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A trinuclear Cu_2Mn complex, $[Mn(CuL)_2(DMF)_2](SCN)_2$, where H_2L is 3,10,18,21-tetraazatetracyclo[20.4.0.0^{4,9}.0^{12,17}]hexacosa-2,10,12,14,16,22,24,26-octaene-19,20-dionate(2−) and DMF is dimethylformamide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.045
wR factor = 0.110
Data-to-parameter ratio = 13.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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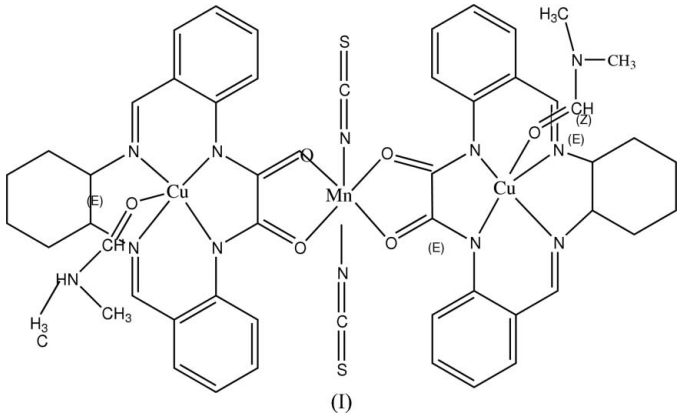
A new trinuclear Cu_2Mn complex, bis(dimethylformamide)bis[μ-3,10,18,21-tetraazatetracyclo[20.4.0.0^{4,9}.0^{12,17}]hexacosa-2,10,12,14,16,22,24,26-octaene-19,20-dionato(2−)]bis(thiocyanato)dicopper(II)manganese(II), $[Cu_2Mn(C_{22}H_{20}N_4O_2)_2(NCS)_2(C_3H_7NO)_2]$, has been synthesized and structurally characterized. The Cu^{II} atom is five-coordinated by four N atoms from the tetraza macrocycle and one dimethylformamide N atom. The central Mn^{II} atom is coordinated by four O atoms of the oxamide group and two N atoms. The Mn^{II} atom lies on a centre of symmetry. The Cu^{II} atoms reside in the cavities of the macrocyclic ligands.

Comment

Investigation of the structures and properties of macrocyclic transition metal complexes has become a fascinating subject in the fields of coordination chemistry, biology and materials science. Macrocyclic ligands have a great advantage over non-cyclic ligands, since their complexes can be thermodynamically stabilized and kinetically retarded toward metal dissociation and subsititution by the so-called 'macrocyclic effect'. Furthermore, the macrocyclic ligand may restrict the type of complex formed. It has been found that the oxamide bridge serves as a pathway through which electron spin interaction takes place and macrocyclic complexes with aromatic rings are held together by intermolecular interactions. Here, we report the preparation and crystal structure of the title trinuclear Cu_2Mn complex, (I).



(I)

The Cu^{II} atom is five-coordinated by four N atoms from the H_2L ligands and one N atom from the dimethylformamide ligand. The central Mn^{II} atom is coordinated by four O atoms and two N atoms. The Mn^{II} atom lies on a centre of symmetry.

Atoms Cu1 and Cu2 reside in the cavities of the macrocyclic complex ligands.

Experimental

The synthesis of the ligand was described previously Zhang *et al.* (2003). A mixture of Cu*L* (0.0430 g, 0.1 mmol) and KSCN (0.0097 g, 0.1 mmol) was added to one side of an H-tube, and $Mn(ClO_4)_2{\cdot}6H_2O$ (0.0181 g, 0.05 mmol) was added to the other side, with a mixture of EtOH and dimethylformamide as the solvent (10:1 *v*/*v*). After two weeks at room temperature, red crystals of (I) suitable for X-ray analysis were obtained.

Crystal data

$[Cu_2Mn(C_{22}H_{20}N_4O_2)_2(NCS)_2{\cdot}(C_3H_7NO)_2]$	$Z = 1$
$M_r = 1189.21$	$D_x = 1.517$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 9.9510$ (19) Å	Cell parameters from 1948 reflections
$b = 11.188$ (2) Å	$\theta = 2.7$–$24.4°$
$c = 13.907$ (3) Å	$\mu = 1.19$ mm^{-1}
$\alpha = 69.960$ (3)°	$T = 293$ (2) K
$\beta = 83.727$ (4)°	Block, red
$\gamma = 63.665$ (3)°	0.24 × 0.16 × 0.12 mm
$V = 1301.9$ (4) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	4570 independent reflections
	3128 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.027$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 25.0°$
	$h = -11 \rightarrow 8$
$T_{min} = 0.780$, $T_{max} = 0.867$	$k = -13 \rightarrow 11$
6623 measured reflections	$l = -15 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0548P)^2 + 0.188P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.045$	
$wR(F^2) = 0.110$	
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.005$
4570 reflections	$\Delta\rho_{max} = 0.44$ e Å^{-3}
342 parameters	$\Delta\rho_{min} = -0.33$ e Å^{-3}
H-atom parameters constrained	

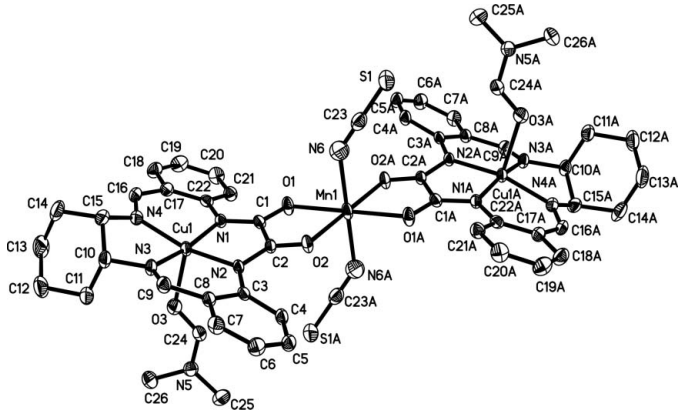


Figure 1
A view of the structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (A) $1-x, 3-y, 1-z$]

H atoms were positioned geometrically, with C—H = 0.93–0.97 Å, and treated as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$, or $1.5U_{eq}(C)$ for methyl H.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

References

Bruker (1997). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2000). *SHELXTL*. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Zhang, L., Wang, S.-B., Yang, G.-M., Tang, J.-K., Liao, D.-Z., Jiang, Z.-H., Yan, S.-P. & Cheng, P. (2003). *Inorg. Chem.* **42**, 1462–1466.