

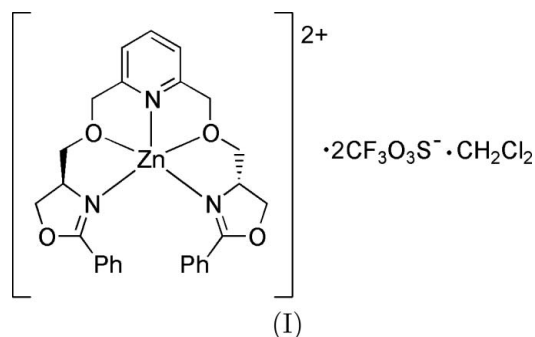
Michael Seitz,^{a*} Manfred Zabel^b
and Oliver Reiser^a^aInstitute for Organic Chemistry, University of Regensburg, Universitätsstrasse 31, D-93051 Regensburg, Germany, and ^bCrystallography Laboratory, University of Regensburg, Universitätsstrasse 31, D-93051 Regensburg, Germany

Correspondence e-mail: michel-seitz@web.de

Key indicators

Single-crystal X-ray study
 $T = 173$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
Disorder in solvent or counterion
 R factor = 0.035
 wR factor = 0.093
Data-to-parameter ratio = 12.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>. (Λ) -[(R,R) -2,6-Bis(2-phenyl-4,5-dihydro-oxazol-4-ylmethoxymethyl)pyridine]zinc(II) bis(trifluoromethanesulfonate) dichloromethane solvateThe structure of the title compound, $[\text{Zn}(\text{C}_{27}\text{H}_{27}\text{N}_3\text{O}_4)](\text{CF}_3\text{O}_3\text{S})_2 \cdot \text{CH}_2\text{Cl}_2$, shows a complex cation with trigonal-bipyramidal geometry around the Zn. The stereochemistry at the metal centre exhibits complete selectivity for the Λ configuration.Received 15 May 2006
Accepted 3 June 2006

Comment

Chiral-at-metal complexes have received a considerable amount of attention in recent years (Knof & von Zelewsky, 1999), due to the impact of asymmetric catalysis, molecular recognition and supramolecular chemistry. For the controlled construction of these species, we have used a chiral pentadentate bis(oxazoline) ligand with a variety of metals, *e.g.* cadmium(II) in enantiopure inorganic-organic hybrid polymers (Seitz *et al.*, 2004), and cadmium(II), iron(II) and manganese(II) for the formation of helical pentagonal-bipyramidal complexes (Seitz, Kaiser *et al.*, 2005). Interestingly, the combination of this ligand with zinc(II) perchlorate results in enantiopure trigonal-bipyramidal dicationic complexes, (II), with complete stereoselectivity for the Λ configuration at the metal, both in solution and in the solid state (Seitz, Stempfhuber *et al.*, 2005). Here, we report the crystal structure of the related title complex, (I), with trifluoromethanesulfonate counterions instead of perchlorate.The complex cation in (I) (Fig. 1) is essentially isostructural with the one previously reported for (II). Both have approximately C_2 symmetry and complete stereoselectivity in the solid state for the Λ configuration with respect to the newly introduced stereogenic centre. The coordination geometry around the Zn atom in (I) can best be described as trigonal-bipyramidal. The three N donors define the trigonal plane, which also contains the metal centre. The N–Zn–N angles are all close to the ideal value of 120° (Table 1). The dihedral angle between this plane and that defined by the two axial ether–O donors and the Zn atom is $73.3(1)^\circ$.

Experimental

Equimolar amounts of (*R,R*)-2,6-bis-(2-phenyl-4,5-dihydrooxazol-4-ylmethoxymethyl)pyridine and anhydrous zinc(II) trifluoromethanesulfonate were dissolved in dry dichloromethane (1 mmol ml⁻¹) and layered with toluene (1 mmol ml⁻¹). The title compound crystallized as colourless needles.

