10.1071/CH21335
Australian Journal of Chemistry

Supplementary Material

An icosanuclear silver(I) cluster supported by bis (thiosemicarbazonato) ligands

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Supporting Information

Crystal structure of glyoxal-bis(4-phenyl-3-thiosemicarbazone) (H_2gtsp).

X-ray Crystallography

Crystals were mounted in low temperature oil then flash cooled to 130 K using an Oxford low temperature device. Intensity data were collected at 130 K with an Oxford XCalibur X-ray diffractometer with Sapphire CCD detector using Cu-Kα radiation (graphite crystal monochromator λ = 1.54184 Å) or a Bruker SMART Apex CCD detector using Mo-Kα radiation (graphite crystal monochromator λ = 0.71073 Å). Data were reduced and corrected for absorption. The structure was solved by direct methods and difference Fourier synthesis using the SHELX suite of programs[1] as implemented within the WINGX software.[2] The large (7310.1 Å^3) amount of solvent accessible voids that accounts for just over 50% of the total volume $Ag^{I}_{20}(Hgtsp)_{16}(gtsp)_2$ consisted of 2058 electrons and is presumably occupied by a combination of DMF and diethylether molecules.[3] CCDC 2128318.

Table S1. Crystallographic data for H_2gtsp.

Crystal Identification	H_2gtsp•0.5Et_2O
Chemical formula	$C_{18}H_{21}N_6O_{0.5}S_2$
M_w	393.53
Crystal System	Triclinic
T/K	130(2)
Space group	$P\bar{1}$
a / Å	8.8060(3)
b / Å	11.8089(5
c / Å	19.1752(7
α / °	77.811(3)
β / °	83.823(3)
γ / °	88.489(3)
V / Å^3	1937.73(13)
Z	4
Independent reflections	7634 [R(int) = 0.0309]
R ($I > 2\sigma(I)$)	0.0398
wR (all data)	0.1110

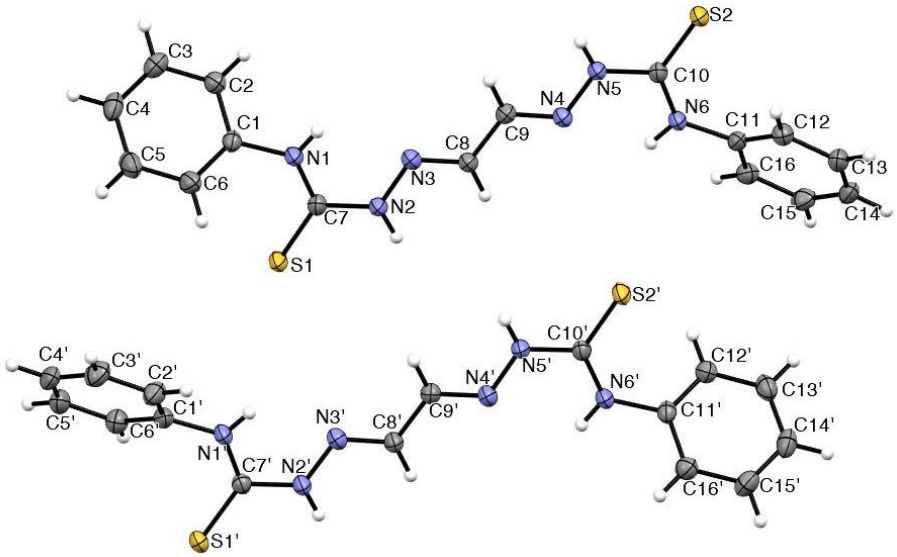

Figure S1. ORTEP representation (50 % ellipsoids) of $(H_2gtsp)_2 \cdot Et_2O$. Selected bond distances; C7-S1 1.6825(19) Å, C7-N2 1.360(2) Å, C10-S2 1.6774(18) Å, C10-N5 1.367(2) Å, C(7')-S(1') 1.6769(18) Å, C10'-S2' 1.6802(18) Å, C7'-N2' 1.367(2) Å, C10'-N5' 1.361(2) Å.

References

[1] G. M. Sheldrick. Crystal structure refinement with SHELXL. Acta Crystallographica, Section C: Structural Chemistry. **2015**, *71*, 3.

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[3] A. L. Spek. PLATON SQUEEZE: a tool for the calculation of the disordered solvent contribution to the calculated structure factors. Acta Crystallographica, Section C: Structural Chemistry. **2015**, *71*, 9.