Supplementary Material (ESI) for Chemical Communications

A banana-shaped dinuclear complex with a tris(benzene-*o*-dithiolato) ligand

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Supporting Information

Single crystals of $(Me_3PhN)_4[Ti_2(\mathbf{1})_2]\cdot 2DMSO\cdot 6DMF$ suitable for an X-ray diffraction analysis were obtained by slow diffusion of diethyl ether into a solution of $(Me_3PhN)_4[Ti_2(\mathbf{1})_2]$ in MeOH/DMF/DMSO (10:1:1, v:v:v) at ambient temperature. X-ray diffraction data were collected at −120(1) °C with a Bruker AXS APEX diffractometer equipped with a rotating Cu anode (CuK_α radiation, $\lambda = 1.54178$ Å).[1] An empirical absorption correction was applied to the raw data ($0.74 \le T \le 0.88$). The structure solution was found with SHELXS[2] and the refinement was carried out with SHELXL[3] using anisotropic thermal parameters for all non-hydrogen atoms, with the exception of atoms O11, N19, C98-C100 belonging to a disordered DMF molecule, which were refined with isotropic thermal parametes. Hydrogen atoms were added to the structure models on calculated positions and were refined as riding atoms (with the exception of hydrogen atoms belonging to the disordered DMF molecule). Additional crystal, data collection and refinement deteils are summarized in Table S1.

Table S1. Crystallographic Data for $(Me_3PhN)_4[Ti_2(\mathbf{1})_2]\cdot 2DMSO\cdot 6DMF$

parameter	
chem. formula	$C_{142}H_{164}N_{28}O_{14}S_{14}Ti_2$
cryst. size, mm	0.10 x 0.075 x 0.04
color of crystal	red
Fw, amu	3031.65
space group	$P\bar{1}$ (no. 2)
a, Å	14.6767(10)
b, Å	21.0095(12)
c, Å	25.8753(14)
α, deg	84.555(4)
β, deg	78.851(4)
γ, deg	87.166(4)
V, Å^3	7788.8(8)
Z	2
radiation, λ, Å	Cu Kα, 1.54178
T, K	153(1)
ρ calcd, g cm^{-3}	1.293
refl. collected/$2\Theta_{max}$	45721/144.8
unique reflns, R_{int}	26396, 0.0687
refl. obs. ($I>2\sigma(I)$)	16405
no. of params/restr	1802/0
μ, mm^{-1}	3.167
*R*1 ($I>2\sigma(I)$)	0.0900
*wR*2 (all data)	0.2586
GOF	0.997
resid density, e Å^{-3}	+1.18/−1.25

1 *SMART*, Bruker AXS, **2000**.
2 *SHELXS-97*, G. M. Sheldrick, *Acta Crystallogr.* **1990**, *A46*, 467–473.
3 *SHELXL-97*, G. M. Sheldrick, *Acta Crystallogr.* **2008**, *A64*, 112–122.