

Dichlorido[*N,N,N',N'*-tetramethylcyclohexane-1,2-diamine- κ^2 *N,N'*]zinc(II)

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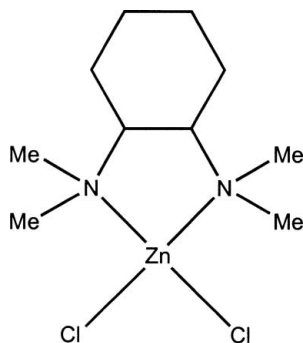
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{N}-\text{C}) = 0.012$ Å; disorder in main residue; R factor = 0.067; wR factor = 0.159; data-to-parameter ratio = 20.4.

In the title compound, $[\text{ZnCl}_2(\text{C}_{10}\text{H}_{22}\text{N}_2)]$, the Zn^{II} ion coordinates to the N atoms of tetramethylcyclohexane-1,2-diamine and to two chloride ions in an approximately tetrahedral arrangement. The $\text{N}-\text{Zn}-\text{N}$ and $\text{Cl}-\text{Zn}-\text{Cl}$ planes are approximately orthogonal, with a dihedral angle of $89.7(2)^\circ$ between them. Four C atoms of the cyclohexane ring, together with their attached H atoms, are disordered equally over two sites.

Related literature

For the use of tetramethylcyclohexane-1,2-diamine in asymmetric addition, see: Cabello *et al.* (2005); Kizirian *et al.* (2005). For related structures, see: Roh *et al.* (2004); Pavlova *et al.* (2003).



Experimental

Crystal data

$[\text{ZnCl}_2(\text{C}_{10}\text{H}_{22}\text{N}_2)]$
 $M_r = 306.59$
 Monoclinic, $P2_1/n$
 $a = 8.2566(6)$ Å
 $b = 14.1915(13)$ Å
 $c = 12.9584(9)$ Å
 $\beta = 107.504(6)^\circ$

$V = 1448.1(2)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 2.04$ mm⁻¹
 $T = 293(2)$ K
 $0.40 \times 0.40 \times 0.35$ mm

Data collection

Enraf–Nonius CAD-4 four-circle diffractometer
 Absorption correction: ψ scan (ABSCALC; McArdle & Daly, 1999)
 $T_{\text{min}} = 0.46$, $T_{\text{max}} = 0.49$
 2918 measured reflections

2687 independent reflections
 2388 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.011$
 3 standard reflections
 frequency: 60 min
 intensity decay: 0.2%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.067$
 $wR(F^2) = 0.159$
 $S = 1.27$
 2687 reflections

132 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.45$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.49$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Zn–N2	2.073 (7)	Zn–Cl2	2.199 (2)
Zn–N1	2.086 (6)	Zn–Cl1	2.219 (2)
N2–Zn–N1	87.1 (2)	N2–Zn–Cl1	110.38 (19)
N2–Zn–Cl2	114.97 (19)	N1–Zn–Cl1	109.88 (18)
N1–Zn–Cl2	115.24 (18)	Cl2–Zn–Cl1	115.83 (10)

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD* (McArdle, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* (McArdle, 1995); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2341).

References

- Cabello, N., Kizirian, J.-C., Gille, S., Alexakis, A., Bernardinelli, G., Pinchard, L. & Caille, J.-C. (2005). *Eur. J. Org. Chem.* **22**, 4835–4842.
 Enraf–Nonius (1989). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
 Kizirian, J.-C., Cabello, N., Pinchard, L., Caille, J.-C. & Alexakis, A. (2005). *Tetrahedron*, **61**, 8939–8946.
 McArdle, P. (1995). *J. Appl. Cryst.* **28**, 65.
 McArdle, P. (1999). *XCAD*. National University of Ireland, Galway, Ireland.
 McArdle, P. & Daly, P. (1999). *ABSCALC*. National University of Ireland, Galway, Ireland.
 Pavlova, S. V., Wen, Y.-S. & Chan, S. I. (2003). *Acta Cryst.* **E59**, m792–m793.
 Roh, S. G., Yoon, J. U. & Jeong, J. H. (2004). *Polyhedron*, **23**, 2063–2067.
 Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

supplementary materials

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Dichlorido[*N,N,N',N'*-tetramethylcyclohexane-1,2-diamine- κ^2 *N,N'*]zinc(II)

