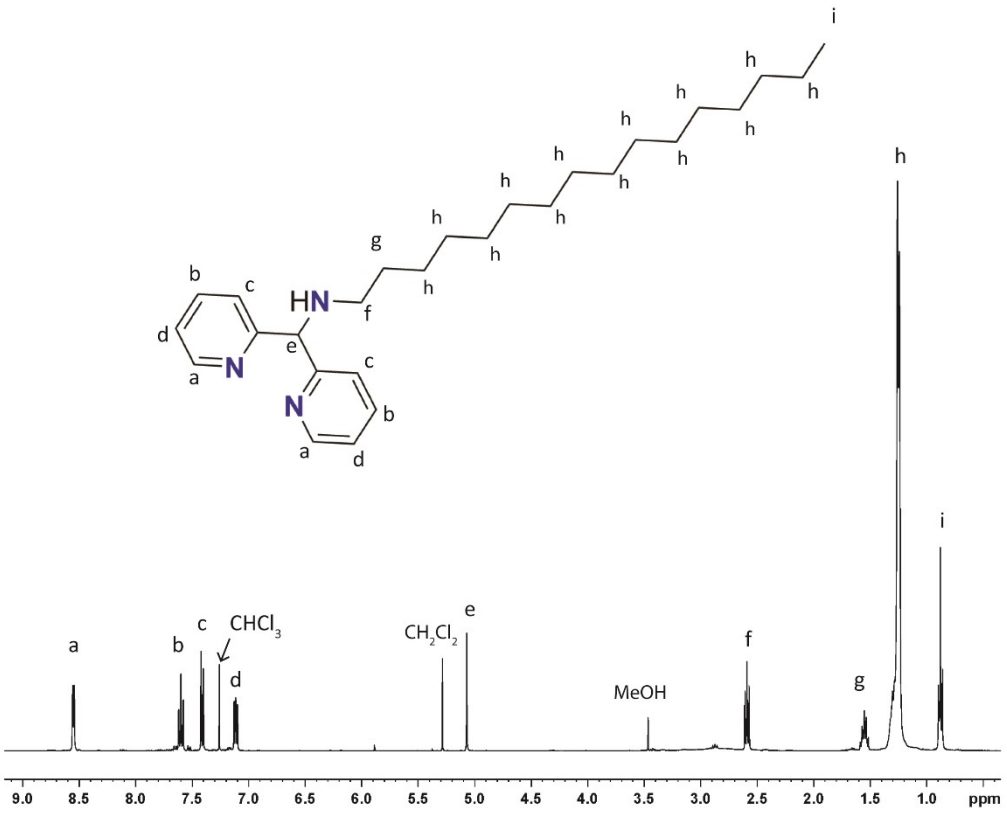


Figure S75 ^{1}H NMR spectrum of LC_{16} in $CDCl_3$ with TMS internal reference.

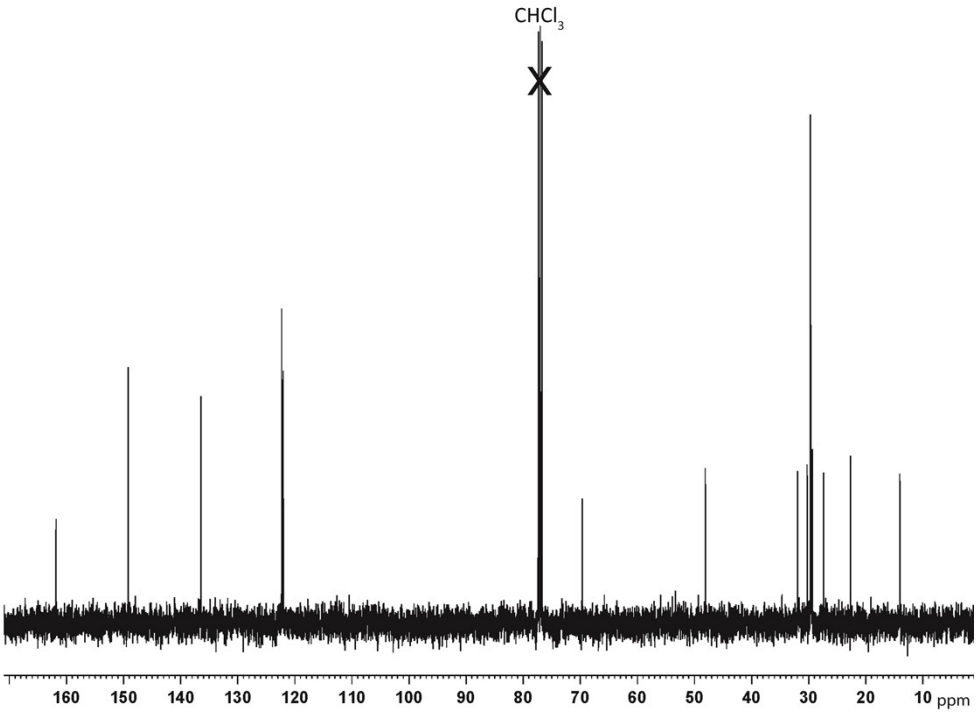


Figure S76 ^{13}C NMR spectrum of LC_{16} in $CDCl_3$ with TMS internal reference.

Mass spectrometry

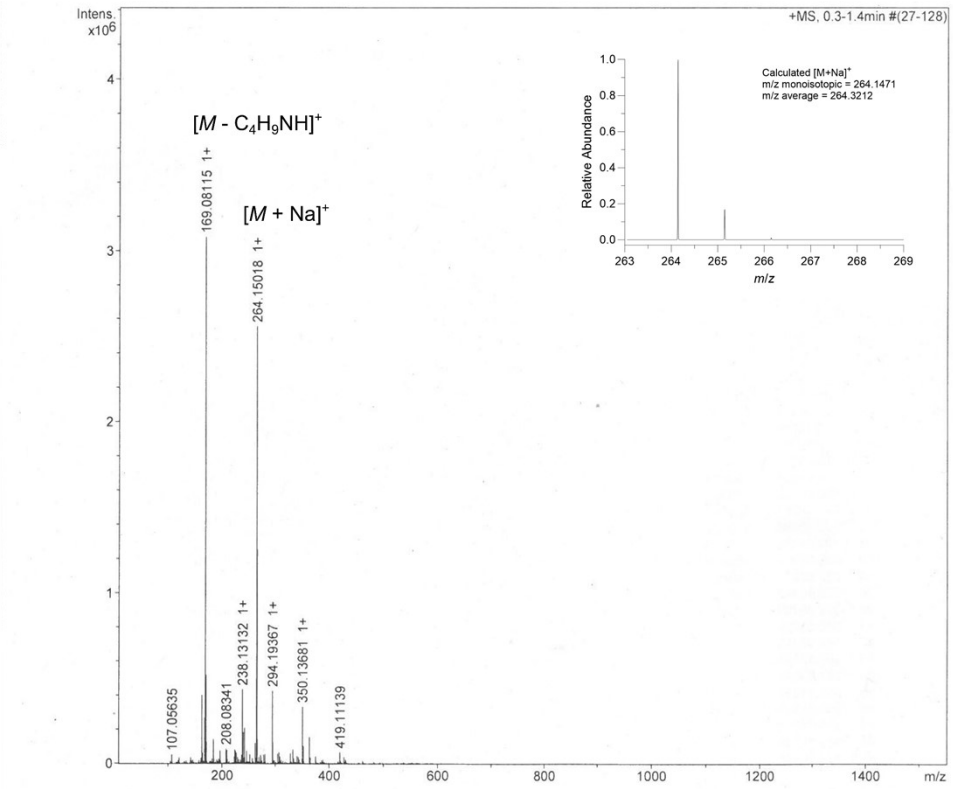


Figure S77 Mass spectrum for LC_4 in MeOH (ESI^+).

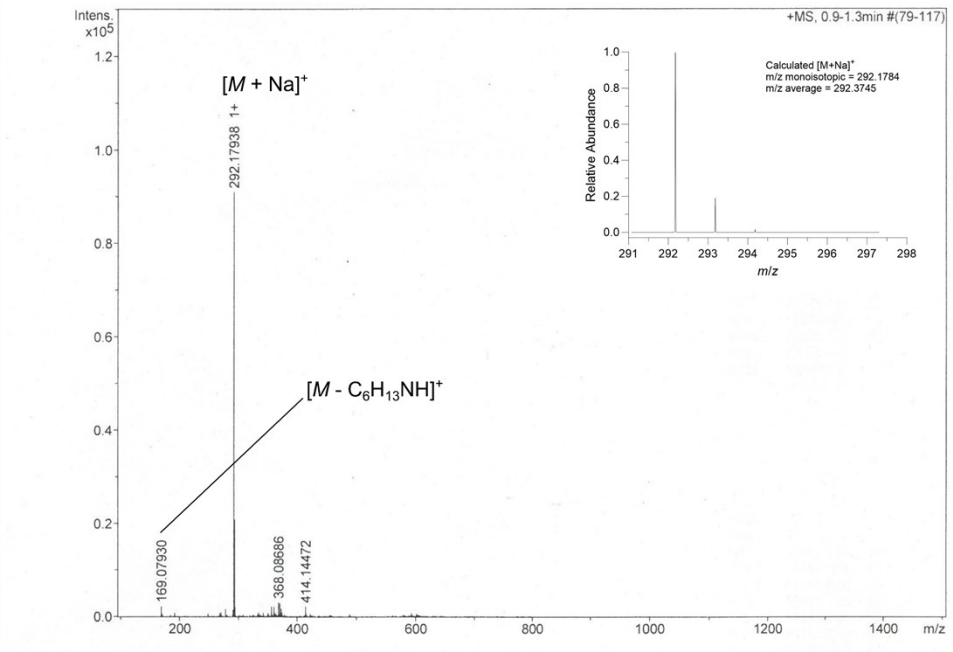


Figure S78 Mass spectrum for LC_6 in MeOH (ESI^+).

