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Bis{*N*-[(dimethylamino)dimethylsilyl]-2,6-dimethylanilido-κ^2N,N'}zinc(II)

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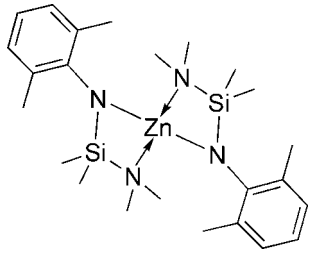
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.009 Å; R factor = 0.064; wR factor = 0.161; data-to-parameter ratio = 16.9.

The title zinc amide, $[Zn(C_{12}H_{21}N_2Si)_2]$, which was synthesized by the metathetical reaction of $[LiN(SiMe_2NMe_2)(2,6\text{-}Me_2C_6H_3)]_2$ with zinc dichloride, has the Zn atom *N*,*N*′-chelated by the *N*-silylated anilide ligand in a square-planar environment. There are two independent molecules in the asymmetric unit; in both, the $Zn-N_{amine}$ bonds are longer than the $Zn-N_{anilide}$ bonds.

Related literature

For related compounds which show linear and tetrahedral coordination, see Schumann *et al.* (2000); Engelhardt *et al.* (1991). For applications of zinc amides, see Amstrong *et al.* (2002) and for their synthesis by MOVCD, see Maile *et al.* (2005).



Experimental

Crystal data

$[Zn(C_{12}H_{21}N_2Si)_2]$
M_r = 508.17
Triclinic, $P\overline{1}$
a = 9.600 (5) Å
b = 10.447 (5) Å
c = 27.338 (5) Å
α = 88.654 (5)°
β = 86.151 (5)°
γ = 89.858 (5)°
V = 2735 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.00 mm^{-1}
T = 293 (2) K
0.25 × 0.20 × 0.20 mm

Data collection

Bruker SMART area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.788, T_{max} = 0.825
11316 measured reflections
9429 independent reflections
5229 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.161
S = 0.90
9429 reflections
559 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.83 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1999); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2346).

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supplementary materials

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Bis{*N*-[(dimethylamino)dimethylsilyl]-2,6-dimethylanilido-$\kappa^2 N,N'$}zinc(II)

J. Chen, K.-N. Cao and J. Guo

Comment

Zinc amides were a class of transamination reagents (Amstrong *et al.*, 2002). They were also useful in preparing the zinc thin film through the MOVCD method (Maile *et al.*, 2005).

The title compound is monomeric, and is similar to bis[(*N*-trimethylsilyl)-2,6-dimethylanilido]zinc and bis[(*N*-dimethylaminodimethylsilyl)-2,6-diisopropylanilido]zinc (Schumann *et al.*, 2000). The ligand has an N—Si—N chelating group, which is presumed to be a "quasi" conjugated unit owing to *d*–π interaction between Si and N atoms. The Zn center is chelated, with an average N—Zn—N bite angle of 74°. Compared with the rigid N—C—N chelating unit in the amidinate ligand, the N—Si—N group is much more flexible. The Zn—$N_{anilido}$ bonds are in the normal range whereas the Zn—N_{amino} bonds are more than 2.40 Å (Engelhardt *et al.*, 1991). The linear N1—Zn1—N3 is nearly linear; this feature has also been observed in bis[(*N*-trimethylsilyl)-2,6-dimethylanilido]zinc. In the present compound, for both independent molecules, the two ligands are arranged in *trans* to each other. The [NZnN] planes are approximately coplanar. In the reported bis[(*N*-dimethylaminodimethylsilyl)-2,6-diisopropylanilido]zinc, the ligands are *cis* to each other in the tetrahedron around zinc. Evidently, the steric effect of the aromatic substituents plays an important role in influencing the geometry of zinc in this class of zinc amides.

Experimental

A solution of Li^{n}Bu in hexane (2.8 *M*, 1.9 ml, 5.37 mmol) was added into a solution of [NH($SiMe_2NMe_2$)(2,6-$Me_2C_6H_3$)] (1.22 g, 5.37 mmol) in Et_2O (25 ml) at 273 K. The mixture was stirred at room temperature for 2 h and then $ZnCl_2$ (0.61 g, 2.70 mmol) was added at 273 K. The resulting solution was stirred at room temperature overnight. The filtered solution was concentrated to give the title compound as colorless crystals. Yield: 0.72 g (53%).