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Comment

Chiral *N,N,N',N'*-tetramethylcyclohexane-1,2-diamine has been used as enantioselective additive for the asymmetric addition of aryl or alkyl lithium to pro-chiral imines (Cabello *et al.*, 2005; Kizirian *et al.*, 2005). Crystal structures of zinc complexes containing non-macrocyclic cyclohexane-1,2-diamine as ligand are very rare (Roh *et al.*, 2004). Herein, we report the crystal structure of the Zn^{II} complex bearing *N,N,N',N'*-tetramethylcyclohexane-1,2-diamine and two chloride anions. The geometry around Zn^{II} is a near tetrahedron while the Cu(II) complex bearing the same ligand has a distorted square-planar geometry (Pavlova *et al.*, 2003). The angles between N—Zn—N and Cl—Zn—Cl planes are 89.7 (2)°.

Experimental

To a solution of ZnCl₂ (0.084 g, 0.61 mmol) in THF (10 ml) was added dropwise a solution of *trans*-(1*R*,2*R*)-*N,N,N',N'*-tetramethylcyclohexane-1,2-diamine (0.93 g, 0.61 mmol) in THF (10 ml). The mixture was stirred for 2 days at room temperature. The solvent was removed and the residue was washed with ether to give a white solid. Colorless crystals was obtained from methanol solution. Yield; 1.40 g (75%). Anal. Calcd. for C₁₀H₂₂Cl₂N₂Zn: C, 39.18; H, 7.23; N, 9.14. Found: C, 39.15; H, 7.24; N, 9.10%. ¹H NMR (CDCl₃); δ 2.45(m, 4H, CHDA), 2.08(m, 2H, CHDA), 1.86(m, 2H, CHDA), 1.25(m, 1H, CHDA), 1.13(m, 1H, CHDA). 2.27(s, 12H, CH₃).

Refinement

The C3, C5, C6 and C8 carbon atoms of the cyclohexane ring are disordered over two positions. They were refined isotropically at half occupancies. All H-atoms were positioned geometrically and refined using a riding model with $d(\text{C—H}) = 0.98 \text{ \AA}$, $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$ for CH, 0.97 \AA , $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$ for CH₂ and 0.96 \AA , $U_{\text{iso}} = 1.5U_{\text{eq}}(\text{C})$ for CH₃ atoms.

Figures

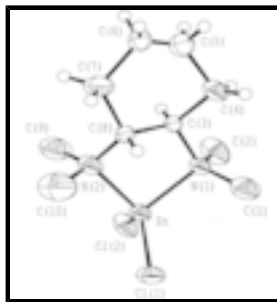


Fig. 1. A view of Dichloro[*trans*-(1*R*,2*R*)-*N,N,N',N'*-tetramethylcyclohexane-1,2-diamine- κ^2 *N,N'*]zinc(II). Displacement ellipsoids are drawn at the 40% probability level. Hydrogen atoms at methyl groups are omitted for clarity.