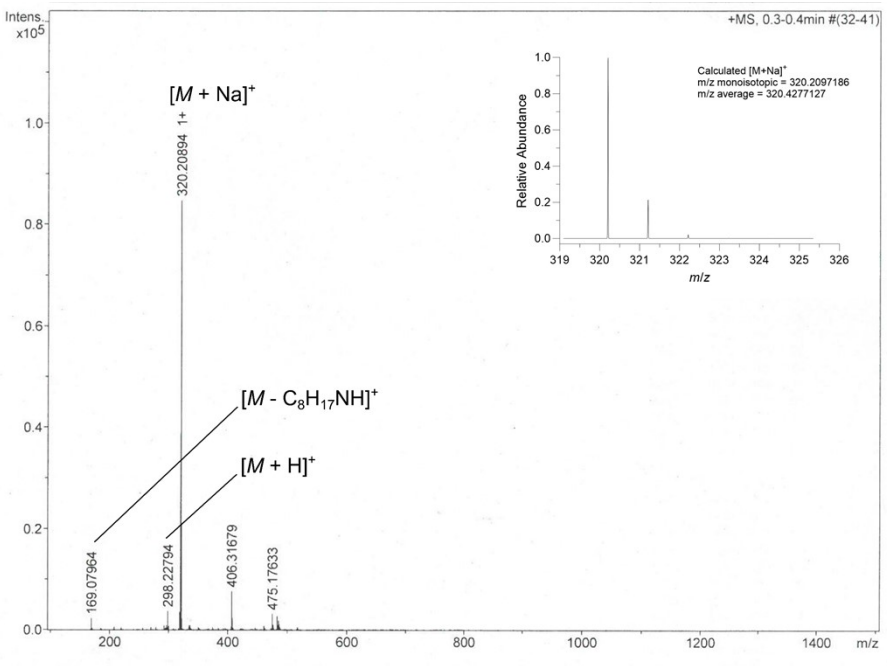


Figure S79 Mass spectrum for LC_8 in MeOH (ESI^+).

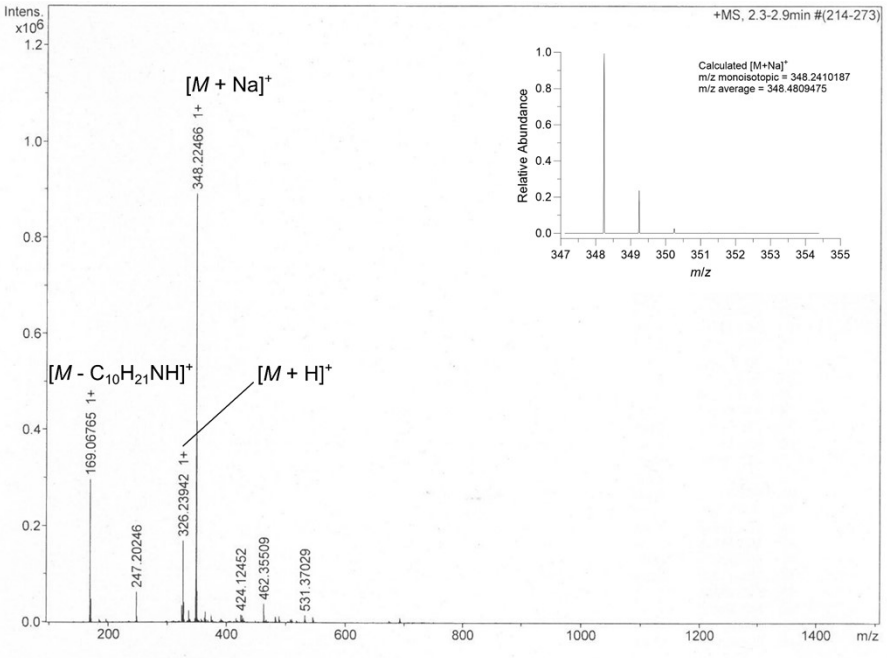


Figure S80 Mass spectrum for LC_{10} in MeOH (ESI^+).

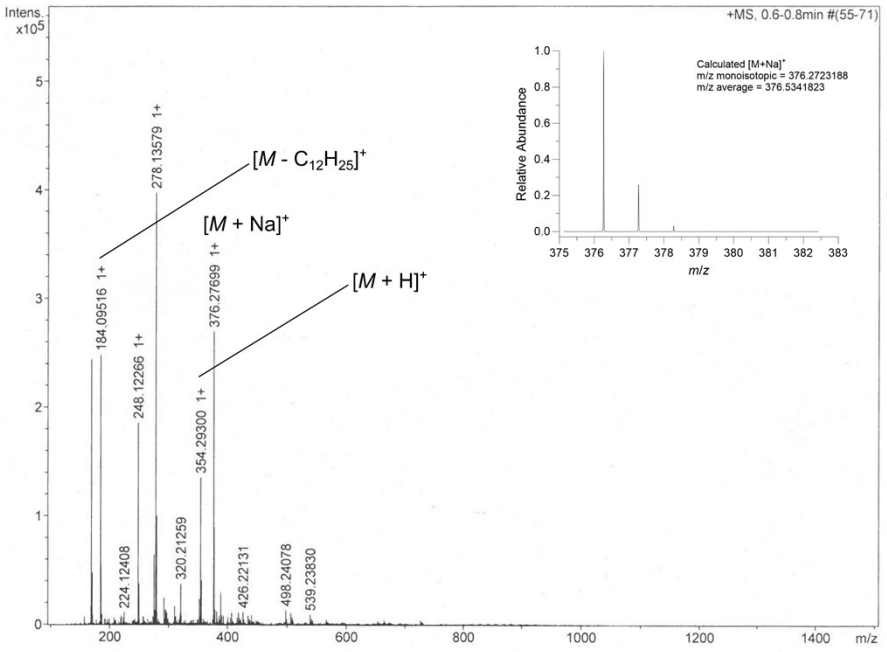


Figure S81 Mass spectrum for LC_{12} in MeOH (ESI^+).

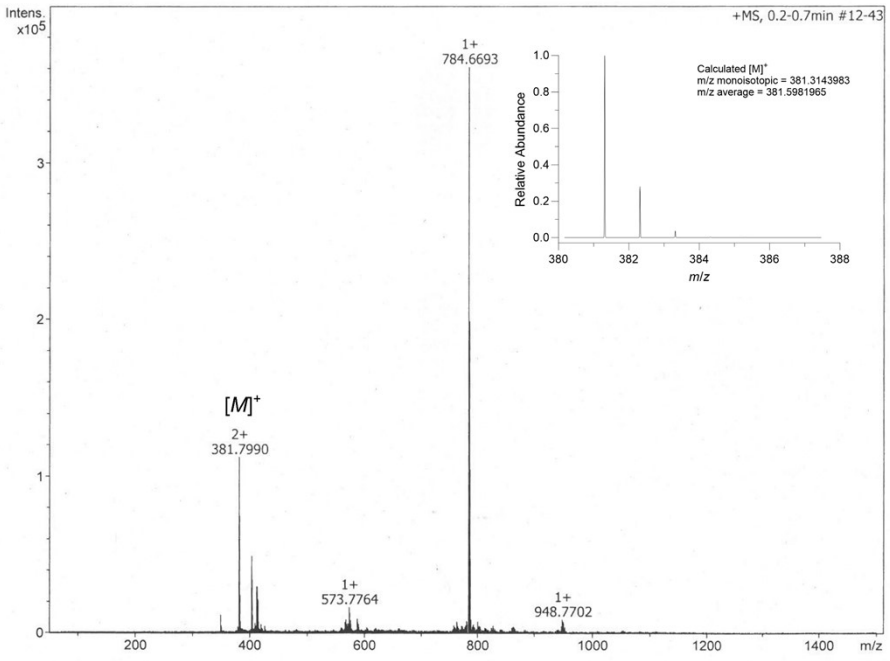


Figure S82 Mass spectrum for LC_{14} in MeOH (ESI^+).

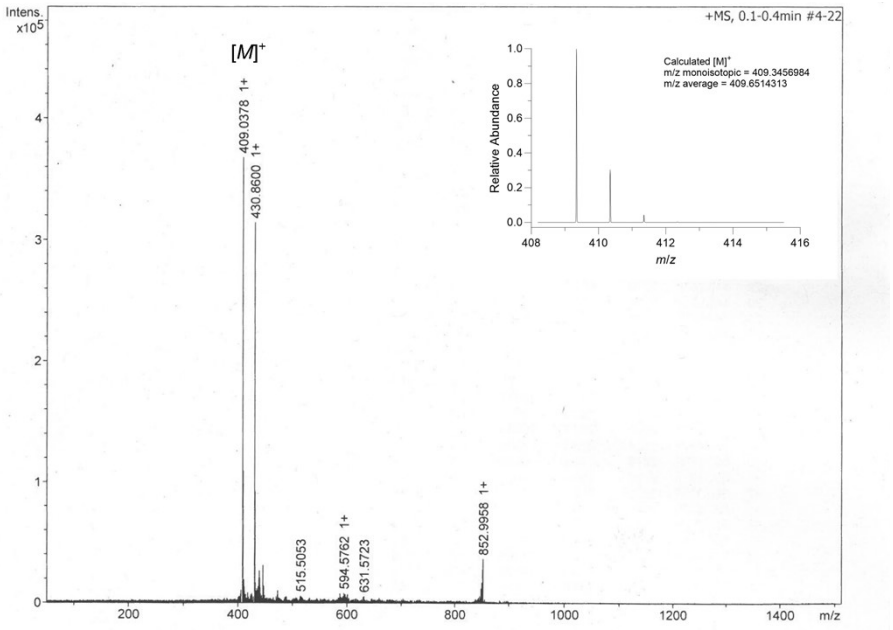


Figure S83 Mass spectrum for LC_{16} in MeOH (ESI^+).

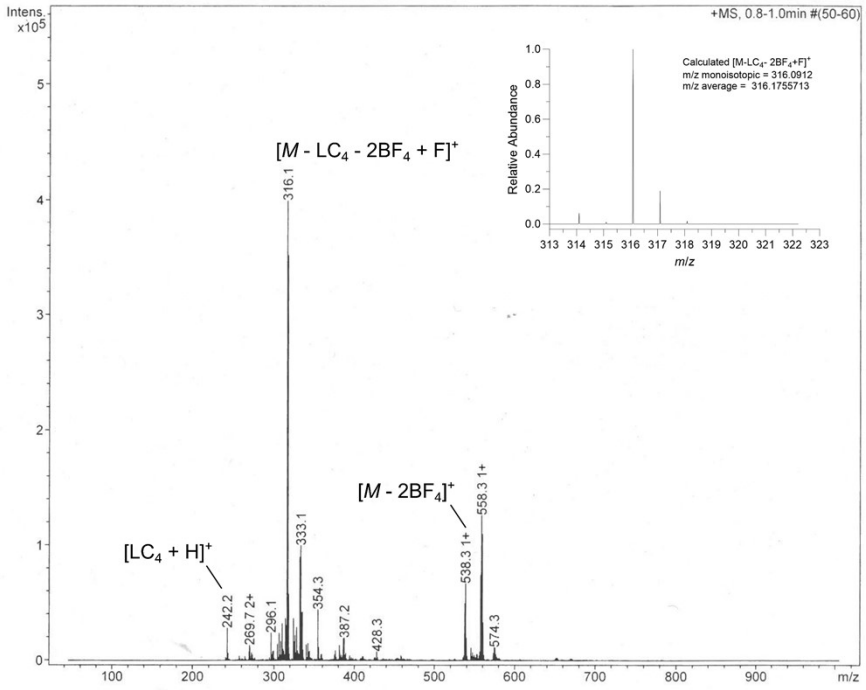


Figure S84 Mass spectrum for **$1C_4$** in MeOH (ESI^+).