Refinement

The methyl H atoms were then constrained to an ideal geometry, with C—H distances of 0.96 Å and U_{iso}(H) = 1.2U_{eq}(C), but each group was allowed to rotate freely about its C–C bond. The other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

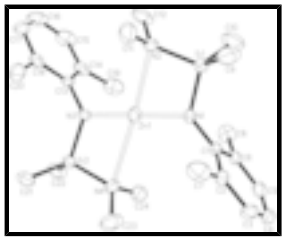


Fig. 1. **Fig. 1**. The molecular structure, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted.

Bis{*N*-[(dimethylamino)dimethylsilyl]-2,6-dimethylanilido-$\kappa^2 N, N'$}zinc(II)

Crystal data

$[Zn(C_{12}H_{21}N_2Si)_2]$	$Z = 4$
$M_r = 508.17$	$F_{000} = 1088$
Triclinic, $P\bar{1}$	$D_x = 1.234$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71069$ Å
$a = 9.600$ (5) Å	Cell parameters from 2236 reflections
$b = 10.447$ (5) Å	$\theta = 2.3$–24.1º
$c = 27.338$ (5) Å	$\mu = 1.00$ mm^{-1}
$\alpha = 88.654$ (5)º	$T = 293$ (2) K
$\beta = 86.151$ (5)º	Block, yellow
$\gamma = 89.858$ (5)º	0.25 × 0.20 × 0.20 mm
$V = 2735$ (2) Å^3	

Data collection

Bruker SMART area-detector diffractometer	9429 independent reflections
Radiation source: fine-focus sealed tube	5229 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.039$
$T = 293$(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 1.5$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -11 \rightarrow 6$
$T_{min} = 0.788$, $T_{max} = 0.825$	$k = -12 \rightarrow 12$
11316 measured reflections	$l = -32 \rightarrow 31$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.064$	H-atom parameters constrained
$wR(F^2) = 0.161$	$w = 1/[\sigma^2(F_o^2) + (0.0712P)^2]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.90$	$(\Delta/\sigma)_{max} = 0.001$
9429 reflections	$\Delta\rho_{max} = 0.83$ e Å^{-3}
559 parameters	$\Delta\rho_{min} = -0.61$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	1.0352 (5)	0.6368 (5)	0.3752 (2)	0.0338 (13)
C2	1.1110 (6)	0.6002 (5)	0.3311 (2)	0.0420 (15)
C3	1.2407 (7)	0.5422 (6)	0.3349 (3)	0.064 (2)
H3A	1.2900	0.5162	0.3064	0.077*
C4	1.2982 (7)	0.5218 (6)	0.3782 (3)	0.067 (2)
H4A	1.3845	0.4816	0.3791	0.080*
C5	1.2288 (7)	0.5608 (6)	0.4207 (3)	0.0572 (18)
H5A	1.2694	0.5489	0.4504	0.069*
C6	1.0982 (6)	0.6178 (5)	0.4196 (2)	0.0418 (15)
C7	1.0520 (7)	0.6223 (6)	0.2833 (2)	0.071 (2)
H7A	1.1165	0.5925	0.2577	0.106*
H7B	1.0355	0.7122	0.2784	0.106*
H7C	0.9655	0.5766	0.2827	0.106*
C8	1.0288 (7)	0.6650 (6)	0.4672 (2)	0.0624 (19)
H8A	0.9398	0.7021	0.4611	0.094*
H8B	1.0868	0.7285	0.4804	0.094*
H8C	1.0158	0.5945	0.4902	0.094*
C9	0.7235 (7)	0.4972 (6)	0.3337 (3)	0.094 (3)
H9A	0.6774	0.4248	0.3497	0.141*
H9B	0.8136	0.4717	0.3199	0.141*
H9C	0.6685	0.5294	0.3080	0.141*
C10	0.6932 (8)	0.5531 (8)	0.4405 (3)	0.111 (3)
H10A	0.6541	0.4697	0.4367	0.166*
H10B	0.6250	0.6068	0.4572	0.166*
H10C	0.7739	0.5458	0.4593	0.166*
C11	0.5859 (7)	0.7736 (6)	0.3195 (3)	0.075 (2)