Dichlorido[*N,N,N',N'*-tetramethylcyclohexane-1,2-diamine- κ^2 *N,N'*]zinc(II)

Crystal data

[ZnCl ₂ (C ₁₀ H ₂₂ N ₂)]	$F_{000} = 640$
$M_r = 306.59$	$D_x = 1.406 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
Hall symbol: -P 2yn	$\lambda = 0.71073 \text{ \AA}$
$a = 8.2566 (6) \text{ \AA}$	Cell parameters from 25 reflections
$b = 14.1915 (13) \text{ \AA}$	$\theta = 9.2\text{--}13.3^\circ$
$c = 12.9584 (9) \text{ \AA}$	$\mu = 2.04 \text{ mm}^{-1}$
$\beta = 107.504 (6)^\circ$	$T = 293 (2) \text{ K}$
$V = 1448.1 (2) \text{ \AA}^3$	Block, colorless
$Z = 4$	$0.40 \times 0.40 \times 0.35 \text{ mm}$

Data collection

Enraf-Nonius CAD-4 four-circle diffractometer	$R_{\text{int}} = 0.011$
Radiation source: fine-focus sealed tube	$\theta_{\text{max}} = 25.5^\circ$
Monochromator: graphite	$\theta_{\text{min}} = 2.2^\circ$
$T = 293(2) \text{ K}$	$h = -9 \rightarrow 9$
scintillation counter scans	$k = -17 \rightarrow 0$
Absorption correction: ψ scan (ABSCALC; McArdle & Daly, 1999)	$l = 0 \rightarrow 15$
$T_{\text{min}} = 0.46, T_{\text{max}} = 0.49$	3 standard reflections
2918 measured reflections	every 60 min
2687 independent reflections	intensity decay: 0.2%
2388 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.067$	H-atom parameters constrained
$wR(F^2) = 0.159$	$w = 1/[\sigma^2(F_o^2) + (0.0001P)^2 + 8.9534P]$
$S = 1.28$	where $P = (F_o^2 + 2F_c^2)/3$
2687 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
132 parameters	$\Delta\rho_{\text{max}} = 0.45 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.49 \text{ e \AA}^{-3}$
	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Zn	0.24797 (10)	0.14548 (6)	0.43395 (6)	0.0467 (3)	
C11	0.2396 (3)	0.07751 (16)	0.58652 (15)	0.0690 (6)	
C12	0.4590 (3)	0.24418 (18)	0.4487 (2)	0.0833 (8)	
N1	0.0079 (7)	0.1968 (4)	0.3495 (5)	0.0476 (14)	
N2	0.2142 (8)	0.0459 (5)	0.3122 (5)	0.0562 (16)	
C1	-0.0956 (11)	0.2038 (8)	0.4228 (8)	0.089 (3)	
H1A	-0.0499	0.2517	0.4759	0.106*	
H1B	-0.0949	0.1444	0.4585	0.106*	
H1C	-0.2101	0.2198	0.3824	0.106*	
C2	0.0250 (13)	0.2904 (6)	0.3069 (10)	0.099 (4)	
H2A	0.1000	0.2872	0.2630	0.119*	
H2B	0.0708	0.3332	0.3659	0.119*	
H2C	-0.0845	0.3124	0.2639	0.119*	
C3	-0.0397 (18)	0.1419 (11)	0.2458 (12)	0.049 (3)*	0.50
H3	0.0088	0.1744	0.1952	0.059*	0.50
C3'	-0.0814 (17)	0.1143 (10)	0.2794 (11)	0.040 (3)*	0.50
H3'	-0.1085	0.0666	0.3263	0.048*	0.50
C4	-0.2412 (9)	0.1412 (6)	0.1940 (7)	0.067 (2)	
H4A	-0.2954	0.1121	0.2428	0.080*	
H4B	-0.2846	0.2047	0.1779	0.080*	
C5	-0.273 (3)	0.0825 (16)	0.0888 (18)	0.087 (6)*	0.50
H5A	-0.3913	0.0641	0.0708	0.105*	0.50
H5B	-0.2676	0.1282	0.0343	0.105*	0.50
C5'	-0.330 (2)	0.0612 (12)	0.1266 (14)	0.060 (4)*	0.50
H5C	-0.3988	0.0852	0.0572	0.072*	0.50
H5D	-0.4062	0.0322	0.1617	0.072*	0.50
C6	-0.211 (3)	0.0220 (16)	0.0704 (17)	0.073 (5)*	0.50
H6A	-0.1929	0.0326	0.0007	0.088*	0.50
H6B	-0.2887	-0.0307	0.0617	0.088*	0.50
C6'	-0.204 (3)	-0.0172 (17)	0.1069 (19)	0.087 (6)*	0.50
H6C	-0.2395	-0.0770	0.1295	0.104*	0.50
H6D	-0.2240	-0.0213	0.0293	0.104*	0.50
C7	-0.0311 (12)	-0.0100 (7)	0.1544 (7)	0.075 (3)	
H7A	-0.0397	-0.0760	0.1715	0.090*	
H7B	0.0549	-0.0052	0.1175	0.090*	
C8	0.033 (2)	0.0454 (12)	0.2630 (14)	0.053 (4)*	0.50
H8	-0.0157	0.0142	0.3142	0.064*	0.50
C8'	0.0396 (18)	0.0717 (11)	0.2248 (13)	0.045 (3)*	0.50
H8'	0.0642	0.1207	0.1783	0.054*	0.50
C9	0.3344 (12)	0.0601 (9)	0.2507 (8)	0.099 (4)	
H9A	0.3239	0.0095	0.2000	0.118*	
H9B	0.4480	0.0613	0.2994	0.118*	
H9C	0.3104	0.1189	0.2124	0.118*	
C10	0.2425 (18)	-0.0485 (7)	0.3608 (10)	0.117 (5)	
H10A	0.1814	-0.0942	0.3089	0.140*	