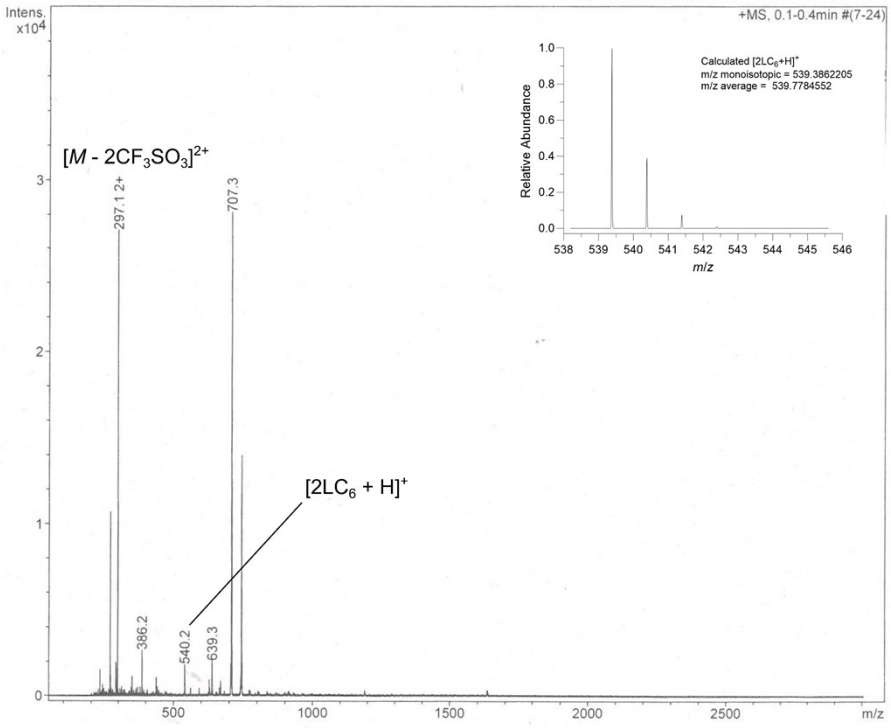


Figure S85 Mass spectrum for **1C$_6$** in MeOH (ESI$^+$).

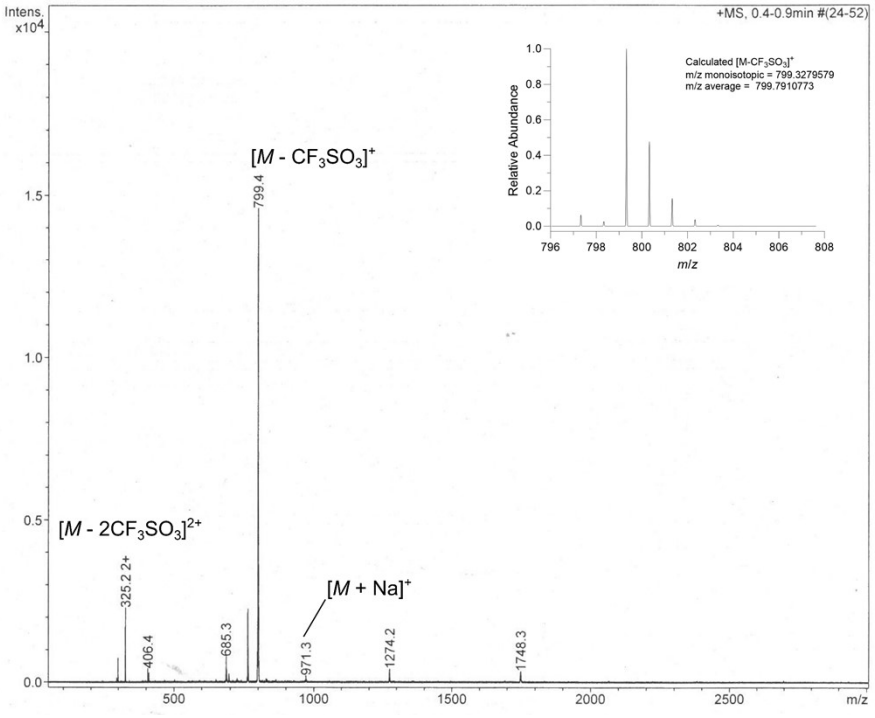


Figure S86 Mass spectrum for **1C$_8$** in MeOH (ESI$^+$).

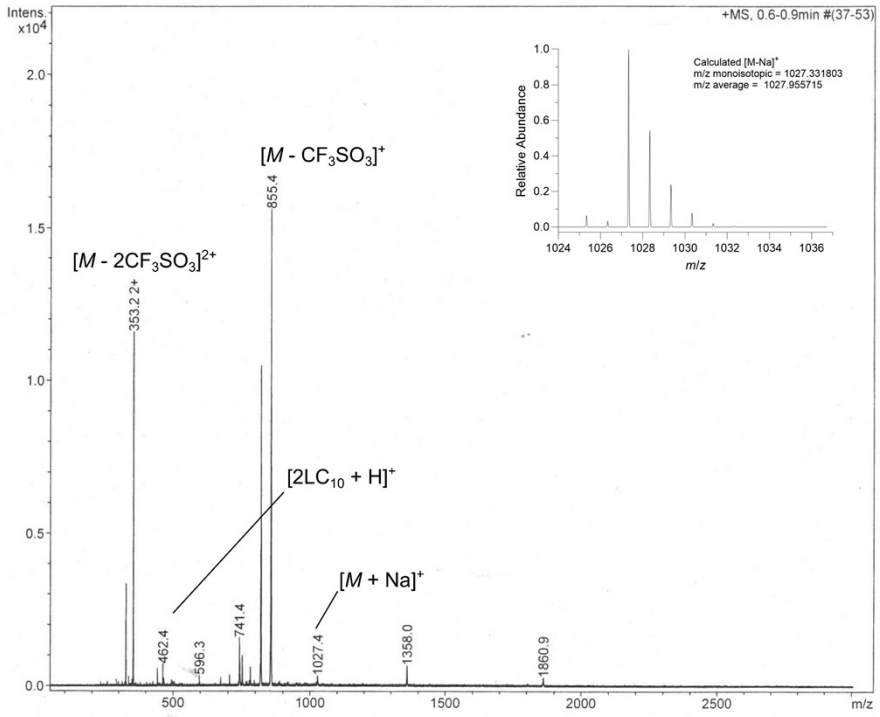


Figure S87 Mass spectrum for **1C$_{10}$** in MeOH (ESI$^+$).

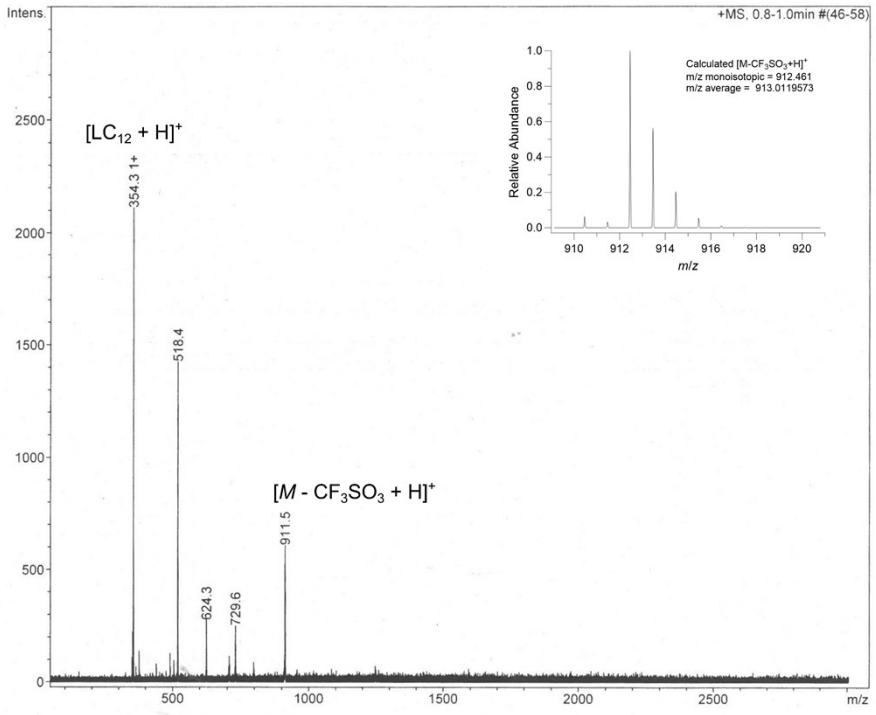


Figure S88 Mass spectrum for **1C$_{12}$** in MeOH (ESI$^+$).

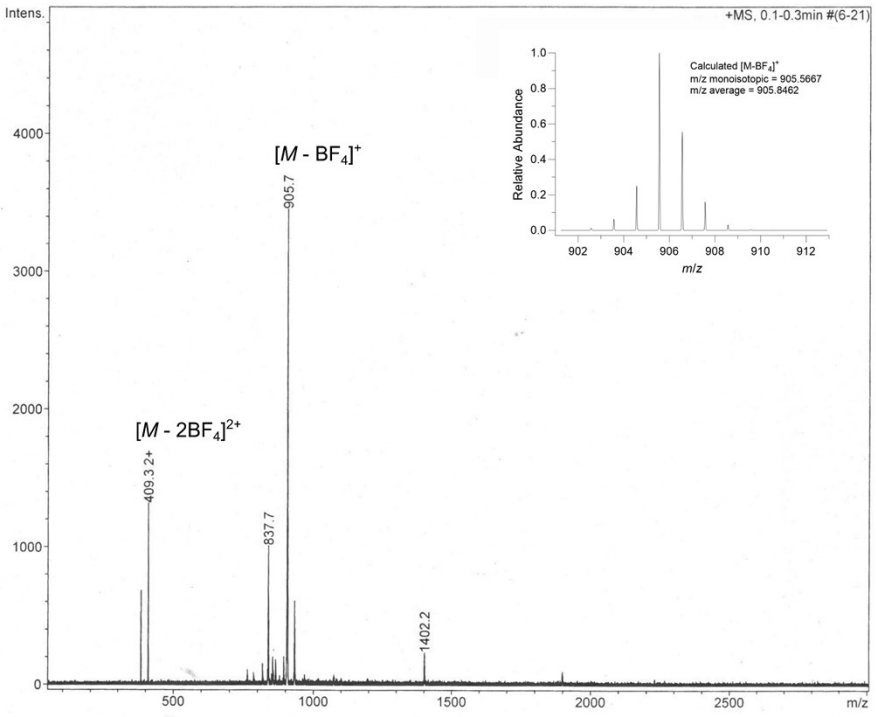


Figure S89 Mass spectrum for **1C$_{14}$** in MeOH (ESI$^+$).

