## Supporting Information for:

# Above Room Temperature Spin Transition in a Metallo-supramolecular Coordination Oligomer/Polymer

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## *1. General experimental methods:*

1,4-phenyldiboronicacid, and $Pd(PPh_3)_4$ were obtained from Aldrich. $Fe(BF_4)_2$ hydrate was purchased from Aldrich and used as received. 1,4-Dioxane, dichloromethane and methanol solvents were used as received without any further purification.$^1$H and $^{13}$C NMR spectroscopic data were recorded on a Bruker DPX 300 spectrometer with solvent proton as internal standard. Infrared spectra were recorded using KBr pressed pellets on Perkin Elmer Spectrum GX FT-IR spectrometer. MALDI-TOF MS data were acquired with a Voyager-DE PRO Bio spectrometry work station. Elemental analyses were carried out on a Vario MICRO cube. ESI-MS analyses were performed on a BRUKER - DALTONICS FT-ICR mass spectrometer.

## *2. Magnetic susceptibility:*

Temperature dependent static susceptibilities of complex **1** were recorded using MPMS-5S (Quantum Design) SQUID magnetometer over a temperature range of 4.5 ↔ 380 K (both cooling and warming mode) in a homogeneous 1000 Oe external magnetic field. The magnetic field dependence of the molar magnetic susceptibility $\chi$ was not found. Gelatin capsules were used as sample containers for measurements taken in the temperature range of 4.5 ↔ 380 K. The very small diamagnetic contribution of the gelatin capsule had a negligible contribution to the overall magnetization, which was dominated by the sample. The magnetic measurement was performed in the temperature range of 4.5 ↔ 380 K at 2 K/min heating and cooling rate. The diamagnetic corrections of the molar magnetic susceptibilities were applied using well-known Pascal's constants. The high spin mol fraction [$n_{HS} = (\chi_M T)/(\chi T)_{HS}$] was calculated by taking the value of $(\chi T)_{HS}$ as 3.5 emu K mol$^{-1}$.

### *3. Single Crystal X-ray diffraction:*

X-ray data collection was performed on a STOE IPDS II diffractometer with graphite monochromated Mo Kα radiation at 200 K. The structure was solved by direct methods (SHELX-97). Refinement was done with anisotropic temperature factors for all non-hydrogen atoms.

### *4. Mössbauer studies:*

The Mössbauer spectral absorber contained *ca*. 50 mg/cm$^2$ of complex **1**, and the spectra were measured between in the temperature range of 182–300 K on a constant-acceleration spectrometer that utilized a room-temperature rhodium matrix cobalt-57 source and was calibrated at room temperature with alpha-iron foil.