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H10B	0.2029	-0.0502	0.4233	0.140*
H10C	0.3616	-0.0629	0.3819	0.140*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn	0.0422 (4)	0.0500 (5)	0.0456 (5)	-0.0030 (4)	0.0101 (3)	0.0028 (4)
Cl1	0.0779 (14)	0.0781 (14)	0.0414 (10)	-0.0194 (11)	0.0034 (9)	0.0103 (9)
Cl2	0.0577 (13)	0.0751 (15)	0.119 (2)	-0.0192 (11)	0.0298 (13)	0.0030 (14)
N1	0.044 (3)	0.046 (3)	0.048 (3)	0.006 (3)	0.007 (3)	0.002 (3)
N2	0.053 (4)	0.065 (4)	0.057 (4)	0.010 (3)	0.026 (3)	0.003 (3)
C1	0.061 (6)	0.135 (10)	0.076 (6)	0.025 (6)	0.029 (5)	0.009 (6)
C2	0.090 (7)	0.059 (6)	0.138 (10)	0.012 (5)	0.016 (7)	0.047 (6)
C4	0.048 (4)	0.069 (5)	0.069 (5)	0.006 (4)	-0.004 (4)	0.010 (5)
C7	0.087 (7)	0.075 (6)	0.059 (5)	-0.015 (5)	0.018 (5)	-0.022 (5)
C9	0.074 (6)	0.153 (11)	0.083 (7)	-0.005 (7)	0.046 (6)	-0.028 (7)
C10	0.205 (15)	0.053 (6)	0.103 (9)	0.016 (8)	0.062 (9)	-0.003 (6)

Geometric parameters (\AA , $^\circ$)