H11A	0.4975	0.7307	0.3197	0.113*
H11B	0.6499	0.7366	0.2953	0.113*
H11C	0.5736	0.8629	0.3117	0.113*
C12	0.5408 (7)	0.8041 (6)	0.4062 (3)	0.079 (3)
H12A	0.4549	0.7577	0.4051	0.119*
H12B	0.5235	0.8939	0.4013	0.119*
H12C	0.5783	0.7898	0.4375	0.119*
C13	0.7081 (5)	1.1005 (5)	0.3849 (2)	0.0330 (13)
C14	0.6785 (6)	1.1050 (6)	0.4358 (2)	0.0508 (17)
C15	0.5536 (8)	1.1586 (6)	0.4535 (3)	0.067 (2)
H15A	0.5339	1.1608	0.4873	0.080*
C16	0.4586 (7)	1.2082 (7)	0.4235 (3)	0.072 (2)
H16A	0.3765	1.2453	0.4365	0.087*
C17	0.4865 (6)	1.2022 (5)	0.3738 (3)	0.0545 (18)
H17A	0.4210	1.2330	0.3529	0.065*
C18	0.6106 (6)	1.1510 (5)	0.3542 (2)	0.0407 (15)
C19	0.7750 (7)	1.0437 (7)	0.4702 (2)	0.070 (2)
H19A	0.8559	1.0116	0.4518	0.105*
H19B	0.7279	0.9742	0.4879	0.105*
H19C	0.8031	1.1058	0.4929	0.105*
C20	0.6336 (6)	1.1462 (6)	0.2990 (2)	0.0566 (17)
H20A	0.5553	1.1844	0.2842	0.085*
H20B	0.6431	1.0587	0.2894	0.085*
H20C	0.7170	1.1925	0.2885	0.085*
C21	0.9967 (6)	1.1994 (6)	0.2865 (2)	0.064 (2)
H21A	1.0406	1.2816	0.2881	0.096*
H21B	0.9040	1.2104	0.2759	0.096*
H21C	1.0501	1.1474	0.2636	0.096*
C22	1.0357 (7)	1.2420 (6)	0.3927 (2)	0.065 (2)
H22A	1.0743	1.3158	0.3751	0.098*
H22B	1.1035	1.2066	0.4134	0.098*
H22C	0.9538	1.2665	0.4123	0.098*
C23	1.1972 (7)	0.9651 (6)	0.3033 (3)	0.079 (2)
H23A	1.2501	0.8886	0.3088	0.118*
H23B	1.2596	1.0366	0.2982	0.118*
H23C	1.1450	0.9555	0.2748	0.118*
C24	1.1655 (6)	0.9534 (6)	0.3908 (3)	0.066 (2)
H24A	1.2235	0.8795	0.3851	0.099*
H24B	1.0953	0.9343	0.4166	0.099*
H24C	1.2218	1.0235	0.4001	0.099*
N1	0.9057 (4)	0.6959 (4)	0.37359 (15)	0.0332 (11)
N2	0.6412 (4)	0.7597 (4)	0.36734 (16)	0.0398 (12)
N3	0.8352 (4)	1.0458 (4)	0.36536 (15)	0.0322 (11)
N4	1.0997 (5)	0.9877 (4)	0.34669 (18)	0.0447 (12)
Si1	0.74471 (17)	0.62499 (15)	0.37901 (6)	0.0430 (4)
Si2	0.98807 (16)	1.11987 (14)	0.34818 (6)	0.0385 (4)
Zn1	0.86701 (7)	0.86979 (6)	0.36550 (2)	0.0404 (2)
C25	0.8211 (5)	0.8591 (5)	0.1183 (2)	0.0347 (13)
C26	0.8934 (6)	0.9011 (5)	0.1581 (2)	0.0410 (15)