***Figure S1.*** *FTIR Spectra of ligand* ***L*** *and iron(II) chain* **1**

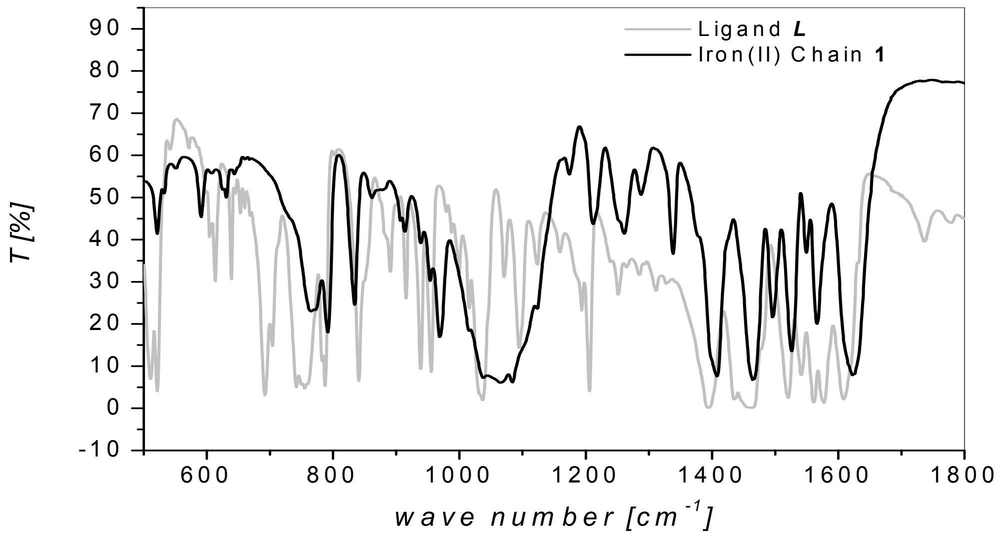


***Figure S2.*** *$^1$H-NMR Spectrum of **L***

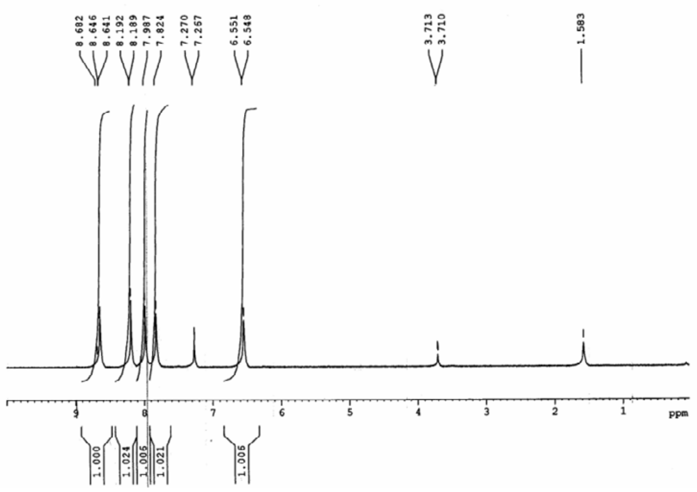
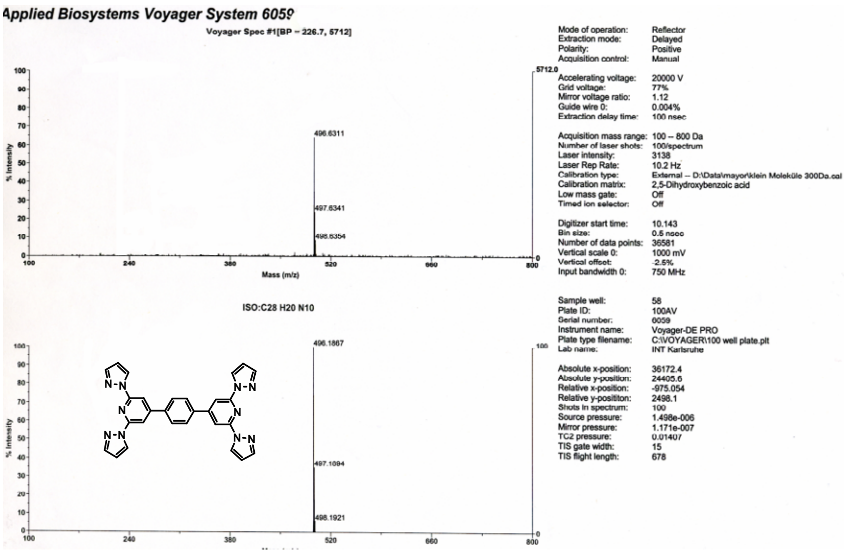