Zn—N2	2.073 (7)	C4—H4A	0.9700
Zn—N1	2.086 (6)	C4—H4B	0.9700
Zn—Cl2	2.199 (2)	C5—C6	1.06 (2)
Zn—Cl1	2.219 (2)	C5—H5A	0.9700
N1—C1	1.461 (10)	C5—H5B	0.9700
N1—C2	1.462 (10)	C5'—C6'	1.59 (3)
N1—C3	1.500 (15)	C5'—H5C	0.9700
N1—C3'	1.528 (14)	C5'—H5D	0.9700
N2—C8	1.438 (16)	C6—C7	1.62 (2)
N2—C9	1.462 (10)	C6—H6A	0.9700
N2—C10	1.468 (11)	C6—H6B	0.9700
N2—C8'	1.585 (16)	C6'—C7	1.38 (2)
C1—H1A	0.9600	C6'—H6C	0.9700
C1—H1B	0.9600	C6'—H6D	0.9700
C1—H1C	0.9600	C7—C8'	1.482 (16)
C2—H2A	0.9600	C7—C8	1.559 (17)
C2—H2B	0.9600	C7—H7A	0.9700
C2—H2C	0.9600	C7—H7B	0.9700
C3—C8	1.49 (2)	C8—H8	0.9800
C3—C4	1.596 (16)	C8'—H8'	0.9800
C3—H3	0.9800	C9—H9A	0.9600
C3'—C4	1.494 (14)	C9—H9B	0.9600
C3'—C8'	1.513 (19)	C9—H9C	0.9600
C3'—H3'	0.9800	C10—H10A	0.9600
C4—C5'	1.485 (18)	C10—H10B	0.9600
C4—C5	1.55 (2)	C10—H10C	0.9600
N2—Zn—N1	87.1 (2)	H4A—C4—H4B	108.9
N2—Zn—Cl2	114.97 (19)	C6—C5—C4	132 (2)

N1—Zn—C12	115.24 (18)	C6—C5—H5A	104.3
N2—Zn—C11	110.38 (19)	C4—C5—H5A	104.3
N1—Zn—C11	109.88 (18)	C6—C5—H5B	104.3
C12—Zn—C11	115.83 (10)	C4—C5—H5B	104.3
C1—N1—C2	109.0 (8)	H5A—C5—H5B	105.6
C1—N1—C3	124.9 (9)	C4—C5'—C6'	113.4 (14)
C2—N1—C3	99.4 (9)	C4—C5'—H5C	108.9
C1—N1—C3'	99.6 (8)	C6'—C5'—H5C	108.9
C2—N1—C3'	123.8 (8)	C4—C5'—H5D	108.9
C3—N1—C3'	28.4 (6)	C6'—C5'—H5D	108.9
C1—N1—Zn	109.4 (5)	H5C—C5'—H5D	107.7
C2—N1—Zn	109.3 (5)	C5—C6—C7	119 (2)
C3—N1—Zn	103.9 (6)	C5—C6—H6A	107.6
C3'—N1—Zn	104.9 (6)	C7—C6—H6A	107.6
C8—N2—C9	123.0 (10)	C5—C6—H6B	107.6
C8—N2—C10	101.3 (10)	C7—C6—H6B	107.6
C9—N2—C10	108.2 (8)	H6A—C6—H6B	107.0
C8—N2—C8'	23.6 (7)	C7—C6'—C5'	120.9 (17)
C9—N2—C8'	101.5 (8)	C7—C6'—H6C	107.1
C10—N2—C8'	120.7 (9)	C5'—C6'—H6C	107.1
C8—N2—Zn	103.0 (7)	C7—C6'—H6D	107.1
C9—N2—Zn	111.2 (6)	C5'—C6'—H6D	107.1
C10—N2—Zn	109.2 (6)	H6C—C6'—H6D	106.8
C8'—N2—Zn	105.7 (6)	C6'—C7—C8'	119.7 (13)
N1—C1—H1A	109.5	C6'—C7—C8	117.7 (13)
N1—C1—H1B	109.5	C8'—C7—C8	23.9 (7)
H1A—C1—H1B	109.5	C6'—C7—C6	26.3 (11)
N1—C1—H1C	109.5	C8'—C7—C6	107.8 (11)
H1A—C1—H1C	109.5	C8—C7—C6	117.4 (11)
H1B—C1—H1C	109.5	C6'—C7—H7A	83.8
N1—C2—H2A	109.5	C8'—C7—H7A	131.0
N1—C2—H2B	109.5	C8—C7—H7A	108.0
H2A—C2—H2B	109.5	C6—C7—H7A	108.0
N1—C2—H2C	109.5	C6'—C7—H7B	126.8
H2A—C2—H2C	109.5	C8'—C7—H7B	92.1
H2B—C2—H2C	109.5	C8—C7—H7B	108.0
C8—C3—N1	111.0 (12)	C6—C7—H7B	108.0
C8—C3—C4	112.4 (12)	H7A—C7—H7B	107.2
N1—C3—C4	109.8 (10)	N2—C8—C3	112.5 (13)
C8—C3—H3	107.8	N2—C8—C7	115.4 (11)
N1—C3—H3	107.8	C3—C8—C7	108.5 (13)
C4—C3—H3	107.8	N2—C8—H8	106.7
C4—C3'—C8'	108.4 (11)	C3—C8—H8	106.7
C4—C3'—N1	113.9 (10)	C7—C8—H8	106.7
C8'—C3'—N1	108.4 (10)	C7—C8'—C3'	114.1 (12)
C4—C3'—H3'	108.7	C7—C8'—N2	111.3 (11)
C8'—C3'—H3'	108.7	C3'—C8'—N2	110.2 (11)
N1—C3'—H3'	108.7	C7—C8'—H8'	107.0
C5'—C4—C3'	114.3 (10)	C3'—C8'—H8'	107.0