C27	1.0259 (6)	0.9538 (5)	0.1489 (3)	0.0514 (17)
H27A	1.0741	0.9815	0.1751	0.062*
C28	1.0869 (7)	0.9657 (5)	0.1023 (3)	0.061 (2)
H28A	1.1746	1.0029	0.0969	0.073*
C29	1.0176 (6)	0.9223 (5)	0.0639 (3)	0.0554 (18)
H29A	1.0600	0.9288	0.0323	0.066*
C30	0.8862 (6)	0.8690 (5)	0.0708 (2)	0.0388 (14)
C31	0.8312 (6)	0.8870 (6)	0.2093 (2)	0.0610 (19)
H31A	0.8950	0.9197	0.2315	0.091*
H31B	0.8133	0.7981	0.2169	0.091*
H31C	0.7452	0.9341	0.2125	0.091*
C32	0.8160 (6)	0.8165 (6)	0.0280 (2)	0.0593 (18)
H32A	0.7262	0.7827	0.0390	0.089*
H32B	0.8725	0.7495	0.0135	0.089*
H32C	0.8047	0.8837	0.0040	0.089*
C33	0.5070 (6)	0.9918 (6)	0.0798 (3)	0.066 (2)
H33A	0.4639	1.0680	0.0927	0.099*
H33B	0.4493	0.9558	0.0563	0.099*
H33C	0.5969	1.0126	0.0642	0.099*
C34	0.4760 (6)	0.9561 (6)	0.1889 (2)	0.070 (2)
H34A	0.4386	1.0393	0.1818	0.105*
H34B	0.5563	0.9651	0.2077	0.105*
H34C	0.4065	0.9059	0.2075	0.105*
C35	0.3731 (7)	0.7072 (6)	0.0787 (2)	0.0622 (19)
H35A	0.2835	0.7466	0.0757	0.093*
H35B	0.3644	0.6161	0.0761	0.093*
H35C	0.4376	0.7394	0.0530	0.093*
C36	0.3194 (6)	0.7024 (6)	0.1662 (2)	0.064 (2)
H36A	0.2368	0.7529	0.1628	0.096*
H36B	0.3559	0.7183	0.1974	0.096*
H36C	0.2967	0.6133	0.1644	0.096*
C37	0.4909 (5)	0.3918 (5)	0.13763 (19)	0.0317 (13)
C38	0.4016 (6)	0.3444 (5)	0.1037 (2)	0.0405 (15)
C39	0.2770 (6)	0.2864 (5)	0.1205 (2)	0.0486 (16)
H39A	0.2181	0.2545	0.0980	0.058*
C40	0.2395 (6)	0.2756 (5)	0.1696 (3)	0.0531 (18)
H40A	0.1565	0.2349	0.1802	0.064*
C41	0.3232 (6)	0.3240 (5)	0.2029 (2)	0.0495 (17)
H41A	0.2960	0.3179	0.2361	0.059*
C42	0.4501 (5)	0.3829 (5)	0.1873 (2)	0.0380 (14)
C43	0.4373 (6)	0.3560 (6)	0.0493 (2)	0.0563 (18)
H43A	0.5258	0.3981	0.0433	0.084*
H43B	0.3665	0.4052	0.0342	0.084*
H43C	0.4424	0.2722	0.0356	0.084*
C44	0.5376 (6)	0.4409 (6)	0.2248 (2)	0.0510 (16)
H44A	0.6198	0.4787	0.2085	0.076*
H44B	0.5643	0.3754	0.2475	0.076*
H44C	0.4845	0.5056	0.2421	0.076*
C45	0.8064 (7)	0.3256 (6)	0.0441 (2)	0.073 (2)

