Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis[μ-2-(2,4-difluorophenyl)-1,3-bis-(1,2,4-triazol-1-yl)propan-2-olato]-$\kappa^8N^2,O:O,N^{2'}$-bis[(acetato-κ^2O,O')nickel(II)]

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.035
wR factor = 0.098
Data-to-parameter ratio = 12.0

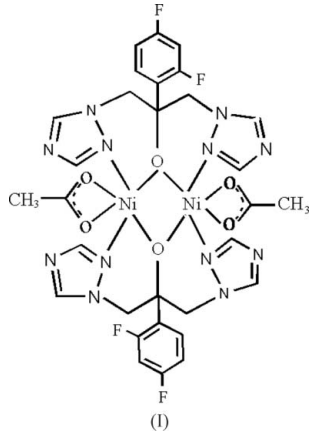
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 15 June 2006
Accepted 8 July 2006

In the title centrosymmetric binuclear nickel(II) complex, $[Ni_2(C_{13}H_{11}F_2N_6O)_2(C_2H_3O_2)_2]$, the two Ni atoms, each attached to an acetate ligand, are linked by two fluconazole molecules. Each Ni atom is six-coordinated by two N atoms from the triazole groups and two bridging O atoms from the deprotonated hydroxyl groups of two different fluconazole ligands and two O atoms from the bidentate acetic anion, exhibiting a distorted octahedral geometry.

Comment

Fungal diseases in man have increased significantly with the advent of an expanding population of immunosuppressed patients and with the introduction of sophisticated life-saving medical procedures. Fluconazole, 2-(2,4-difluorophenyl)-1,3-bis(1,2,4-triazol-1-yl)propan-2-ol, a good antifungal agent in the treatment of candidiasis, has attracted much interest among researchers (Cyr *et al.*, 1996; Heald *et al.*, 1996; Jacob *et al.*, 2003). It is highly active against a variety of fungal pathogens that cause systemic mycoses (Saag & Dismukes, 1988) and is effective in preventing fungal infections in patients undergoing bone marrow transplantation (Goodman *et al.*, 1992). With two symmetrical 1,2,4-triazole groups, fluconazole is expected to form stable complexes with various transition metal ions. Recently, interactions between metal ions and drugs have become of great interest (Ali *et al.*, 2002). In some cases, the highest activity of a drug is associated with the existence of a metal ion (Agh-Atabay *et al.*, 2003; Castilo-Blum & Barba-Behrens, 2000; Inoue *et al.*, 2002; Patel *et al.*, 2002; Tavman *et al.*, 2000). However, metal–fluconazole complexes have rarely been structurally characterized. We report here the title binuclear nickel(II)–fluconazole complex, (I).



(I)

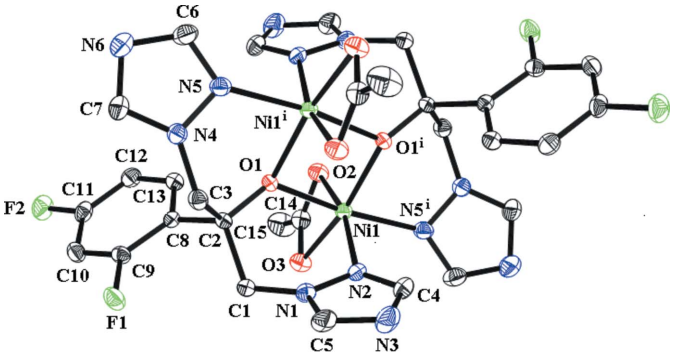


Figure 1
The structure of (I), with the atomic numbering scheme and displacement ellipsoids at the 30% probability level. H atoms have been omitted for clarity. [Symmetry code: (i) $2-x, -y, 1-z$.]

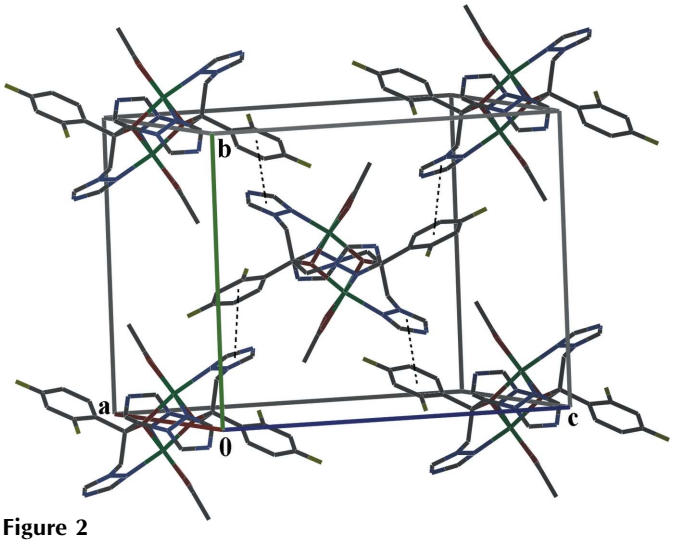


Figure 2
The π–π stacking interactions in (I) (dashed lines). H atoms have been omitted.