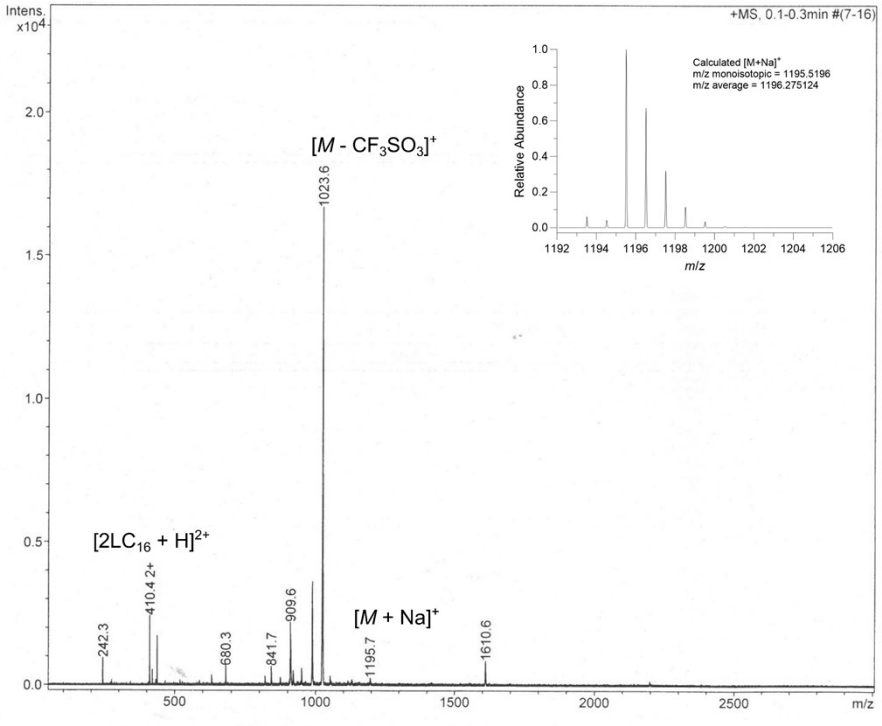


Figure S90 Mass spectrum for **1C$_{16}$** in MeOH (ESI$^+$).

Density Functional Theory

Table S6 Selected bond lengths and parameters for **1C$_4$** determined by X-ray crystallography at 100 K and DFT geometry optimization (BP86/def2-TZVP).

Bond(s)	**1C$_4$**	
	Exp.	**DFT**
Lengths (Å)		
Fe1-N1	1.967(18)	1.925
Fe1-N2	1.982(19)	1.958
Fe1-N3	2.045(18)	2.051
Fe1-N4	1.953(18)	1.925
Fe1-N5	1.985(18)	1.960
Fe1-N6	2.066(18)	2.047
Fe-N av.	1.999	1.978
Angles (°)		
N1-Fe1-N4	100.11(8)	99.97
N2-Fe1-N5	179.04(7)	178.95
N1-Fe1-N2	86.82(7)	87.80
N2-Fe1-N3	81.03(7)	80.97
N3-Fe1-N6	97.61(7)	95.81
$\sum^a$ (°)	82.92	76.21

[a] Octahedral distortion parameter derived from the equation: Σ, (= N-Fe-N) where perfect octahedrons produce a value $\Sigma = 0°$ and deviation from this value coincides with structural deformation of the coordination polyhedron.

Example Orca Input Files

Geometry Optimization

```
! UKS RIJK B3LYP def2-TZVP AutoAux D3BJ Opt TightSCF DefGrid2 SlowConv NormalPrint Pal8
! CPCM(solvent_code)

%maxcore 3000

%scf
MaxIter 700
End

*xyzfile charge spin-multiplicity xyz_filename.xyz
```

Vibrational spectroscopy

```
! UKS RIJCOSX B3LYP ZORA ZORA-def2-TZVP NumFreq AutoAux DefGrid2 SlowConv TightSCF Pal8
! LargePrint CPCM(solvent_code)

%scf
MaxIter 700
end

%maxcore 3000

%elprop
Polar 1
end

*xyzfile charge spin_multiplicity xyz_filename.xyz
```

UV-vis spectroscopy

```
! UKS RIJCOSX B3LYP ZORA ZORA-def2-TZVP AutoAux DefGrid2 SlowConv
! TightSCF Pal8 NormalPrint UNO CPCM(solvent_code)

%scf
MaxIter 700
end

%maxcore 3000

%tddft
NRoots 60
MaxDim 5
end

*xyzfile charge spin_multiplicity xyz_filename.xyz
```

Optimised XYZ Coordinates for Orca Calculations

LC_4 (acetone)

Charge = 0, Spin Multiplicity = 1

N	-0.12609812708998	1.98677222982502	-0.02119291165896
N	-0.15744108426452	-0.71340961305141	-2.15889779383406
N	-1.95093060394499	-0.28702760932997	-0.10827988473683
H	-2.04032065293161	-1.21079451559141	-0.53911895295100
C	0.40228699833939	3.13785955990470	0.42439093764803
H	1.37572983549051	3.06178037682080	0.91781844683439
C	-0.22056783275050	4.38087338818241	0.28219944660243
H	0.25820380824074	5.28357788143272	0.66284673929488
C	-1.46085456715755	4.42830925521003	-0.35453701942639
H	-1.98682246443636	5.37565490984337	-0.48269460439769
C	-2.02076915633071	3.23706116787131	-0.81834005885933
H	-2.99395098245587	3.22764200548859	-1.31188637333734
C	-1.32378754523644	2.03846878853227	-0.63126907331746
C	-1.89664813172324	0.71979717792821	-1.15965694607329
H	-2.90739082554871	0.95969010472128	-1.55397496896107
C	-1.06322540093950	0.25995483432990	-2.35024378406965
C	-1.25000662729055	0.87914981426391	-3.59456024732705
H	-2.00786655502580	1.65653572203253	-3.70570760748767
C	-0.46073544162332	0.48730637911294	-4.67251553005802
H	-0.58731206733623	0.95379778346475	-5.65066979607708
C	0.48937600455778	-0.51912323977141	-4.47824833652002
H	1.12958118310501	-0.86050263573435	-5.29219057890577
C	0.59528346783745	-1.08890962983513	-3.21008777568155
H	1.31839533215302	-1.88739911126245	-3.02059155927160
C	-3.04648119043915	-0.05359355503282	0.83292892562241
H	-2.89025389597349	0.93759539697394	1.28856069179695
H	-4.03404006357329	-0.00791921417280	0.32101286827306
C	-3.08447008176522	-1.13193516721505	1.91277343336417
H	-3.17436011698256	-2.11658363082369	1.42233741774576
H	-2.11973822986813	-1.13377700248255	2.44791928795058
C	-4.23535541014591	-0.95994985115729	2.91199727231009

H	-5.19409651881404	-0.96639873952285	2.36562194808711
H	-4.25638089670336	-1.83740469773448	3.57805523430758
C	-4.13707443385259	0.31202148352236	3.76082643495048
H	-4.21455062362321	1.22085935447119	3.14647053914925
H	-4.94049511711679	0.34985909179930	4.51089080697952
H	-3.17506760878024	0.35228366998612	4.29550778003513

LC_4 (DMSO)

Charge = 0, Spin Multiplicity = 1

N	-0.07298305539911	2.20468267524045	-0.29711829032912
N	-0.79484954626806	-1.07441232043612	-2.39505332318982
N	-1.82921471189767	-0.19484350783673	-0.06649893032884
H	-1.81522561890545	-1.13294499600383	-0.48068910326728
C	0.37580898444987	3.39030612082551	0.14252767811410
H	1.42425868737147	3.42434215800639	0.45311125535951
C	-0.41667082693867	4.54065797438582	0.21217162534499
H	0.00450272510164	5.47688657370850	0.57949008623781
C	-1.74617293142375	4.45265414079344	-0.19873653044932
H	-2.40230395286717	5.32350756102121	-0.15976714658004
C	-2.22339603247451	3.22372177187525	-0.66046319705687
H	-3.25664355752427	3.10871170012340	-0.99168481538360
C	-1.35877087839187	2.12596677953885	-0.69318517100435
C	-1.84578328244528	0.76424542632111	-1.16844090459993
H	-2.88160552428676	0.91265811582538	-1.55107759181383
C	-1.03062412805770	0.24673353614315	-2.34917129821020
C	-0.60560946157051	1.11744890349081	-3.36255455863286
H	-0.81441290993854	2.18541029737265	-3.29006983335805
C	0.08523491364576	0.59876772876380	-4.45468330339409
H	0.42541740111953	1.25678210266137	-5.25571135256474
C	0.33679343327735	-0.77570166405554	-4.50402330063646
H	0.87679206360870	-1.22556205384811	-5.33742894844983
C	-0.12317994777834	-1.56666461564573	-3.45281683403929
H	0.05122022172629	-2.64616831984358	-3.45161570079800
C	-2.96710762782914	-0.04311179894686	0.84106433681365

H	-2.92707896325317	0.97104100925125	1.27027182819886
H	-3.93797394438312	-0.11659530100372	0.30237371024567
C	-2.92250530307553	-1.08775624426236	1.95381408854930
H	-2.87735397712717	-2.08952679658837	1.49302437405747
H	-1.98740517371536	-0.96092425760258	2.52544697048688
C	-4.12439253013441	-1.02265934046187	2.90497493880154
H	-5.05345442936522	-1.15722683674410	2.32491351889652
H	-4.07026253055872	-1.87668161759486	3.59908862296919
C	-4.20622676645420	0.27698381380925	3.71210468351784
H	-4.34762788503943	1.15283905895096	3.06219867589204
H	-5.04667455345322	0.25158661073007	4.42106421030742
H	-3.28275400374422	0.43696777503571	4.29064393829370

LC_4 (acetonitrile)

Charge = 0, Spin Multiplicity = 1

N	-0.06895079067409	2.20218910697738	-0.29887369087938
N	-0.79250895400779	-1.07342723060965	-2.39221941519823
N	-1.83156854694608	-0.19335489465825	-0.06727944714994
H	-1.81570820575330	-1.13184606870772	-0.48028752259934
C	0.38278207560175	3.38637730458661	0.14155062289278
H	1.43184584098476	3.41790360314792	0.45032476524269
C	-0.40754905429683	4.53801163749153	0.21435054445666
H	0.01615500861433	5.47312297333280	0.58161601177869
C	-1.73809767130764	4.45274696542663	-0.19369047405217
H	-2.39273896015182	5.32459892491539	-0.15197041287240
C	-2.21834532783048	3.22525594964730	-0.65613701376126
H	-3.25262199474335	3.11262336352980	-0.98499117085850
C	-1.35550217825234	2.12621008698036	-0.69251289875035
C	-1.84613532604657	0.76565337877832	-1.16852450238713
H	-2.88145921667163	0.91760402485396	-1.55135006326621
C	-1.03150326693166	0.24727150401989	-2.34913340661493
C	-0.60992302458843	1.11666918279894	-3.36499410497359
H	-0.82133783686868	2.18428687882041	-3.29436560740144
C	0.08069991751884	0.59726043298363	-4.45686168254800