H45A	0.8503	0.2429	0.0445	0.110*
H45B	0.8659	0.3852	0.0254	0.110*
H45C	0.7187	0.3196	0.0294	0.110*
C46	0.8057 (6)	0.2434 (5)	0.1506 (3)	0.068 (2)
H46A	0.8533	0.1766	0.1327	0.102*
H46B	0.7175	0.2121	0.1646	0.102*
H46C	0.8616	0.2701	0.1764	0.102*
C47	1.0029 (6)	0.5425 (6)	0.0775 (2)	0.0612 (19)
H47A	1.0530	0.6156	0.0877	0.092*
H47B	0.9645	0.5619	0.0466	0.092*
H47C	1.0655	0.4710	0.0739	0.092*
C48	0.9316 (6)	0.5383 (6)	0.1637 (2)	0.0577 (18)
H48A	0.9926	0.6112	0.1617	0.087*
H48B	0.9801	0.4656	0.1765	0.087*
H48C	0.8509	0.5564	0.1851	0.087*
N5	0.6876 (4)	0.8031 (4)	0.12634 (15)	0.0322 (11)
N6	0.4247 (4)	0.7370 (4)	0.12669 (17)	0.0382 (12)
N7	0.6194 (4)	0.4531 (4)	0.12183 (15)	0.0297 (10)
N8	0.8880 (5)	0.5102 (4)	0.11487 (17)	0.0423 (12)
Si3	0.52800 (16)	0.87462 (14)	0.13026 (6)	0.0385 (4)
Si4	0.77609 (16)	0.38238 (14)	0.10839 (6)	0.0372 (4)
Zn2	0.64533 (7)	0.62880 (6)	0.12387 (2)	0.0391 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.031 (3)	0.022 (3)	0.048 (4)	0.002 (2)	−0.001 (3)	−0.001 (3)
C2	0.039 (4)	0.027 (3)	0.059 (4)	0.001 (3)	0.004 (3)	−0.008 (3)
C3	0.044 (5)	0.043 (4)	0.103 (6)	−0.001 (3)	0.026 (4)	−0.020 (4)
C4	0.032 (4)	0.032 (4)	0.137 (8)	−0.001 (3)	−0.006 (5)	0.002 (5)
C5	0.045 (4)	0.039 (4)	0.090 (5)	−0.009 (3)	−0.026 (4)	0.012 (4)
C6	0.036 (4)	0.029 (3)	0.061 (4)	−0.006 (3)	−0.014 (3)	0.006 (3)
C7	0.076 (5)	0.077 (5)	0.056 (5)	−0.006 (4)	0.026 (4)	−0.017 (4)
C8	0.070 (5)	0.064 (5)	0.054 (4)	−0.006 (4)	−0.012 (4)	−0.003 (4)
C9	0.043 (5)	0.055 (5)	0.186 (9)	−0.003 (4)	−0.008 (5)	−0.058 (5)
C10	0.067 (6)	0.135 (8)	0.127 (8)	−0.033 (5)	−0.007 (5)	0.078 (6)
C11	0.075 (5)	0.060 (5)	0.092 (6)	−0.005 (4)	−0.032 (4)	0.018 (4)
C12	0.057 (5)	0.053 (4)	0.121 (7)	−0.015 (4)	0.049 (5)	−0.020 (4)
C13	0.024 (3)	0.028 (3)	0.045 (4)	−0.003 (2)	0.009 (3)	−0.001 (3)
C14	0.047 (4)	0.045 (4)	0.058 (4)	−0.009 (3)	0.018 (3)	−0.007 (3)
C15	0.070 (5)	0.068 (5)	0.060 (5)	−0.009 (4)	0.031 (4)	−0.026 (4)
C16	0.043 (5)	0.057 (5)	0.113 (7)	−0.001 (4)	0.032 (5)	−0.025 (5)
C17	0.035 (4)	0.037 (4)	0.091 (5)	0.000 (3)	0.001 (4)	−0.008 (4)
C18	0.040 (4)	0.022 (3)	0.060 (4)	−0.003 (3)	0.009 (3)	−0.007 (3)
C19	0.073 (5)	0.094 (6)	0.041 (4)	−0.013 (4)	0.012 (4)	−0.012 (4)
C20	0.053 (4)	0.044 (4)	0.073 (5)	0.008 (3)	−0.003 (3)	−0.004 (3)
C21	0.051 (4)	0.056 (4)	0.080 (5)	−0.006 (3)	0.025 (4)	0.014 (4)
C22	0.061 (5)	0.044 (4)	0.089 (5)	−0.019 (3)	0.011 (4)	−0.017 (4)

