Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Spin-Induced Electron Transmission through Metal-Organic Chiral Crystals

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**Materials and methods**: All the chemicals including amino acids were purchased from Sigma Aldrich (purity > 98%). Water was processed using a Millipore purification system (Biological Industries, Beit Haemeck, Israel) with a minimum resistivity of 18.2 MΩ cm.

**Crystal preparation and data collection for the Co(II)-Phe crystal:**

The Co(II)-Phe crystal suitable for SCXRD was immersed in Paratone–N oil, mounted in a MiTeGen loop and flash-frozen in liquid nitrogen at 100 K. The Data was collected with a Rigaku XtaLab Synergy R rotating anode source and a HyPix-Arc 150 detector using CuKα radiation (1.54184 Å). The Data was collected as ω scans using 'CrysAlisPro 1.171.41.111a (Rigaku OD, 2021)'. Data were integrated and reduced in CrysAlisPro. The structure was solved by direct methods (SHELXT-2018)[1] and refined by full-matrix least-squares methods against $F^2$ (SHELXL-2013)[2] as implemented in Olex2 (Dolomanov 2016).[3] The Mercury 2020.3.0 software was used for molecular graphics.

**Table S1**. Crystallographic data collection and refinement statistics for Co(II)-Phe crystal.

| **Compound** | **Co(II)-Phe** |
|---|---|
| CCDC number | 2283838 |
| Crystal description | Pink colour plate |
| Diffractometer | Rigaku XtaLab Synergy R |
| Temperature (K) | 100 |
| Chemical formula | $C_{18}H_{24}CoN_2O_6$ |
| Formula weight (g/mol) | 423.32 |
| Wavelength (Å) | 1.54184 |
| Crystal system | Monoclinic |
| Space group | $P12_11$ |
| a (Å) | 4.8214 (2) |
| b (Å) | 32.8351 (12) |
| c (Å) | 6.0176 (2) |
| α (°) | 90 |
| β (°) | 105.571 (4) |
| γ (°) | 90 |
| Volume ($Å^3$) | 917.68 (6) |
| Z | 2 |
| $\rho_{calc}$ ($g/cm^3$) | 1.532 |
| μ ($mm^{-1}$) | 7.672 |
| F(000) | 442.0 |
| 2θ range for data collection (°) | 9.998 to 149.504 |
| Index ranges | $-6 \leq h \leq 6$, $-41 \leq k \leq 41$, $-7 \leq l \leq 7$ |
| Data/restraints/parameters | 3645/0/257 |
| Goodness-of-fit on $F^2$ | 1.053 |
| Final R indexes [I>=2σ (I)] | $R_1 = 0.0388$, $wR_2 = 0.0946$ |

**Superconducting Quantum Interference Device (SQUID) Measurements:**

For a paramagnet containing identical ions with a partially filled electron shell, the following expression for the Curie constant is known (eq.31.49 in [12]).

$$C = \frac{N_A \mu_B^2}{3k_B} g_{(JLS)}^2 [J(J+1)] \qquad (1s) ,$$

where $N_A$ is the Avogadro number, $\mu_B$ is the Bohr magneton, $k_B$ is the Boltzmann constant, $g_{(JLS)}$ is the Lande factor, and $J$, $L$, and $S$ are the total, orbital, and spin quantum numbers, respectively. For $Co^{2+}$ ions, we assumed here that $L$ =0 and therefore that $J$ =$S$=3/2 and $g$ =2, since for transition metal ions of the iron group we can usually neglect the spin-orbit coupling in comparison with the effect of the crystal field on their outer d-electrons.

**Magnetic Conductive Atomic Force Microscopy (mc-AFM):** For the samples for the mc-AFM measurement, the substrate surfaces were prepared by evaporating an 8 nm Ti adhesive layer, followed by a 100 nm layer of nickel and an 8 nm layer of gold on top of a $Si/SiO_2$ wafer with a 2 μm thermal silicon oxide layer. The magnetic field was used to enable field-induced electron spin injections from the surface to the crystal by magnetizing the Ni/Au surface. Prior to transferring crystals to the Ni/Au surface, all surfaces were cleaned by boiling them first in acetone and then in ethanol for 10 min, followed by a UV-ozone cleaning for 15 min and a final incubation in warm ethanol for 30 min. The solution of the crystal was drop-casted on the surface and kept in vacuum before proceeding to the mc-AFM measurements.

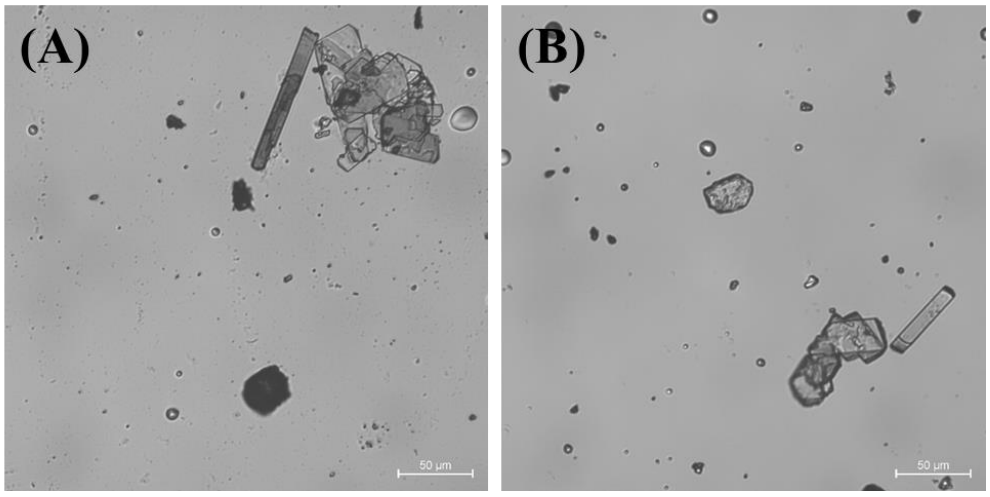


**Figure S1:** Optical micrograph of (A) an L-Phenylalanine-$Co^{2+}$ crystal and (B) a D-Phenylalanine-$Co^{2+}$ crystal.

## References

1. Sheldrick, G. M. SHELXT – Integrated Space-Group and Crystal Structure Determination. *Acta Cryst. A*, 2015, **71**, 3-8.

2. Sheldrick, G. M. Crystal Structure Refinement with SHELXL. *Acta Cryst. C*, 2015, **71**, 3-8.

3. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. OLEX2: A Complete Structure Solution, Refinement and Analysis Program. *J. Appl. Cryst.*, 2009, **42**, 339-341.