H	0.41817535728959	1.25407036625052	-5.26002266254062
C	0.33559802848763	-0.77666759853903	-4.50338509480714
H	0.87563722441926	-1.22692990635254	-5.33655061797043
C	-0.12095150420155	-1.56635988220178	-3.44971220529406
H	0.05609262850700	-2.64543117942541	-3.44603553546994
C	-2.96984626179457	-0.04180273713741	0.83992526653654
H	-2.93052983900969	0.97277644565380	1.26809140857017
H	-3.94031875317842	-0.11673975891008	0.30072267826827
C	-2.92463201589210	-1.08585504326655	1.95313695188468
H	-2.87712069119608	-2.08763929046857	1.49265845266652
H	-1.99052859856259	-0.95702028044184	2.52591495149119
C	-4.12762743586622	-1.02265068750344	2.90304840636975
H	-5.05599407975959	-1.16008152043957	2.32255950276418
H	-4.07200344280206	-1.87603954938093	3.59787918774286
C	-4.21274960994180	0.27722103769311	3.70940271695477
H	-4.35285072932293	1.15287775878502	3.05893311334021
H	-5.05521476622953	0.25139878952328	4.41593799413707
H	-3.29090362259521	0.43783807484614	4.29033936229802

$[1C_4]^{2+}$ (acetone, low-spin)

Charge = 2+, Spin Multiplicity = 1

Fe	-0.00275056688370	-0.00031475420174	0.00555486835053
N	0.02539506889496	1.89581654777562	-0.32744727741677
N	1.95327484901598	0.03256513951454	-0.08533644867743
N	0.22879895246675	-0.08837926405194	-2.02952384392522
H	0.69298888081006	-0.97813029835316	-2.25090991340546
N	-0.00670240477960	0.00063317178388	1.93027810522090
N	-1.95920079207457	-0.06170262736089	0.07469009138573
N	-0.26102326956902	-2.01643823431507	0.26991704287405
H	-0.75041233545055	-2.37817076077230	-0.55838360213209
C	-0.54776974852264	2.88392671801925	0.39498559133607
H	-1.06190721742002	2.58305747566708	1.30681566679087
C	-0.49305620721666	4.21216818577772	-0.01357546865911
H	-0.96669304694853	4.97796690603493	0.59954346230557

C	0.16218459259078	4.53871491805591	-1.20398381681225
H	0.20878877457401	5.57224863292109	-1.54665345695853
C	0.74899751302689	3.51694795545376	-1.95543197201247
H	1.26217383571804	3.72072477388910	-2.89504247329180
C	0.66081382915352	2.21334192781694	-1.48843040665335
C	1.26181534107732	0.99218586560072	-2.14088034349323
H	1.57992421631735	1.18486769680125	-3.17466278592463
C	2.40065535353161	0.54466728053615	-1.26356228338459
C	3.74980869420467	0.66539899244825	-1.56755542715942
H	4.05102702851479	1.07133455288805	-2.53290860145554
C	4.68792579876991	0.26056314913863	-0.61573105228887
H	5.75510750121455	0.33563330783976	-0.82357526696598
C	4.23232664405294	-0.23815515140211	0.60676710381063
H	4.92721173572250	-0.55598716245479	1.38285054589180
C	2.86551705393975	-0.34009329198915	0.83912059583786
H	2.48438195734934	-0.72843051783327	1.78045638414366
C	-0.87506198769225	0.07843503977098	-3.01131553631980
H	-1.46762855229863	0.95765241798564	-2.72565342988575
H	-0.42806795861005	0.29609652611857	-3.99425307921458
C	-1.74994040060482	-1.16651566606926	-3.08614796382770
H	-1.14847690932232	-2.00796905244735	-3.47057879842243
H	-2.07831912840985	-1.44466256238193	-2.07460741389980
C	-2.99273142699235	-0.96665940151541	-3.96343625669443
H	-3.61405793604485	-1.87229094042620	-3.88747685456002
H	-3.59420930508117	-0.14384190190688	-3.54183322010864
C	-2.68248699028376	-0.68338281857333	-5.43583719034360
H	-2.13571550303847	0.26193861457790	-5.56460091567931
H	-2.06813622027589	-1.48759134941730	-5.86953087768882
H	-3.60802574916883	-0.61202403643901	-6.02464963719441
C	0.59113555498907	0.87428233286473	2.77062673564172
H	1.10695258990157	1.71638381586891	2.31098355756256
C	0.55937681686404	0.69862331135010	4.14983939125472
H	1.05384135277085	1.42765307546057	4.79070435506471
C	-0.09908550480988	-0.41078687710852	4.68674630949124

H	-0.12781259549133	-0.57199239856590	5.76420407898233
C	-0.71263470848107	-1.31818338934619	3.81875352130721
H	-1.22970557776031	-2.20343951980615	4.18836658245111
C	-0.64527378750934	-1.08144962611750	2.45308485289964
C	-1.27426674003771	-1.92554819939001	1.37232562872761
H	-1.59971476330320	-2.90667406755918	1.74398956198353
C	-2.41113688677239	-1.12482622439283	0.79296364860331
C	-3.76195010856959	-1.39168820792973	0.97094853644972
H	-4.06865790372778	-2.26464508974208	1.54657142537043
C	-4.69529334606860	-0.52564479256718	0.39734593752362
H	-5.76340695498274	-0.71054856723252	0.50995041360545
C	-4.23453346248928	0.58155395493643	-0.31884508633556
H	-4.92652098804620	1.28925803385017	-0.77351273924921
C	-2.86662970719704	0.78593004198443	-0.45850607510636
H	-2.48027820953718	1.64233268435082	-1.00620409166313
C	0.82962156105556	-2.98161492703304	0.56927951870288
H	1.43797407942047	-2.57576962420480	1.38673524890470
H	0.37142288461650	-3.91472270151820	0.93998982407868
C	1.65944028472623	-3.28278118552651	-0.67306382920040
H	0.97457427377995	-3.58364211782299	-1.48385794620542
H	2.17949121323044	-2.37403155244517	-1.01327271135509
C	2.69167768505202	-4.39409021759840	-0.44151839596916
H	2.17331343885073	-5.30067684573698	-0.08712482218767
H	3.13981477715730	-4.65403961959881	-1.41297501834696
C	3.80165338817735	-4.01083026506522	0.54106034485784
H	3.40512475397417	-3.79514947323156	1.54407761250628
H	4.53424554179645	-4.82406511909801	0.64246946442760
H	4.33655278216374	-3.11442595653329	0.19367429973049

$[1C_4]^{2+}$ (DMSO, low-spin)

Charge = 2+, Spin Multiplicity = 1

Fe	-0.00271815397271	-0.00100860432675	0.00495609235322
N	0.02515161051844	1.89502566640111	-0.32786484200685
N	1.95316921145284	0.03219940376655	-0.08619946270876

N	0.22815947206332	-0.08876584246977	-2.03014123697502
H	0.69193809030373	-0.97851315126494	-2.25232753046079
N	-0.00648354473987	0.00012954654973	1.92955757958751
N	-1.95895005759889	-0.06261628445012	0.07421712013964
N	-0.26027254227314	-2.01711857924967	0.26978236289552
H	-0.74907844966903	-2.37998551335882	-0.55834736525197
C	-0.54803924582528	2.88292217673496	0.39479575057479
H	-1.06221864414708	2.58191105646410	1.30654568371146
C	-0.49340487540104	4.21120832002118	-0.01362031735537
H	-0.96717930203924	4.97679541101991	0.59966627777429
C	0.16174951195680	4.53796561662343	-1.20403653323947
H	0.20817976025358	5.57155060236968	-1.54662544976183
C	0.74857823843055	3.51636849291161	-1.95568402455811
H	1.26165726528173	3.71990952300423	-2.89539288113133
C	0.66047655201247	2.21271113854758	-1.48883035946340
C	1.26121354535271	0.99167308950836	-2.14165468183867
H	1.57916402241962	1.18442218924947	-3.17543129904516
C	2.40015996416538	0.54437219508955	-1.26449749578748
C	3.74921382392818	0.66536724115293	-1.56883320587234
H	4.04976580273108	1.07123361714175	-2.53441482342400
C	4.68758606746168	0.26078004127734	-0.61718387839640
H	5.75472079471773	0.33594428453345	-0.82531181250189
C	4.23233989680471	-0.23788111570293	0.60548636158707
H	4.92733895082631	-0.55558633365370	1.38152351764085
C	2.86560927093431	-0.34011157010740	0.83818139679517
H	2.48491766115395	-0.72853957537035	1.77963969223094
C	-0.87557388056593	0.07914825907629	-3.01186281972428
H	-1.46786993207960	0.95841477348466	-2.72583359664403
H	-0.42801554549562	0.29733421190181	-3.99440949023644
C	-1.75102409438538	-1.16531015056167	-3.08793091679687
H	-1.15007118607115	-2.00652733927033	-3.47351828914590
H	-2.07910259126297	-1.44490056729165	-2.07676867845223
C	-2.99408238703552	-0.96325441858396	-3.96426767642787
H	-3.61646605977553	-1.86825767457770	-3.88892574816116

H	-3.59420698694547	-0.14002703554869	-3.54155026956479
C	-2.68424797730729	-0.67880262221069	-5.43659108539904
H	-2.13550209080459	0.26553801773926	-5.56415586645933
H	-2.07142449846824	-1.48363636753539	-5.87135766644508
H	-3.60998529672980	-0.60490823310308	-6.02491914044239
C	0.59142946055876	0.87393828580096	2.76964727325199
H	1.10729229179463	1.71592124422327	2.30985966821313
C	0.55972373349424	0.69846508564701	4.14888164599737
H	1.05437412232197	1.42760018155348	4.78949294094523
C	-0.09874869956207	-0.41085255928242	4.68601103801223
H	-0.12732854691311	-0.57194465471227	5.76350558967348
C	-0.71237297930516	-1.31838633869750	3.81823316786724
H	-1.22942671773753	-2.20372672888213	4.18764982731713
C	-0.64506052761092	-1.08184055502600	2.45253664573405
C	-1.27373191846838	-1.92630938019932	1.37193673352450
H	-1.59910856489541	-2.90739215038837	1.74364947624128
C	-2.41060607964823	-1.12571907260376	0.79262397847995
C	-3.76135044251941	-1.39279143687853	0.97083150784711
H	-4.06747617139134	-2.26589397595628	1.54652894195124
C	-4.69486003686470	-0.52691158155688	0.39730578945907
H	-5.76294603148393	-0.71202666704910	0.50997379331946
C	-4.23434315850277	0.58035861526056	-0.31896288561442
H	-4.92636278583321	1.28798337853097	-0.77371092951464
C	-2.86649580208386	0.78497973545110	-0.45882328572578
H	-2.48052851475387	1.64144823034015	-1.00666078167539
C	0.83032275353136	-2.98189050893902	0.57067684728074
H	1.43775433303573	-2.57562189579757	1.38859256545877
H	0.37159472394843	-3.91472545169824	0.94139408174697
C	1.66116265114257	-3.28394664000225	-0.67071612515878
H	0.97689100411916	-3.58501739282393	-1.48184914897203
H	2.18176335608194	-2.37576429917997	-1.01138505595234
C	2.69287305384904	-4.39530632656106	-0.43727273402065
H	2.17404797339579	-5.30112508052262	-0.08147567502122
H	3.14128512594517	-4.65680983823721	-1.40823940242286

