Supporting Information

Metallotectons: Comparison of Molecular Networks Built from Racemic and Enantiomerically Pure Tris(dipyrrinato)cobalt(III) Complexes

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Contents:

I. Solubility Tests

Triacid *rac*-**1a** (4.2 mg) was added to *N*,*N*'-diethylformamide (DEF) (75 μL), and the resulting suspension was stirred vigorously at 20 °C for 4 h before being filtered through a 45 μm nylon syringe filter. The saturated filtrate was diluted by adding 10 μL to MeOH (20 mL). The absorption spectrum was recorded using a cell of 1 cm pathlength, giving $A_{468\ nm}$ = 1.0. Using a value of $\varepsilon_{468\ nm}$ = 57,000 $M^{-1}cm^{-1}$ gave a concentration of 18 μM for the diluted solution, and 10 μL of saturated solution therefore contains 0.37 μmol of triacid *rac*-**1a**. This gave a concentration of a saturated solution of triacid *rac*-**1a** in DEF of 0.037 M.

The same procedure using enantiomerically pure triacid Δ-**1a** (10 mg) gave a saturated solution in DEF with a concentration of 0.16 M.

II. X-Ray Crystallographic Details

X-ray diffraction data were collected with Cu K_α radiation using a Bruker Smart 6000 CCD diffractometer equipped with an FR591 rotating anode generator. The structures were solved by direct methods using SHELXS-97 and refined with SHELXL-97.[1] All non-hydrogen atoms were refined anisotropically, except where noted below. Hydrogen atoms were placed in ideal positions and refined as riding atoms, except for those of certain guest molecules, where they were not included in the model (see below).

The percentage of volume accessible to guests was estimated by the PLATON program.[2] PLATON calculates the accessible volume by allowing a spherical probe of variable radius to roll over the van der Waals surface of the network. PLATON uses a default value of 1.20 Å for the radius of the probe, which is an appropriate model for small guests such as water.

Refinement Details

Complex *rac*-**1a.** The included molecules of H_2O (O100 − O103) are disordered over several sites. Their O atoms were refined anisotropically, and their H atoms were excluded in the model.

Complex *rac*-**1c.** The S atoms of two of the included molecules of DMSO proved to be disordered over two positions (S501/S502 and S201/S202). O801 corresponds to an included

molecule of H_2O with half occupancy. The H atoms of this molecule were not included in the model.

Complex *rac*-**1d.** The included molecule of CH_2Cl_2 was found to be disordered over two positions in a 70/30 ratio. The H atoms of this molecule were not included in the model.

ORTEP View of the Structure of Trinitrile Λ-1b

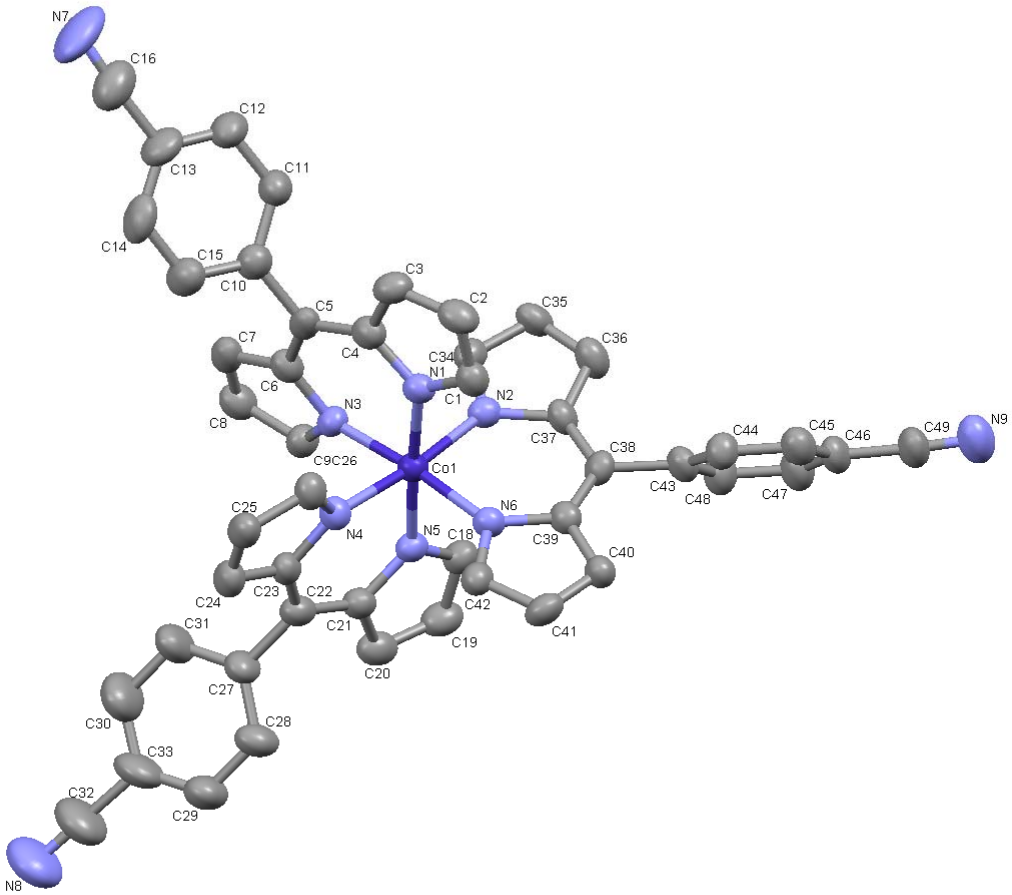

Figure S1. ORTEP view of the molecular structure of trinitrile Λ-**1b** in crystals grown from $CHCl_3$/pentane, showing the numbering scheme. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are shown at the 50% level.

References

1. Sheldrick, G. M. SHELXS-97, *Program for the Solution of Crystal Structures* and SHELXL-97, *Program for the Refinement of Crystal Structures*; Universität Göttingen: Germany, 1997.
2. Spek, A. L. *PLATON*, A Multipurpose Crystallographic Tool; Utrecht University: Utrecht, The Netherlands, 2001. van der Sluis, P.; Spek, A. L. *Acta Crystallogr*. **1990**, *A46*, 194.