***Figure S3.*** *MALDI-TOF MS data of **L***



```
Mode of operation:        Reflector
Extraction mode:          Delayed
Polarity:                 Positive
Acquisition control:      Manual

Accelerating voltage:     20000 V
Grid voltage:             77%
Mirror voltage ratio:     1.12
Guide wire 0:             0.004%
Extraction delay time:    100 nsec

Acquisition mass range:   100 -- 800 Da
Number of laser shots:    100/spectrum
Laser intensity:          3138
Laser Rep Rate:           10.2 Hz
Calibration type:         External -- D:\Data\mayor\klein Moleküle 300Da.cal
Calibration matrix:       2,5-Dihydroxybenzoic acid
Low mass gate:            Off
Timed ion selector:       Off

Digitizer start time:     10.143
Bin size:                 0.5 nsec
Number of data points:    36581
Vertical scale 0:         1000 mV
Vertical offset:          -2.5%
Input bandwidth 0:        750 MHz

Sample well:              58
Plate ID:                 100AV
Serial number:            6059
Instrument name:          Voyager-DE PRO
Plate type filename:      C:\VOYAGER\100 well plate.plt
Lab name:                 INT Karlsruhe

Absolute x-position:      36172.4
Absolute y-position:      24405.6
Relative x-position:      -975.054
Relative y-posititon:     2498.1
Shots in spectrum:        100
Source pressure:          1.498e-006
Mirror pressure:          1.171e-007
TC2 pressure:             0.01407
TIS gate width:           15
TIS flight length:        678
```

***Figure S4.*** *FT-ICR Spectrum of* ***1*** *in (MeOH/DMF/$CH_3CN$). Inset show the calculated spectra (blue line) and the experimentally observed doubly charged (black line) high molecular weight peaks.*

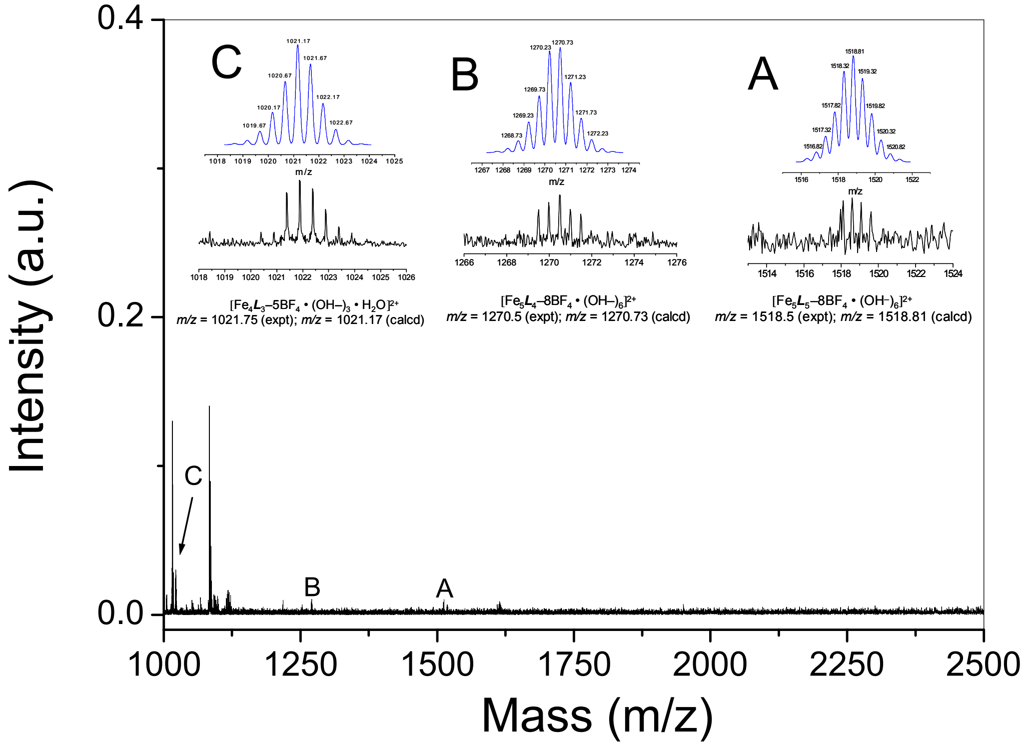


***Figure S4.*** *FT-ICR Spectrum of **1** in (MeOH/DMF/$CH_3CN$). Inset show the calculated spectra (blue line) and the experimentally observed doubly charged (black line) high molecular weight peaks.*