The molecular structure of the complex (I) is shown in Fig. 1. Selected bond lengths and angles are shown in Table 1. Compound (I) crystallizes in the space group *Pbca*, with one Ni^{II} ion, one fluconazole ligand and one bidentate-coordinated acetate anion in the asymmetric unit. The centrosymmetric molecule of (I) contains two symmetrical fluconazole ligands, each of which links two Ni^{II} centres *via* its deprotonated hydroxyl group and two triazole groups. The Ni^{II} centre exhibits a distorted octahedral geometry, defined by two N atoms from the triazole ligands and two O atoms from the hydroxyl groups of two different fluconazole ligands, and two O atoms from the acetate anion. The Ni···Ni distance is 3.0512 (9) Å and the dihedral angle between the two triazole planes in the same fluconazole ligand is 65.4 (9)°.

The complex molecules are assembled into a three-dimensional supramolecular architecture by π–π stacking interactions. As shown in Fig. 2, one triazole ring forms a π–π stacking interaction with the substituted phenyl ring from an adjacent complex molecule, with a centroid-to-centroid distance of 3.87 Å.

Experimental

A mixture of $Ni(OAc)_2{\cdot}4H_2O$ (0.5 mmol, 0.125 g), fluconazole (0.5 mmol, 0.153 g) and DMF (5 ml; DMF is *N*,*N*′-dimethylformamide) was sealed in a Teflon-lined autoclave and heated at 383 K for 3 d, followed by slow cooling to room temperature. The resulting green crystals were filtered off and washed with DMF. Analysis, calculated for $C_{30}H_{28}F_4N_{12}Ni_2O_6$: C 42.55, H 3.31, N 19.86%; found: C 42.68, H 3.29, N 19.77%. Selected FT–IR (KBr, cm^{-1}): 3120 (*m*), 3055 (*m*), 1616 (*s*), 1554 (*s*), 1459 (*s*), 1420 (*s*), 1290 (*s*), 1148 (*s*), 1053 (*s*), 958 (*s*), 877 (*m*), 677 (*s*).

Crystal data

$[Ni_2(C_{13}H_{11}F_2N_6O)_2(C_2H_3O_2)_2]$	$Z = 4$
$M_r = 846.06$	$D_x = 1.699$ Mg m^{-3}
Orthorhombic, *Pbca*	Mo $K\alpha$ radiation
$a = 13.617$ (2) Å	$\mu = 1.23$ mm^{-1}
$b = 13.883$ (2) Å	$T = 298$ (2) K
$c = 17.501$ (3) Å	Prism, green
$V = 3308.4$ (9) $Å^3$	0.43 × 0.38 × 0.28 mm

Data collection

Siemens SMART area-detector diffractometer	16325 measured reflections
φ and ω scans	2925 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	2011 reflections with $I > 2\sigma(I)$
$T_{min} = 0.60$, $T_{max} = 0.72$	$R_{int} = 0.049$
	$\theta_{max} = 25.0°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0325P)^2 + 4.3678P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.035$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.098$	$\Delta\rho_{max} = 0.36$ e $Å^{-3}$
$S = 1.11$	$\Delta\rho_{min} = -0.30$ e $Å^{-3}$
2925 reflections	
244 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	2.033 (2)	Ni1—N2	2.077 (3)
Ni1—O1^{i}	2.034 (2)	Ni1—O2	2.102 (3)
Ni1—N5^{i}	2.073 (3)	Ni1—O3	2.130 (2)
O1—Ni1—O1^{i}	82.78 (9)	N5^{i}—Ni1—N2	92.20 (12)
O1—Ni1—N5^{i}	170.08 (10)	O1^{i}—Ni1—O2	100.65 (9)
O1^{i}—Ni1—N5^{i}	87.76 (10)	N2—Ni1—O2	164.66 (10)
O1—Ni1—N2	85.60 (10)	O1^{i}—Ni1—O3	163.26 (10)
O1^{i}—Ni1—N2	94.49 (10)	O2—Ni1—O3	62.61 (10)

Symmetry code: (i) $-x+2, -y, -z+1$.

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic H atoms, C—H = 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for methylene H atoms, and C—H = 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

This work was supported by the Natural Science Fund Council of China (NSFC; grant Nos. 20331010 and 90406002) and the Specialized Research Fund for the Doctoral Programme of Higher Education (SRFDP; grant No. 20030007014).

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Received 21 June 2007; accepted 25 July 2007

In the paper by Gong, Tang, Hou, Zha & Hu [*Acta Cryst.* (2006), E**62**, m1827–m1829], the first address is incomplete. The correct full address if given here.

  DOI:10.1107/S1600536807036549