Acta Crystallographica Section C
**Crystal Structure Communications**
ISSN 0108-2701

# Bis(di-$\mu$-acetato-aqua{2-[*N*-ethyl-*N*-(2-hydroxy-4-methylbenzyl)aminomethyl]-1-methylbenzimidazole}nickel)nickel(II) tetrahydrate

## Cassandra J. Martin *et al.*

**Electronic paper**
This paper is published electronically. It meets the data-validation criteria for publication in Acta Crystallographica Section C. The submission has been checked by a Section C Co-editor though the text in the 'Comments' section is the responsibility of the authors.

Acta Crystallographica Section C
**Crystal Structure Communications**
ISSN 0108-2701

# Bis(di-$\mu$-acetato-aqua{2-[*N*-ethyl-*N*-(2-hydroxy-4-methylbenzyl)aminomethyl]-1-methylbenzimidazole}nickel)nickel(II) tetrahydrate

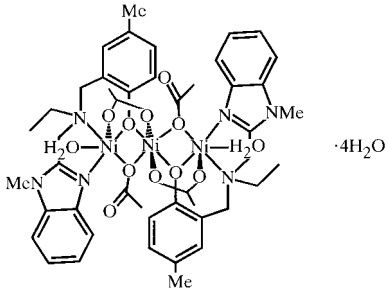
**Cassandra J. Martin,[a] David C. R. Hockless,[b] Max R. Taylor[a] and Lisandra L. Martin[a]***

[a]School of Chemistry, Physics and Earth Sciences, The Flinders University of South Australia, GPO Box 2100, Adelaide, 5001 SA, Australia, and [b]Research School of Chemistry, Australian National University, Canberra, ACT 0200, Australia
Correspondence e-mail: lisa.martin@flinders.edu.au

Received 19 September 2000
Accepted 23 October 2000

Data validation number: IUC0000300

The previously unknown title compound, tetra-$\mu$-acetato-1:2$\kappa^2O$;1:2$\kappa^2O$:$O'$;2:3$\kappa^2O$;2:3$\kappa^2O$:$O'$-diaqua-1$\kappa O$,3$\kappa O$-bis($\mu$-2-{[*N*-ethyl-*N*-(2-hydroxy-5-methylbenzyl)amino]methyl}-1-methyl-1*H*-benzimidazole)-1$\kappa^3N^3$,*N*,*O*:2$\kappa O$;3$\kappa^3N^3$,*N*,*O*:2$\kappa O$-trinickel(II) tetrahydrate, $[Ni_3(C_{18}H_{22}N_3O)_2(C_2H_3O_2)_4(H_2O)_2]\cdot 4H_2O$, (I), is a centrosymmetric linear trinuclear nickel(II) complex, where the Ni atoms are in an octahedral coordination and the ligand heteroatoms act so as to model amino acid residues.




(I)

## Experimental

2-{[*N*-Ethyl-*N*-(2-hydroxy-5-methylbenzyl)amino]methyl}-1-methyl-1*H*-benzimidazole (*L*; 0.224 g, 0.725 mmol) dissolved in methanol (7 ml) was added slowly to a suspension of $NiBr_2$ (0.231 g, 0.966 mmol) in refluxing methanol. Heating was continued until dissolution of the nickel salt was complete, affording a clear green solution. Sodium acetate (0.277 g, 0.203 mmol) dissolved in methanol (5 ml) was added to the green solution. The solvent was removed under vacuum, resulting in a crude green product. This material was dissolved in acetonitrile and the solution filtered and evaporated to dryness. Recrystallization from methanol/2-propanol resulted in crystals of suitable quality for X-ray structure determination.

*Crystal data*

| | |
|---|---|
| $[Ni_3(C_{18}H_{22}N_3O)_2(C_2H_3O_2)_4(H_2O)_2]\cdot 4H_2O$ | $Z = 1$ |
| $M_r = 1137.15$ | $D_x = 1.419$ Mg m$^{-3}$ |
| Triclinic, $P\overline{1}$ | Cu $K\alpha$ radiation |
| $a = 11.130$ (2) Å | Cell parameters from 25 reflections |
| $b = 11.732$ (2) Å | $\theta = 17.2$–$26.1°$ |
| $c = 12.258$ (2) Å | $\mu = 1.831$ mm$^{-1}$ |
| $\alpha = 99.66$ (2)° | $T = 193$ (2) K |
| $\beta = 110.34$ (1)° | Plate, colourless |
| $\gamma = 110.23$ (1)° | 0.12 × 0.12 × 0.02 mm |
| $V = 1330.6$ (5) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Rigaku AFC-6*R* diffractometer | $R_{int} = 0.031$ |
| $\omega$–$2\theta$ scans | $\theta_{max} = 60.04°$ |
| Absorption correction: $\psi$ scan (North *et al.*, 1968) | $h = -11 \rightarrow 12$ |
| $T_{min} = 0.873$, $T_{max} = 0.965$ | $k = -12 \rightarrow 13$ |
| 4152 measured reflections | $l = -13 \rightarrow 0$ |
| 3940 independent reflections | 3 standard reflections every 150 reflections |
| 2872 reflections with $F > 2.5\sigma(F_o)$' | intensity decay: 0.82% |

*Refinement*

| | |
|---|---|
| Refinement on $F$ | H-atom parameters not refined |
| $R = 0.058$ | $w = 1/\sigma^2(F_o)$ |
| $wR = 0.047$ | $(\Delta/\sigma)_{max} < 0.001$ |
| $S = 1.750$ | $\Delta\rho_{max} = 0.64$ e Å$^{-3}$ |
| 2865 reflections | $\Delta\rho_{min} = -0.68$ e Å$^{-3}$ |
| 322 parameters | |

The coordinates of the two H atoms of the O8 water molecule could not be reliably located and were not included in the refinement.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1994); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1992–1997); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *Xtal*3.4 *CRYLSQ* (Hall *et al.*, 1995); software used to prepare material for publication: *Xtal*3.4 *BONDLA CIFIO*.

## References

Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Hall, S. R., King, G. S. D. & Stewart, J. M. (1995). Editors. *Xtal*3.4 *Reference Manual.* Universities of Western Australia, Australia, and Maryland, USA.
Molecular Structure Corporation (1992–1997). *TEXSAN.* Version 1.7. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
Molecular Structure Corporation (1994). *MSC/AFC Diffractometer Control Software*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.