Crystal data

[Zn(C₂₇H₂₇N₃O₄)](CF₃O₃S)₂·CH₂Cl₂
M_r = 905.99
 Orthorhombic, *P*2₁2₁2₁
a = 8.7347 (6) Å
b = 15.2145 (10) Å
c = 26.9055 (19) Å
V = 3575.6 (4) Å³
Z = 4
D_x = 1.683 Mg m⁻³
 Mo *K*α radiation
 μ = 1.04 mm⁻¹
T = 173 (1) K
 Needle, colourless
 0.72 × 0.24 × 0.18 mm

Data collection

Stoe IPDS diffractometer
 ω scans
 Absorption correction: numerical
 [FACEIT in X-RED (Stoe & Cie, 1996)]
T_{min} = 0.592, *T_{max}* = 0.816
 30057 measured reflections
 6882 independent reflections
 6405 reflections with *I* > 2σ(*I*)
R_{int} = 0.038
θ_{max} = 25.9°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.035
wR [*F*²] = 0.093
S = 1.04
 6882 reflections
 533 parameters
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0601P)^2 + 1.1443P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 (Δ/σ)_{max} < 0.001
 Δρ_{max} = 0.60 e Å⁻³
 Δρ_{min} = -0.35 e Å⁻³
 Absolute structure: Flack (1983),
 with 3002 Friedel pairs
 Flack parameter: 0.001 (10)

Table 1

Selected geometric parameters (Å, °).

Zn1–N3	1.969 (2)	Zn1–O3	2.252 (2)
Zn1–N2	1.976 (2)	Zn1–O1	2.2614 (19)
Zn1–N1	2.033 (3)		
N3–Zn1–N2	134.06 (11)	N1–Zn1–O3	76.43 (9)
N3–Zn1–N1	112.42 (11)	N3–Zn1–O1	109.89 (9)
N2–Zn1–N1	113.50 (10)	N2–Zn1–O1	80.19 (9)
N3–Zn1–O3	80.76 (9)	N1–Zn1–O1	76.34 (9)
N2–Zn1–O3	110.98 (9)	O3–Zn1–O1	152.77 (8)

All H atoms were positioned geometrically and refined as riding, with C–H = 0.93 (aromatic CH), 0.97 (secondary CH₂) and 0.98 Å (tertiary CH), and with *U*_{iso}(H) = 1.2*U*_{eq}(C). Positional disorder in one of the trifluoromethanesulfonate anions was modelled over two positions, with partial occupancies of 0.760 (6) and 0.240 (6).

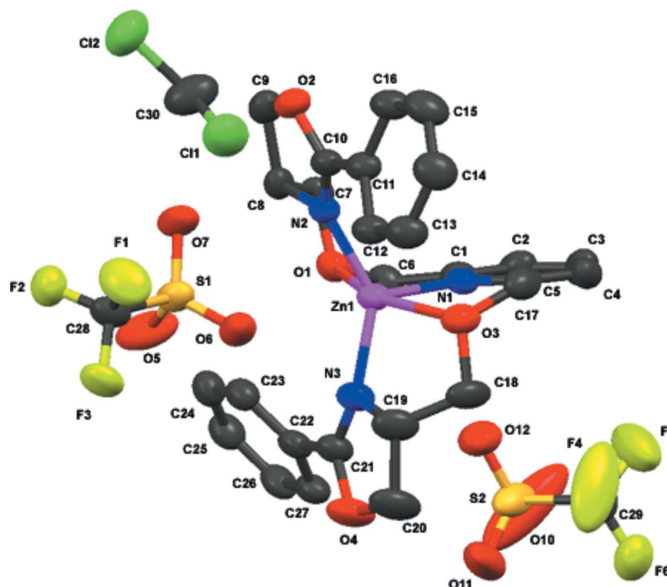


Figure 1

The asymmetric unit of (I), with displacement ellipsoids drawn at the 50% probability level. Only the principal component is shown for the disordered trifluoromethanesulfonate anion and H atoms have been omitted for clarity.

Data collection: *IPDS Software* (Stoe & Cie, 1998); cell refinement: *IPDS Software*; data reduction: *IPDS Software*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *MERCURY* (version 1.4; Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

This work was supported by the German Research Foundation (DFG) as part of the programme SP1118 (RE948/5–2).

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