C23	0.053 (5)	0.074 (5)	0.107 (6)	0.010 (4)	0.015 (4)	−0.029 (5)
C24	0.048 (4)	0.046 (4)	0.105 (6)	−0.008 (3)	−0.012 (4)	−0.001 (4)
N1	0.035 (3)	0.022 (2)	0.043 (3)	0.003 (2)	−0.002 (2)	−0.002 (2)
N2	0.030 (3)	0.039 (3)	0.050 (3)	−0.001 (2)	0.004 (2)	−0.007 (2)
N3	0.027 (3)	0.030 (3)	0.039 (3)	−0.001 (2)	0.008 (2)	−0.001 (2)
N4	0.034 (3)	0.042 (3)	0.057 (3)	0.007 (2)	−0.001 (2)	−0.007 (3)
Si1	0.0330 (10)	0.0317 (9)	0.0642 (12)	−0.0015 (7)	−0.0019 (8)	0.0012 (8)
Si2	0.0325 (10)	0.0299 (9)	0.0517 (10)	−0.0044 (7)	0.0087 (8)	−0.0028 (8)
Zn1	0.0476 (5)	0.0279 (4)	0.0448 (4)	0.0057 (3)	0.0042 (3)	−0.0049 (3)
C25	0.030 (3)	0.017 (3)	0.058 (4)	−0.002 (2)	−0.003 (3)	−0.004 (3)
C26	0.028 (3)	0.024 (3)	0.072 (4)	0.006 (3)	−0.009 (3)	−0.010 (3)
C27	0.033 (4)	0.036 (4)	0.089 (5)	0.006 (3)	−0.023 (4)	−0.018 (3)
C28	0.040 (4)	0.021 (3)	0.121 (7)	−0.006 (3)	0.002 (4)	−0.006 (4)
C29	0.040 (4)	0.033 (4)	0.090 (5)	−0.004 (3)	0.014 (4)	0.006 (4)
C30	0.031 (3)	0.028 (3)	0.056 (4)	−0.002 (3)	0.004 (3)	0.000 (3)
C31	0.049 (4)	0.069 (5)	0.066 (5)	0.006 (3)	−0.004 (3)	−0.026 (4)
C32	0.050 (4)	0.075 (5)	0.050 (4)	0.002 (3)	0.013 (3)	−0.006 (4)
C33	0.040 (4)	0.049 (4)	0.108 (6)	0.006 (3)	0.004 (4)	0.016 (4)
C34	0.052 (5)	0.069 (5)	0.088 (5)	0.006 (4)	0.008 (4)	−0.046 (4)
C35	0.061 (5)	0.046 (4)	0.081 (5)	−0.002 (3)	−0.013 (4)	−0.014 (4)
C36	0.054 (4)	0.046 (4)	0.086 (5)	0.000 (3)	0.031 (4)	0.006 (4)
C37	0.025 (3)	0.023 (3)	0.047 (3)	0.002 (2)	0.006 (3)	−0.001 (3)
C38	0.032 (4)	0.028 (3)	0.060 (4)	−0.003 (3)	0.003 (3)	0.002 (3)
C39	0.042 (4)	0.031 (3)	0.074 (5)	−0.007 (3)	−0.007 (3)	−0.009 (3)
C40	0.032 (4)	0.037 (4)	0.087 (5)	−0.008 (3)	0.020 (4)	0.002 (4)
C41	0.046 (4)	0.041 (4)	0.059 (4)	−0.006 (3)	0.020 (3)	−0.004 (3)
C42	0.030 (3)	0.033 (3)	0.050 (4)	−0.001 (3)	0.007 (3)	0.000 (3)
C43	0.059 (4)	0.052 (4)	0.057 (4)	−0.013 (3)	−0.001 (3)	−0.011 (3)
C44	0.052 (4)	0.054 (4)	0.044 (4)	−0.002 (3)	0.013 (3)	−0.002 (3)
C45	0.053 (5)	0.077 (5)	0.089 (5)	−0.010 (4)	0.022 (4)	−0.045 (4)
C46	0.050 (4)	0.039 (4)	0.114 (6)	0.003 (3)	−0.003 (4)	0.008 (4)
C47	0.045 (4)	0.055 (4)	0.081 (5)	−0.008 (3)	0.014 (4)	0.003 (4)
C48	0.045 (4)	0.044 (4)	0.084 (5)	−0.003 (3)	−0.004 (4)	−0.012 (4)
N5	0.023 (3)	0.026 (2)	0.047 (3)	−0.0041 (19)	0.002 (2)	−0.013 (2)
N6	0.026 (3)	0.032 (3)	0.056 (3)	−0.002 (2)	0.011 (2)	−0.003 (2)
N7	0.023 (2)	0.025 (2)	0.040 (3)	−0.0024 (19)	0.0054 (19)	−0.007 (2)
N8	0.034 (3)	0.039 (3)	0.052 (3)	−0.008 (2)	0.012 (2)	−0.008 (2)
Si3	0.0314 (10)	0.0260 (9)	0.0575 (11)	0.0003 (7)	0.0042 (8)	−0.0088 (8)
Si4	0.0317 (10)	0.0265 (9)	0.0526 (10)	−0.0008 (7)	0.0054 (7)	−0.0075 (7)
Zn2	0.0448 (5)	0.0255 (4)	0.0462 (4)	−0.0073 (3)	0.0047 (3)	−0.0049 (3)