C	3.80270560040594	-4.01083522256373	0.54510405152254
H	3.40552830526851	-3.79264437167134	1.54730746894436
H	4.53491821660187	-4.82426036616247	0.64855517248696
H	4.33796379990307	-3.11522946734682	0.19620840519109

$[1C_4]^{2+}$ (DMSO, high-spin)

Charge = 2+, Spin Multiplicity = 5

Fe	-0.02234724164911	-0.02022527773309	0.00853641088570
N	2.11460011730239	-0.14833023979082	0.00240522950196
N	0.14496201314293	-0.05245531240473	2.15627053244789
N	0.35940309585888	-2.16815477883325	0.47667156435490
H	-0.45239577484518	-2.54734134511184	0.97769268826775
N	-0.51143259885355	2.06074811525880	-0.10367960471921
N	-0.21565048527570	-0.02203575737907	-2.13821064104323
N	-2.22833753009026	-0.04150629791232	-0.32941799341170
H	-2.47426103132798	-0.93827867641453	-0.76448567413083
C	2.99884638954571	0.64867414600256	-0.62260633607396
H	2.58138432570369	1.45372288064115	-1.22941181456549
C	4.37216381744195	0.45396100091591	-0.50329394995110
H	5.06136784786981	1.11765440482339	-1.02393384986326
C	4.83581173014938	-0.60402714385152	0.28274160602870
H	5.90558363937623	-0.78730906764704	0.38697683879660
C	3.91465554540678	-1.43086653657317	0.92995801370932
H	4.23595876175982	-2.26868411480439	1.54870078354390
C	2.55839016556865	-1.17014587984249	0.76541611386903
C	1.45364328229244	-1.95316530184634	1.45842884990251
H	1.85397675322729	-2.89541641684366	1.86112901224409
C	0.90172614552607	-1.09105699379445	2.57877300242043
C	1.17383072751662	-1.31473606261084	3.92448552825617
H	1.78571515332659	-2.16739529271889	4.21903702825804
C	0.64627363114710	-0.43205016584534	4.86969898327076
H	0.83739550912142	-0.58375979107565	5.93223422007430
C	-0.12935061887273	0.64416016699136	4.43285449877807
H	-0.55786508023246	1.35653310695321	5.13687374070521

C	-0.35765586677395	0.79994460115372	3.06873413541482
H	-0.96053663182941	1.62297026622211	2.68422639777427
C	0.72811689133125	-3.11354727576640	-0.60390937656027
H	1.51221286739254	-2.64166088757653	-1.21455590347602
H	1.16454625781971	-4.02498832508001	-0.16220726548231
C	-0.48536039458684	-3.45065287913271	-1.46128520849821
H	-1.22222954410260	-3.99541485397266	-0.84654162145719
H	-0.96666386468217	-2.51367904642933	-1.77789438441471
C	-0.13083345630515	-4.27401031317894	-2.70519119419255
H	-1.04091268109489	-4.38558506791258	-3.31511636726530
H	0.58355377589961	-3.70049200483386	-3.31977879327730
C	0.44600956890511	-5.65905295951796	-2.39728610140745
H	1.40959396127447	-5.59378676778833	-1.87120756545317
H	-0.24309541608109	-6.23799940146179	-1.76286049135373
H	0.61293619941048	-6.22997605115321	-3.32210487174964
C	0.15903725095190	3.10955180925430	0.40456925036558
H	1.06016278637647	2.87900085348360	0.97515362594548
C	-0.27648479511963	4.41836022917978	0.21584849909627
H	0.29001209672706	5.24535570571735	0.64216849479397
C	-1.44608290052132	4.63950576506866	-0.51579745496957
H	-1.81759430307865	5.65281181482582	-0.67107612630402
C	-2.13999812198881	3.54790985924828	-1.04268073077790
H	-3.05731889662283	3.67736708240445	-1.61700061630115
C	-1.63904203027226	2.27028698448758	-0.81623061040561
C	-2.26176064078059	1.00493141898221	-1.38404076069959
H	-3.28145965714150	1.21411081491934	-1.74078272652011
C	-1.39364866330120	0.51668857323043	-2.52887968783837
C	-1.75588865458404	0.62322639846072	-3.86749911732082
H	-2.71790878438761	1.06001496505338	-4.13573090644485
C	-0.87046033740796	0.15324823007847	-4.84003801833204
H	-1.12973181081344	0.21532432761003	-5.89717356685761
C	0.34749235824313	-0.39931956184779	-4.43720350269992
H	1.06672799838990	-0.77616755232061	-5.16352526470770
C	0.63973414182975	-0.46675660303958	-3.07797068790264

H	1.57925428573407	-0.88834036143308	-2.72020510334287
C	-3.18347413011713	0.21109063299454	0.77337678925946
H	-2.85730866617597	1.11728472507611	1.30235640297330
H	-4.18548003568626	0.41892522803895	0.35607137572178
C	-3.25010896512625	-0.98965654951730	1.71091548075137
H	-3.46599267914348	-1.88849642872887	1.10938579906483
H	-2.26472599618646	-1.14835794772748	2.17635281040366
C	-4.31849946517385	-0.83703414815654	2.80071990056699
H	-5.29770516415072	-0.66486346523880	2.32283192864046
H	-4.40268143440183	-1.79358872332578	3.33987904127674
C	-4.02726650666560	0.28299132266122	3.80350121329335
H	-3.97638249295102	1.26733025798609	3.31547993492926
H	-4.81011915308021	0.33468616781676	4.57383556808631
H	-3.06570673808744	0.11383025763335	4.31105124909820

$[1C_4]^{2+}$ (acetonitrile, low-spin)

Charge = 2+, Spin Multiplicity = 1

Fe	-0.00272558101375	-0.00085239914388	0.00509100846130
N	0.02520616834171	1.89520368005929	-0.32777297122170
N	1.95319294114018	0.03228178747542	-0.08600418081547
N	0.22830407947207	-0.08868034411655	-2.03000227333796
H	0.69217499408654	-0.97842900171806	-2.25200691107410
N	-0.00653278922571	0.00024339642248	1.92972019915291
N	-1.95900711175898	-0.06241173950464	0.07432453521852
N	-0.26044128647136	-2.01696560381363	0.26981244819364
H	-0.74937981399542	-2.37957647851255	-0.55835529448624
C	-0.54797978480798	2.88314898692218	0.39483456988312
H	-1.06215012189677	2.58217083134536	1.30660270379726
C	-0.49332831529253	4.21142446390443	-0.01361611263721
H	-0.96707229642338	4.97706013427850	0.59963108197027
C	0.16184595330423	4.53813286527258	-1.20403064353427
H	0.20831500338713	5.57170575831226	-1.54663916937404
C	0.74867236208298	3.51649681484000	-1.95563138356959
H	1.26177380688801	3.72009114381986	-2.89531776671231

C	0.66055286436881	2.21285178911357	-1.48874253604255
C	1.26135027129104	0.99178654717516	-2.14148069428891
H	1.57933690754310	1.18451965071579	-3.17525866606678
C	2.40027214939619	0.54443685271920	-1.26428655348979
C	3.74934854495546	0.66537192304229	-1.56854454051982
H	4.05005232307861	1.07125339449753	-2.53407442323650
C	4.68766274039907	0.26072888641653	-0.61685512696833
H	5.75480812361615	0.33587160627361	-0.82491858211192
C	4.23233647972216	-0.23794380701388	0.60577664231212
H	4.92730987097819	-0.55567658863630	1.38182459341905
C	2.86558801320594	-0.34010706180213	0.83839462060203
H	2.48479592376878	-0.72851322094996	1.77982567843718
C	-0.87545781209543	0.07898680855891	-3.01173978152560
H	-1.46781339692647	0.95824343137315	-2.72579395256151
H	-0.42802675534102	0.29705307490092	-3.99437502958678
C	-1.75078235710494	-1.16558060399369	-3.08752797828916
H	-1.14971719543631	-2.00685336979108	-3.47285442641582
H	-2.07892984343872	-1.44484316989780	-2.07627987661012
C	-2.99378032872997	-0.96401809948942	-3.96407951436931
H	-3.61592672495857	-1.86916246656459	-3.88859949357100
H	-3.59420947013384	-0.14088287681813	-3.54161241241656
C	-2.68385356625450	-0.67983018328005	-5.43642018604309
H	-2.13555290797965	0.26473226717760	-5.56425458957675
H	-2.07068565034260	-1.48452288724914	-5.87094559518394
H	-3.60954640342494	-0.60650741991383	-6.02485764748442
C	0.59136290706890	0.87401673859902	2.76986778785783
H	1.10721388897020	1.71602729774536	2.31011259295859
C	0.55964685094963	0.69850119249844	4.14909720942585
H	1.05425482240085	1.42761281770365	4.78976568665267
C	-0.09882135263215	-0.41083826703805	4.68617666527566
H	-0.12743321721180	-0.57195617595620	5.76366283437707
C	-0.71242861350319	-1.31834164901311	3.81835073516326
H	-1.22948475682683	-2.20366333091979	4.18781295911300
C	-0.64510685735507	-1.08175294205664	2.45266061387758

C	-1.27385108512438	-1.92613866972983	1.37202521667007
H	-1.59924279361117	-2.90723129522940	1.74372760655504
C	-2.41072520403585	-1.12551927275328	0.79270201728304
C	-3.76148478183201	-1.39254466718991	0.97086004494845
H	-4.06774224264235	-2.26561367269542	1.54654150537008
C	-4.69495745506360	-0.52662844489986	0.39731693745095
H	-5.76304947006178	-0.71169591742189	0.50997161083699
C	-4.23438677256846	0.58062532011377	-0.31893528499108
H	-4.92640006079856	1.28826727291200	-0.77366479887185
C	-2.86652689194463	0.78519170855251	-0.45875150232952
H	-2.48047321342409	1.64164516834216	-1.00655815274830
C	0.83016659108911	-2.98182765047748	0.57035933529721
H	1.43780354025319	-2.57565659360096	1.38817419807179
H	0.37155971811509	-3.91472683683966	0.94107066271368
C	1.66078011625570	-3.28367589573718	-0.67124761206697
H	0.97637734775088	-3.58469404106186	-1.48230869921716
H	2.18125924435588	-2.37536395847291	-1.01180472648386
C	2.69260784211785	-4.39502661261075	-0.43823557327293
H	2.17388387600215	-5.30102339488742	-0.08277099487985
H	3.14096772201045	-4.65616767733436	-1.40931155989456
C	3.80246230569164	-4.01084024392608	0.54420279238722
H	3.40542100007714	-3.79323044682003	1.54658953756184
H	4.53476044005725	-4.82422331062987	0.64718891002041
H	4.33764224549648	-3.11504863157230	0.19566565456195