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C5'—C4—C5	31.8 (9)	N2—C8'—H8'	107.0
C3'—C4—C5	113.1 (11)	N2—C9—H9A	109.5
C5'—C4—C3	121.4 (10)	N2—C9—H9B	109.5
C3'—C4—C3	27.6 (6)	H9A—C9—H9B	109.5
C5—C4—C3	104.6 (11)	N2—C9—H9C	109.5
C5'—C4—H4A	79.3	H9A—C9—H9C	109.5
C3'—C4—H4A	83.5	H9B—C9—H9C	109.5
C5—C4—H4A	110.8	N2—C10—H10A	109.5
C3—C4—H4A	110.8	N2—C10—H10B	109.5
C5'—C4—H4B	119.9	H10A—C10—H10B	109.5
C3'—C4—H4B	125.7	N2—C10—H10C	109.5
C5—C4—H4B	110.8	H10A—C10—H10C	109.5
C3—C4—H4B	110.8	H10B—C10—H10C	109.5
N2—Zn—N1—C1	128.6 (6)	N1—C3—C4—C5	-179.8 (12)
Cl2—Zn—N1—C1	-115.1 (6)	C5'—C4—C5—C6	-90 (4)
Cl1—Zn—N1—C1	17.9 (6)	C3'—C4—C5—C6	9(4)
N2—Zn—N1—C2	-112.2 (6)	C3—C4—C5—C6	37 (3)
Cl2—Zn—N1—C2	4.1 (7)	C3'—C4—C5'—C6'	-33.8 (19)
Cl1—Zn—N1—C2	137.2 (6)	C5—C4—C5'—C6'	61 (2)
N2—Zn—N1—C3	-6.8 (8)	C3—C4—C5'—C6'	-4(2)
Cl2—Zn—N1—C3	109.5 (7)	C4—C5—C6—C7	-12 (4)
Cl1—Zn—N1—C3	-117.4 (7)	C4—C5'—C6'—C7	3(3)
N2—Zn—N1—C3'	22.5 (7)	C5'—C6'—C7—C8'	0(3)
Cl2—Zn—N1—C3'	138.8 (6)	C5'—C6'—C7—C8	27 (3)
Cl1—Zn—N1—C3'	-88.2 (7)	C5'—C6'—C7—C6	-69 (3)
N1—Zn—N2—C8	-19.6 (9)	C5—C6—C7—C6'	103 (4)
Cl2—Zn—N2—C8	-136.2 (8)	C5—C6—C7—C8'	-19 (3)
Cl1—Zn—N2—C8	90.5 (8)	C5—C6—C7—C8	5(3)
N1—Zn—N2—C9	113.9 (6)	C9—N2—C8—C3	-82.1 (16)
Cl2—Zn—N2—C9	-2.6 (7)	C10—N2—C8—C3	157.2 (13)
Cl1—Zn—N2—C9	-135.9 (6)	C8'—N2—C8—C3	-55 (2)
N1—Zn—N2—C10	-126.7 (7)	Zn—N2—C8—C3	44.3 (15)
Cl2—Zn—N2—C10	116.8 (7)	C9—N2—C8—C7	43.1 (18)
Cl1—Zn—N2—C10	-16.5 (7)	C10—N2—C8—C7	-77.6 (14)
N1—Zn—N2—C8'	4.6 (7)	C8'—N2—C8—C7	70 (2)
Cl2—Zn—N2—C8'	-112.0 (7)	Zn—N2—C8—C7	169.4 (10)
Cl1—Zn—N2—C8'	114.7 (7)	N1—C3—C8—N2	-55.0 (18)
C1—N1—C3—C8	-93.7 (14)	C4—C3—C8—N2	-178.4 (10)
C2—N1—C3—C8	145.1 (12)	N1—C3—C8—C7	176.1 (10)
C3'—N1—C3—C8	-63.3 (17)	C4—C3—C8—C7	52.7 (17)
Zn—N1—C3—C8	32.4 (14)	C6'—C7—C8—N2	176.4 (15)
C1—N1—C3—C4	31.2 (15)	C8'—C7—C8—N2	-82 (2)
C2—N1—C3—C4	-89.9 (11)	C6—C7—C8—N2	-153.9 (13)
C3'—N1—C3—C4	61.7 (16)	C6'—C7—C8—C3	-56 (2)
Zn—N1—C3—C4	157.3 (8)	C8'—C7—C8—C3	45 (2)
C1—N1—C3'—C4	79.6 (11)	C6—C7—C8—C3	-26.7 (19)
C2—N1—C3'—C4	-41.1 (14)	C6'—C7—C8'—C3'	27 (2)
C3—N1—C3'—C4	-75.5 (18)	C8—C7—C8'—C3'	-65 (2)
Zn—N1—C3'—C4	-167.2 (8)	C6—C7—C8'—C3'	53.0 (17)

