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## Key indicators

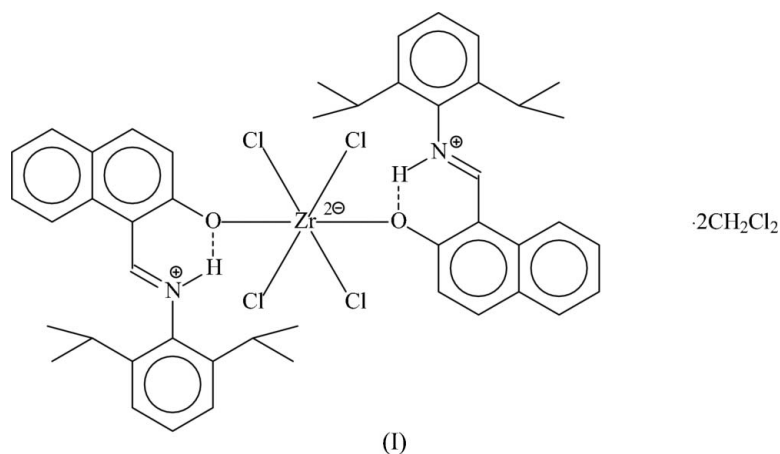
Single-crystal X-ray study  
T = 295 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$   
Disorder in solvent or counterion  
R factor = 0.052  
wR factor = 0.161  
Data-to-parameter ratio = 18.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.***trans*-Tetrachlorobis[1-[(2,6-diisopropylphenyl)iminomethyl]-2-naphtholato- $\kappa\text{O}$ ]zirconium(IV) dichloromethane disolvate**The Zr atom in the title disolvate,  $[\text{ZrCl}_4(\text{C}_{23}\text{H}_{25}\text{NO})_2] \cdot 2\text{CH}_2\text{Cl}_2$ , lies on a special position of  $\bar{1}$  site symmetry in a *trans*- $\text{Cl}_4\text{O}_2\text{Zr}$  octahedral geometry.

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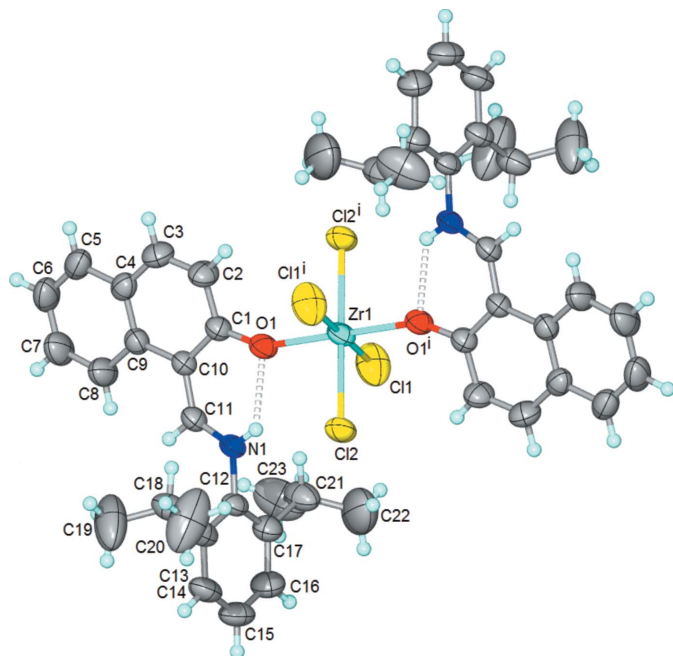
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## Comment

The deprotonated salicylideneamino-2,6-diisopropylbenzene Schiff base *N,O*-chelates to the metal atoms in a large number of metal complexes (Cambridge Structural Database, Version 5.27; Allen, 2002), an example of which is the dichlorozirconium(IV) complex (Strauch *et al.*, 2000). The isopropyl substituent of the diisopropylphenyl unit does not seem to be too sterically demanding in these examples. Similarly, the related Schiff base, 3-[(2,6-diisopropylphenyl)imino]methyl-2-naphthol (Lin *et al.*, 2005), is not expected to be crowded, and neither should the analogous Schiff base with an  $\alpha$ -naphthyl group in place of the 2,6-isopropylphenyl unit, *i.e.* 3-( $\alpha$ -naphthyl)methyl-2-naphthol. Interestingly, in the solid state, 3-( $\alpha$ -naphthyl)methyl-2-naphthol exists in a zwitterionic form, as the hydroxy group has transferred its H atom to the imino group (Gavranic *et al.*, 1996).



3-[(2,6-Diisopropylphenyl)imino]methyl-2-naphthol, when reacted with zirconium(IV) tetrachloride, forms the title 1:2 metal–ligand adduct, (I), in which the ligand has also rearranged itself into a zwitterionic form so as to bind through the negatively-charged hydroxy O atom. The compound crystallizes from dichloromethane as a disolvate (Fig. 1). The metal atom lies on a special position of  $\bar{1}$  site symmetry in a six-coordinate geometry. The bond dimensions of the iminium unit are similar to those found in, for example, zwitterionic 3-( $\alpha$ -naphthyl)methyl-2-naphthol (Gavranic *et al.*, 1996).