$[1C_4]^{3+}$ (DMSO, low-spin)

Charge = 3+, Spin Multiplicity = 2

Fe	-0.01335775523439	0.01735735510606	0.02006750927002
N	0.02278755060980	1.94077886688130	-0.32009382098107
N	1.96638410677577	0.06558323478481	-0.08462617619178
N	0.22472911907118	-0.07616062157795	-2.00171724993875
H	0.69032344797925	-0.96924757226607	-2.21090834438318
N	-0.00884601086649	-0.00466420813360	1.97357575828477
N	-1.99181877003724	-0.03723646099326	0.11944201036724

N	-0.29456485483302	-1.98769901565311	0.26005771781447
H	-0.79383785331918	-2.33338566382153	-0.57094810418953
C	-0.54661614887682	2.91949029395091	0.41229997116719
H	-1.06406126388341	2.62033178329306	1.32268731948025
C	-0.47633235358784	4.24623422811172	0.00516667869103
H	-0.93610145334463	5.01740442456339	0.62107436115177
C	0.17318792629133	4.56033490379438	-1.19093376463545
H	0.22689418494382	5.59370955555855	-1.53337778443113
C	0.74491759168832	3.53837850026198	-1.95400939136693
H	1.24930140676446	3.73950597121546	-2.89829749410311
C	0.65294282502358	2.23802498142228	-1.48490602905306
C	1.24981596575296	1.01189211501271	-2.13321528834162
H	1.54655126671501	1.18831779732841	-3.17451100777586
C	2.39896465774159	0.57416617239524	-1.26549050411081
C	3.74456805643708	0.69425759550250	-1.57546341561020
H	4.04206324123942	1.10362620988729	-2.53996661833142
C	4.68338463301439	0.28153139621795	-0.62735160905829
H	5.74946581519807	0.35636604208747	-0.84040710942445
C	4.23733671597326	-0.22277757455756	0.59379335378366
H	4.93497415691780	-0.54691263977699	1.36419212871573
C	2.87138819316724	-0.31951762455902	0.83736346037393
H	2.49768080992465	-0.71302596515990	1.77915167655974
C	-0.89258825706982	0.06310927749269	-2.98336212521629
H	-1.48230867913835	0.95200214747518	-2.72667425390647
H	-0.42712865062161	0.25682750328949	-3.96171668223823
C	-1.75966256994675	-1.18622739725954	-3.04487297353869
H	-1.13496517428797	-2.04308376536583	-3.34932329768699
H	-2.16069603704805	-1.41741321713778	-2.04795104758943
C	-2.94157890338338	-1.02926446022143	-4.01144530264442
H	-3.57178850619942	-1.92669322272005	-3.91902216077722
H	-3.56258643157091	-0.18006150945485	-3.68054905186470
C	-2.53463994094639	-0.84026922319097	-5.47515381274564
H	-1.97823624266109	0.09540993816767	-5.63064711829974
H	-1.89757979552992	-1.67084221853501	-5.81603145705134

H	-3.42124312327640	-0.80704526718500	-6.12395605064576
C	0.60188319488836	0.86248781196474	2.80625433744794
H	1.12097988847595	1.70505333791060	2.35177365523950
C	0.56940083880317	0.67227446267510	4.18227301050483
H	1.06415918791671	1.39319589444208	4.83100785429063
C	-0.08795983143690	-0.44511985399116	4.70211113951556
H	-0.11235193647224	-0.61867892234219	5.77784784350091
C	-0.70573605233239	-1.34806478608819	3.83220594671601
H	-1.21799032797350	-2.23793061147105	4.19562452741527
C	-0.64744990980382	-1.09366675439243	2.47132364177855
C	-1.29131934896350	-1.91571146008924	1.38127242876895
H	-1.60481296478039	-2.90741337512286	1.72977219432976
C	-2.43437781017728	-1.10290153661981	0.83258379162110
C	-3.78291917778358	-1.35985090710045	1.02488667957275
H	-4.08987095881986	-2.23140880648184	1.60155474995033
C	-4.71253415578698	-0.48221610302033	0.46210780115946
H	-5.78055289783893	-0.65822579475401	0.58807531217707
C	-4.25540121166372	0.62008568276653	-0.25960649976575
H	-4.94617353299240	1.33243851500956	-0.70777993786489
C	-2.88739418710886	0.81917902270164	-0.41221256291432
H	-2.50481273188658	1.67159039653859	-0.96828381566164
C	0.80738250048535	-2.96140605664906	0.52550734742303
H	1.41435401010257	-2.58492370687673	1.35690245936672
H	0.33123350328667	-3.89394172693299	0.87087474781000
C	1.63146044414374	-3.24328366657397	-0.72408061250066
H	0.94393687893190	-3.51594313120657	-1.54190486393017
H	2.17381408474932	-2.33990262252480	-1.04385600739127
C	2.64501893284907	-4.37583307512573	-0.50893859521338
H	2.11072740109976	-5.27649267429191	-0.16438112140983
H	3.08251905379354	-4.62917113495933	-1.48647077217915
C	3.76548678382024	-4.02237516611843	0.47250414927852
H	3.37902612580932	-3.81043344048962	1.48024267232355
H	4.48280827748256	-4.85032940629209	0.56118299523818
H	4.31639873161682	-3.13329638072512	0.13095658187421

$[1C_4]^{3+}$ (DMSO, high-spin)

Charge = 3+, Spin Multiplicity = 6

Fe	-0.00336790523539	-0.02934144384842	-0.01091148749973
N	-0.03752939913776	2.01986866564832	-0.50679154061790
N	2.13120856316564	0.09025500234029	-0.16981162555486
N	0.34202307391968	-0.07054998563145	-2.18399590214327
H	0.81794020924611	-0.94213793201204	-2.45188384073032
N	0.06996167949713	-0.16100698884147	2.08941696430147
N	-2.13736891612135	-0.12606302995615	0.16747881452635
N	-0.38787100624300	-2.17027517535805	0.33250683909673
H	-0.89266537581329	-2.56506887470842	-0.47090228366304
C	-0.61970796831231	3.02902331098857	0.16896700277014
H	-1.18633367877822	2.75908701437952	1.06070835229145
C	-0.49792650352425	4.34609595643231	-0.26027731144021
H	-0.97784614216343	5.14310436839280	0.30548601912288
C	0.23622788658260	4.61408030716962	-1.41756615126576
H	0.33792310982671	5.63689705405648	-1.78075326882317
C	0.83928615218777	3.56138045701918	-2.11242504308002
H	1.42091854629643	3.73118952095408	-3.01792104860424
C	0.68161777058136	2.27222051735930	-1.62558093676757
C	1.33371600831103	1.04242895242608	-2.23161523700146
H	1.67057599132808	1.24774372686602	-3.25702391291536
C	2.49867934676665	0.64328645583098	-1.35030715492974
C	3.82998987221894	0.84565640887699	-1.68393600806036
H	4.08735484776009	1.28830716363915	-2.64563178899758
C	4.81206348033164	0.46711732806377	-0.76430122320255
H	5.86666700198931	0.61145312394744	-0.99927091855803
C	4.42922351334414	-0.09858752766395	0.45253905094997
H	5.16566424724472	-0.40723215854053	1.19271432839386
C	3.07557074344001	-0.27438907569793	0.71802022871243
H	2.73509609898834	-0.72235126912265	1.65001450690913
C	-0.80186419916583	0.13969978127167	-3.11520813144240
H	-1.38126100298372	1.00434153090451	-2.76294527252666

H	-0.38601618382400	0.41034776100076	-4.09891310589069
C	-1.68144646928209	-1.09826111529086	-3.22148869673852
H	-1.09205095676186	-1.92795428435989	-3.64574985856301
H	-1.99988754957681	-1.41173928233086	-2.21700154448168
C	-2.93558556192549	-0.85034195512673	-4.07065270760057
H	-3.56385410138850	-1.75265436593969	-4.01862418793816
H	-3.52119722194432	-0.03859953419157	-3.60734191835086
C	-2.64548061693584	-0.51445594551268	-5.53604517013991
H	-2.09438256966795	0.43162254584321	-5.63837677546512
H	-2.04368010462397	-1.30615069836816	-6.00834899653383
H	-3.57988360984272	-0.41513511116804	-6.10631775478168
C	0.68659614903816	0.66924596065159	2.95221305155752
H	1.25994412301082	1.48991895560481	2.51930799811136
C	0.58920981453938	0.47923109122661	4.32621042978035
H	1.09745236296532	1.16535625917874	5.00182249877615
C	-0.15792099713816	-0.59786765881266	4.80757500968124
H	-0.24071398287391	-0.77490330080321	5.88001508290180
C	-0.79813964115274	-1.45308359506288	3.90565140923368
H	-1.38946002586117	-2.30314943607198	4.24440163250761
C	-0.66312500324069	-1.20257568940620	2.54787854703431
C	-1.35390027166210	-2.00124817775414	1.45714487875148
H	-1.70328805855843	-2.96729074301774	1.84593155162320
C	-2.51328711797924	-1.18388645747218	0.92480542505592
C	-3.84691658242242	-1.46225924950261	1.18692867435636
H	-4.11094210824686	-2.32391705736715	1.79909262207995
C	-4.82160047651014	-0.61978243979686	0.64459526415236
H	-5.87798336827508	-0.81610900715032	0.82829380118318
C	-4.42991965154482	0.47013585300335	-0.13439202118434
H	-5.16116041926000	1.14706604767371	-0.57322895501601
C	-3.07417622647901	0.69064874635217	-0.35122678347516
H	-2.72348072766352	1.52999397603234	-0.94942830726866
C	0.73063679803754	-3.09634516647041	0.66593194842704
H	1.31920088375277	-2.64313772402819	1.47365038576710
H	0.29131988332676	-4.02607248239936	1.06652329288322

