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Supporting information for article:

A synchrotron study of [5,10,15,20-tetrakis(3-cyanophenyl)porphyrinato-κ^4*N*^{5},*N*^{10},*N*^{15},*N*^{20}]copper(II) nitrobenzene trisolvate at 80 K

Dedicated to Professor Wolfgang Seidel on the occasion of his 85th birthday.

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Supporting information for 5,10,15,20-tetra(3-cyanophenyl)porphyrinatocopper(II) nitrobenzene trisolvate at 80 K: a synchrotron study

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1. Electronic spectrum and IR spectrum of CuTCNPP

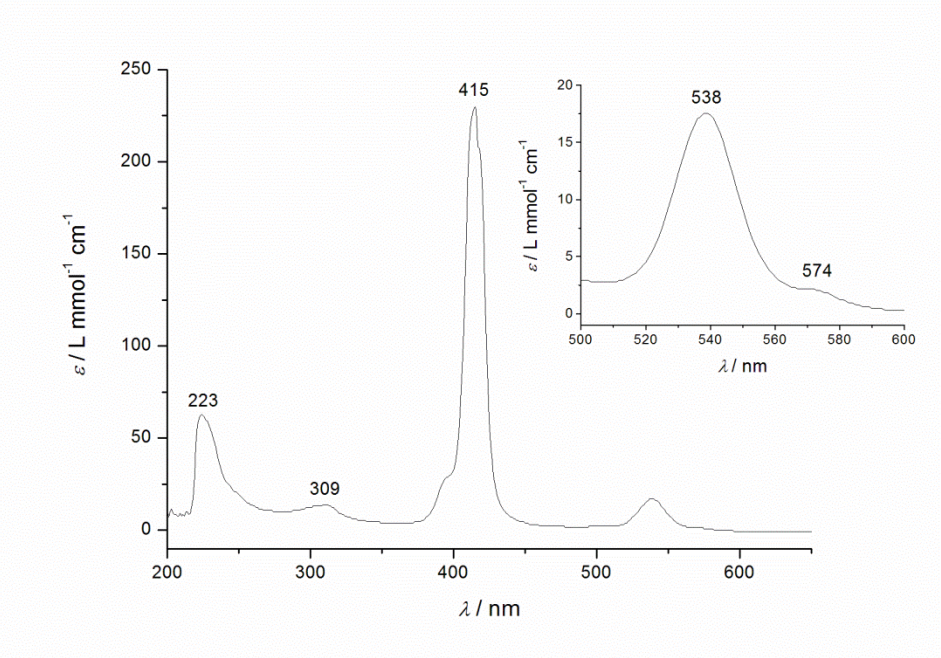

Figure S1 Electronic spectrum of CuTCNPP in dichloromethane (64.4 μM). The inset shows the Q band region. The spectrum was measured in a 2 mm quartz glass cuvette (1 cm for the inset spectrum).

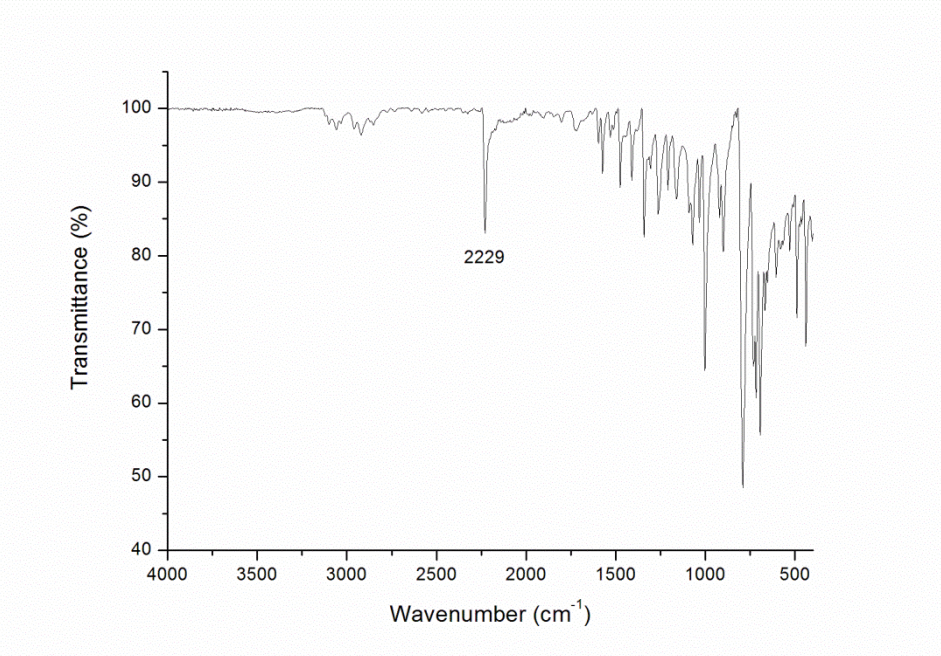

Figure S2 IR spectrum of CuTCNPP. The band at 2229 cm^{-1} can be assigned to the stretching vibration of the cyano groups.

2. Purification of CuTCNPP for spectroscopy

For UV/Vis and IR spectroscopic analyses, a small amount of the product was purified by semi-preparative HPLC, using a Shimadzu LC-20AP pump with a Shimadzu FRC-10 A fraction collector, a YMC-Actus-Pro C18, 150 *x* 20 mm i.d. HPLC column, acetonitrile (90%) / water (10%) mobile phase, 20.0 ml min^{-1} flow rate and UV (220 nm) flow detector. The product fraction was collected and the solvents were removed under reduced pressure by rotary evaporation. The final product used for spectroscopy (purity 99.7 area %) was analysed using an analytical HPLC system with an Eclipse Plus 1.8 µm C18 column, 50 *x* 4.6 mm i.d., acetonitrile (90%) / water (10%) mobile phase, 1 ml min^{-1} flow rate and UV (220 nm) flow detector.