C1—N1—C3'—C8'	-159.6 (11)	C6'—C7—C8'—N2	152.6 (15)
C2—N1—C3'—C8'	79.7 (13)	C8—C7—C8'—N2	61 (2)
C3—N1—C3'—C8'	45.4 (16)	C6—C7—C8'—N2	178.4 (11)
Zn—N1—C3'—C8'	-46.4 (12)	C4—C3'—C8'—C7	-56.2 (16)
C8'—C3'—C4—C5'	60.1 (15)	N1—C3'—C8'—C7	179.6 (10)
N1—C3'—C4—C5'	-179.1 (11)	C4—C3'—C8'—N2	177.7 (10)
C8'—C3'—C4—C5	25.3 (17)	N1—C3'—C8'—N2	53.6 (14)
N1—C3'—C4—C5	146.2 (12)	C8—N2—C8'—C7	-73 (2)
C8'—C3'—C4—C3	-51.7 (16)	C9—N2—C8'—C7	84.1 (12)
N1—C3'—C4—C3	69.2 (17)	C10—N2—C8'—C7	-35.4 (15)
C8—C3—C4—C5'	-26.1 (19)	Zn—N2—C8'—C7	-159.7 (9)
N1—C3—C4—C5'	-150.3 (12)	C8—N2—C8'—C3'	54 (2)
C8—C3—C4—C3'	56.5 (17)	C9—N2—C8'—C3'	-148.3 (12)
N1—C3—C4—C3'	-67.6 (16)	C10—N2—C8'—C3'	92.2 (13)
C8—C3—C4—C5	-55.6 (17)	Zn—N2—C8'—C3'	-32.2 (13)

Fig. 1