C	1.57981284605325	-3.40861713685786	-0.55865845563920
H	0.91767750470144	-3.76653955255410	-1.36385810505040
H	2.06595984145657	-2.49099973874448	-0.92529301980999
C	2.65590000662555	-4.46448347170812	-0.27033012331963
H	2.17358594222890	-5.37021529693286	0.13321604934712
H	3.11165187059771	-4.75722515171930	-1.22855136846590
C	3.75143381542849	-3.98440349132550	0.68543334814423
H	3.34694132629611	-3.70991431270612	1.67070561248551
H	4.50535420163818	-4.76831033142862	0.84437064706618
H	4.26489188739707	-3.10127473037189	0.27661065355632

***trans*-[1C$_4$]$^{2+}$ (DMSO, low-spin)**

Charge = 2+, Spin Multiplicity = 1

Fe	0.13308523438603	-0.04360095748709	-0.07016363385542
N	2.08601348425836	-0.10556443498499	0.15529639608228
N	-0.10584476709564	-0.11204097532305	1.87892414016788
N	0.36963700724150	-2.05383147202547	0.26831421647258
H	-0.51628615872248	-2.40518677275814	0.64993781285290
N	0.41147959296332	0.16333927639216	-2.00930132246539
N	-1.80709889009305	-0.12642303141829	-0.35597991843321
N	-0.29728329318261	1.95419529739128	-0.25665586309750
H	-0.92017314663037	2.20570775571251	0.51936938199701
C	3.04153061209663	0.65039694011886	-0.42770525971144
H	2.70179060636111	1.45095872796776	-1.07779069327090
C	4.39793380401003	0.41894547372251	-0.22915795328972
H	5.12368264589735	1.06553647943157	-0.72056320257362
C	4.80171113337309	-0.63506236143156	0.59212300673670
H	5.85903338789403	-0.83695918935397	0.76254756447960
C	3.82109239880304	-1.44362272805033	1.17102086342597
H	4.07850416534930	-2.30002169941299	1.79389830383490
C	2.48675256129129	-1.15577453769850	0.92131386811494
C	1.31684149131062	-1.95271043396283	1.42865884534811
H	1.62274285965056	-2.93165255473560	1.82272849806897
C	0.58362696314572	-1.13201065316898	2.45327551966742

C	0.58812573329107	-1.36551475039297	3.82219632156361
H	1.16121218031351	-2.20022064901785	4.22514638840076
C	-0.16088849634799	-0.52328550931567	4.64544662257851
H	-0.18128665029511	-0.67758840478661	5.72414712376979
C	-0.90104127485077	0.50515251385051	4.05709916479819
H	-1.51752976275640	1.17377180196608	4.65638258355681
C	-0.85805093797894	0.67621749775487	2.67831377770782
H	-1.45039176028100	1.45582465200116	2.20307531287120
C	0.80048626734264	-3.05071780758844	-0.74640241905151
H	1.75218543147294	-2.71603583245266	-1.18045281762055
H	1.00643757628030	-4.00103366929280	-0.22848379673117
C	-0.27833277060239	-3.23298268393637	-1.80750289988826
H	-1.16320464645620	-3.69494899789134	-1.33671736309208
H	-0.59757655202717	-2.24463073234574	-2.16804581231969
C	0.18057907815383	-4.08692378567536	-2.99484060504267
H	-0.62570882132108	-4.09055551292143	-3.74470724009101
H	1.04515829643611	-3.59823168525186	-3.47505447280115
C	0.54006723397802	-5.52923913526701	-2.62676313382295
H	1.40846750684170	-5.57582137909546	-1.95336315451870
H	-0.30229642559443	-6.02644543812903	-2.12121629550196
H	0.78699077081772	-6.11388525394841	-3.52453881717179
C	1.26227578397387	-0.48722860929296	-2.83354691102308
H	1.86091406796174	-1.27916279763202	-2.39343545665037
C	1.38424463608436	-0.16670331901617	-4.18077462082204
H	2.07950091110673	-0.73286186254647	-4.79924404617626
C	0.61854880466711	0.87335015550535	-4.71135595927975
H	0.69905883480890	1.14585468264178	-5.76356942410838
C	-0.23770487577991	1.57375961101285	-3.85936152506619
H	-0.83690283126973	2.41294017286601	-4.21198085495072
C	-0.30750654288852	1.19596541607992	-2.52572145359597
C	-1.16216671578745	1.85794984334395	-1.48012666665375
H	-1.54724438245709	2.83094166466970	-1.81480891843710
C	-2.26761580399099	0.91138147297723	-1.10163018033446
C	-3.60289426469632	1.05243738296207	-1.45666360050352

H	-3.91379728519619	1.90627916678942	-2.05815941863960
C	-4.51587747257031	0.09283463959855	-1.01603286868075
H	-5.57174292994514	0.17282329836504	-1.27417815778415
C	-4.05357631705118	-0.95860382997471	-0.22056895752982
H	-4.73205043364073	-1.71983045910734	0.16300429753127
C	-2.70217895873435	-1.03326319147392	0.09528637783089
H	-2.33065249636994	-1.83059955327259	0.73659723088043
C	0.69830300439120	3.05394249918158	-0.34459218434128
H	1.40038116407401	2.81933408818946	-1.15389307031292
H	0.17046513170539	3.97647542519949	-0.64151868904430
C	1.38844123543811	3.26560636132227	0.99706540296458
H	0.60898301755517	3.45188617765636	1.75463479843164
H	1.90775469023090	2.34414461531576	1.30250194446093
C	2.36769468046533	4.44681744769126	0.98570586503467
H	1.83714947308163	5.34993176622023	0.64006229672544
H	2.67487664725562	4.64900105243233	2.02350178921363
C	3.61513188857034	4.21779742250303	0.12785899171618
H	3.36070747944464	4.03448441060205	-0.92649431185262
H	4.27968796297928	5.09304275124316	0.15936501643960
H	4.18520909785928	3.34969258575893	0.49043449741258

***trans*-[1C$_4$]$^{2+}$ (DMSO, high-spin)**

Charge = 2+, Spin Multiplicity = 5

Fe	0.13244473776919	-0.04513074137670	-0.07830231578666
N	2.25755252338665	-0.25708365304065	0.18726433503220
N	-0.03573353195716	-0.12637306375480	2.08987091319060
N	0.39354472811415	-2.18977913735121	0.43593589619270
H	-0.47471451867653	-2.56460800761360	0.83296482423587
N	0.38803316885395	0.32174674965624	-2.18392301483353
N	-2.00300419797693	-0.10499676174605	-0.48021905885662
N	-0.46289253929383	2.08488657659854	-0.30551404166747
H	-1.10072260583485	2.34762024030593	0.45400564530776
C	3.25262669786634	0.46819205610074	-0.35488095828176
H	2.95990342074961	1.25808795903464	-1.04657905233619

C	4.59050848512597	0.22140200158094	-0.06178538428626
H	5.36595693502949	0.83374350876215	-0.52033244049062
C	4.90813123554875	-0.81824671551118	0.81520079932476
H	5.94738981381229	-1.03918752110441	1.05977850577416
C	3.87660207637766	-1.58416084800163	1.36283665872220
H	4.07960522503303	-2.41620737265966	2.03709627398970
C	2.56484133090748	-1.27504584814599	1.02040955795168
C	1.35678909761956	-2.02040069708391	1.55635772233901
H	1.66818543357010	-2.98008254575175	1.99491415990367
C	0.67375634269415	-1.15833986834015	2.60005458052596
C	0.78012397826400	-1.38703430781551	3.96875256182697
H	1.36157598209865	-2.23411372588008	4.33304153963095
C	0.12374203821590	-0.52122958821837	4.84479084805245
H	0.18492365803725	-0.67586888587909	5.92225521489029
C	-0.62188246069580	0.53654670034940	4.31857079012714
H	-1.15823657619596	1.22924824063912	4.96611819435496
C	-0.67933723560523	0.69727304770094	2.93727336812977
H	-1.25860087903689	1.50557483381786	2.49090426456517
C	0.85590430673102	-3.11390659451452	-0.62602822988360
H	1.77275635406606	-2.69451702254701	-1.06679612567522
H	1.12552148665466	-4.08435104658593	-0.17812071770697
C	-0.22394285822673	-3.27382374026364	-1.69056723874533
H	-1.10915450565029	-3.75184303912539	-1.23694943106028
H	-0.54398977796268	-2.27340525268354	-2.02179227187268
C	0.23824838760636	-4.08741583477567	-2.90477700580880
H	-0.56222164158320	-4.06091506116494	-3.66043516374596
H	1.10906718322688	-3.58720380525402	-3.36144956766112
C	0.58686790270876	-5.54424903507425	-2.58613326962545
H	1.44716267663770	-5.62046254710002	-1.90529411209752
H	-0.26366597844217	-6.05564738345501	-2.10922146026441
H	0.84106447806707	-6.09691763296647	-3.50213910162121
C	1.19503106184989	-0.30263970463263	-3.06217861568583
H	1.82503820723187	-1.09935574243849	-2.66657896771668
C	1.23208409107241	0.04716060480642	-4.40844137879120

H	1.89678455178990	-0.48648880777420	-5.08663736607293
C	0.41432825044446	1.08650678062190	-4.85846914834222
H	0.42753083528573	1.38847323647323	-5.90606984592362
C	-0.41322662489886	1.74349056661043	-3.94569765195343
H	-1.05942675772138	2.56651749887339	-4.25061110005741
C	-0.39682356392293	1.33217735366906	-2.61718319318396
C	-1.27812458571992	1.93649348169065	-1.53989779157529
H	-1.69767403679835	2.89224721968820	-1.88745423702624
C	-2.39069241359077	0.95611534950710	-1.22379416721006
C	-3.69520264460706	1.10817165532629	-1.68434637444491
H	-3.96039023205571	1.98040938122397	-2.28189480374331
C	-4.63756594741184	0.13145025640012	-1.35936447642782
H	-5.66822138855251	0.22340885093857	-1.70271665748290
C	-4.24155896477648	-0.95872034389646	-0.58048106051074
H	-4.94707448440183	-1.73928205512391	-0.29779010267187
C	-2.91766277639248	-1.03876258209905	-0.15893061247097
H	-2.57205069458056	-1.87107625384967	0.45432441474917
C	0.58853260242333	3.12418638059591	-0.40341830241794
H	1.29659424638154	2.81261419045399	-1.18376997561658
H	0.13878334020349	4.07755668913331	-0.73298271801982
C	1.27838681448031	3.30504425733715	0.94439152379115
H	0.50716878634934	3.52932095799261	1.69980462452432
H	1.74783616877194	2.35477815576738	1.24817076835178
C	2.32320607292340	4.42811128113175	0.94061384142494
H	1.84778526651986	5.35977246808914	0.59051578889273
H	2.63452469748779	4.61359652944125	1.98041525518974
C	3.56112728396568	4.12550879385296	0.09197643716631
H	3.30412072775736	3.95798231216678	-0.96438361593752
H	4.27825732991487	4.95797293710658	0.12959167983002
H	4.07343527294299	3.22342754615491	0.45830140860282

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