**Figure 1**

A plot of zwitterionic (I). The disordered dichloromethane molecule is not shown. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii. The dashed lines indicate the intramolecular hydrogen bond. [Symmetry code: (i) =  $\frac{1}{2} - x, \frac{1}{2} - y, 1 - z$ .]

## Experimental

The Schiff base was synthesized from 2-hydroxy-1-naphthaldehyde and 2,6-diisopropylaniline according to the literature procedure of Lin *et al.* (2005). The zirconium compound was synthesized using Schlenk techniques under a nitrogen atmosphere. The Schiff base (3.31 g, 10.5 mmol) was dissolved in tetrahydrofuran (THF; 100 ml) at 183 K. In an attempt to deprotonate the Schiff base, an *n*-butyllithium solution in hexane (0.683 g, 10.5 mmol) was added to the THF solution. The solution was allowed to warm to room temperature over a period of 2 h before being added to a solution of zirconium tetrachloride (1.17 g, 5.0 mmol) in THF (100 ml) at 183 K. The mixture was allowed to warm to room temperature. The solution was stirred overnight and then the solvent was removed under vacuum to give a solid, to which dichloromethane (60 ml) was added. The solid material that separated was collected and washed with dichloromethane. The solid material was discarded; the dichloromethane filtrate was concentrated to afford the crude product, (I), which was purified by recrystallization from dichloromethane to give yellow crystals in about 60% yield. CHN elemental analysis, calculated for  $C_{47}H_{52}N_2O_2Cl_6Zr$ : C 57.55, H 5.34, N 2.86%; found: C 57.39, H 5.07, N 2.82%. These values are those of a mono- rather than a bis(dichloromethane) solvate.

### Crystal data

$[ZrCl_4(C_{23}H_{25}NO)_2] \cdot 2CH_2Cl_2$	$Z = 4$
$M_r = 1065.75$	$D_x = 1.363 \text{ Mg m}^{-3}$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 17.700 (1) \text{ \AA}$	$\mu = 0.66 \text{ mm}^{-1}$
$b = 16.897 (1) \text{ \AA}$	$T = 295 (2) \text{ K}$
$c = 18.190 (1) \text{ \AA}$	Block, yellow
$\beta = 107.286 (1)^\circ$	$0.25 \times 0.20 \times 0.16 \text{ mm}$
$V = 5194.6 (5) \text{ \AA}^3$	

### Data collection

Bruker APEXII area-detector diffractometer	15120 measured reflections
$\varphi$ and $\omega$ scans	5829 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	4410 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.852, T_{\max} = 0.902$	$R_{\text{int}} = 0.018$
	$\theta_{\max} = 27.5^\circ$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0967P)^2 + 2.9123P]$
$R[F^2 > 2\sigma(F^2)] = 0.052$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.161$	$(\Delta/\sigma)_{\max} = 0.001$
$S = 1.02$	$\Delta\rho_{\max} = 0.53 \text{ e \AA}^{-3}$
5829 reflections	$\Delta\rho_{\min} = -0.36 \text{ e \AA}^{-3}$
309 parameters	
H atoms treated by a mixture of independent and constrained refinement	

**Table 1**

Selected geometric parameters ( $\text{\AA}, ^\circ$ ).

Zr1—O1	2.058 (2)	Zr1—Cl1	2.449 (1)
Zr1—Cl2	2.459 (1)		
O1—Zr1—O1 <sup>i</sup>	180	Cl1—Zr1—Cl1 <sup>i</sup>	180
O1—Zr1—Cl1	89.09 (7)	Cl1—Zr1—Cl2	89.28 (5)
O1—Zr1—Cl1 <sup>i</sup>	90.91 (7)	Cl1—Zr1—Cl2 <sup>i</sup>	90.72 (5)
O1—Zr1—Cl2	87.02 (6)	Cl2—Zr1—Cl2 <sup>i</sup>	180
O1—Zr1—Cl2 <sup>i</sup>	92.98 (6)		

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

The dichloromethane molecule is disordered over two sites, the occupancies being in a 0.72 (1):0.28 (1) ratio. The C—Cl distance was restrained to 1.79 (1)  $\text{\AA}$  and the Cl $\cdots$ Cl distance to 2.92 (1)  $\text{\AA}$ . Additionally, the displacement parameters of the disordered atoms were restrained to be nearly isotropic.

The iminium H atom was located and refined with an N—H distance restraint of 0.85 (1)  $\text{\AA}$ ; its displacement parameter was freely refined. The remaining H atoms were placed in calculated positions (C—H = 0.93–0.98  $\text{\AA}$ ) and were included in the refinement in the riding-model approximation, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Data collection: SMART (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: X-SEED (Barbour, 2001); software used to prepare material for publication: SHELXL97.

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