Geometric parameters (Å, °)

C1—N1	1.389 (6)	C25—C26	1.408 (7)
C1—C6	1.403 (7)	C25—N5	1.411 (6)
C1—C2	1.426 (7)	C26—C27	1.391 (7)
C2—C3	1.393 (8)	C26—C31	1.490 (8)
C2—C7	1.471 (8)	C27—C28	1.369 (9)
C3—C4	1.350 (9)	C27—H27A	0.9300

C3—H3A	0.9300	C28—C29	1.368 (9)
C4—C5	1.371 (9)	C28—H28A	0.9300
C4—H4A	0.9300	C29—C30	1.380 (7)
C5—C6	1.389 (8)	C29—H29A	0.9300
C5—H5A	0.9300	C30—C32	1.505 (8)
C6—C8	1.512 (8)	C31—H31A	0.9600
C7—H7A	0.9600	C31—H31B	0.9600
C7—H7B	0.9600	C31—H31C	0.9600
C7—H7C	0.9600	C32—H32A	0.9600
C8—H8A	0.9600	C32—H32B	0.9600
C8—H8B	0.9600	C32—H32C	0.9600
C8—H8C	0.9600	C33—Si3	1.843 (6)
C9—Si1	1.864 (6)	C33—H33A	0.9600
C9—H9A	0.9600	C33—H33B	0.9600
C9—H9B	0.9600	C33—H33C	0.9600
C9—H9C	0.9600	C34—Si3	1.871 (6)
C10—Si1	1.862 (7)	C34—H34A	0.9600
C10—H10A	0.9600	C34—H34B	0.9600
C10—H10B	0.9600	C34—H34C	0.9600
C10—H10C	0.9600	C35—N6	1.474 (7)
C11—N2	1.449 (7)	C35—H35A	0.9600
C11—H11A	0.9600	C35—H35B	0.9600
C11—H11B	0.9600	C35—H35C	0.9600
C11—H11C	0.9600	C36—N6	1.469 (6)
C12—N2	1.469 (7)	C36—H36A	0.9600
C12—H12A	0.9600	C36—H36B	0.9600
C12—H12B	0.9600	C36—H36C	0.9600
C12—H12C	0.9600	C37—C42	1.390 (7)
C13—C18	1.393 (8)	C37—C38	1.404 (7)
C13—C14	1.404 (8)	C37—N7	1.428 (6)
C13—N3	1.422 (6)	C38—C39	1.387 (7)
C14—C15	1.385 (8)	C38—C43	1.507 (7)
C14—C19	1.495 (9)	C39—C40	1.368 (8)
C15—C16	1.360 (10)	C39—H39A	0.9300
C15—H15A	0.9300	C40—C41	1.360 (8)
C16—C17	1.372 (9)	C40—H40A	0.9300
C16—H16A	0.9300	C41—C42	1.402 (7)
C17—C18	1.385 (7)	C41—H41A	0.9300
C17—H17A	0.9300	C42—C44	1.505 (7)
C18—C20	1.511 (8)	C43—H43A	0.9600
C19—H19A	0.9600	C43—H43B	0.9600
C19—H19B	0.9600	C43—H43C	0.9600
C19—H19C	0.9600	C44—H44A	0.9600
C20—H20A	0.9600	C44—H44B	0.9600
C20—H20B	0.9600	C44—H44C	0.9600
C20—H20C	0.9600	C45—Si4	1.872 (6)
C21—Si2	1.860 (6)	C45—H45A	0.9600
C21—H21A	0.9600	C45—H45B	0.9600
C21—H21B	0.9600	C45—H45C	0.9600

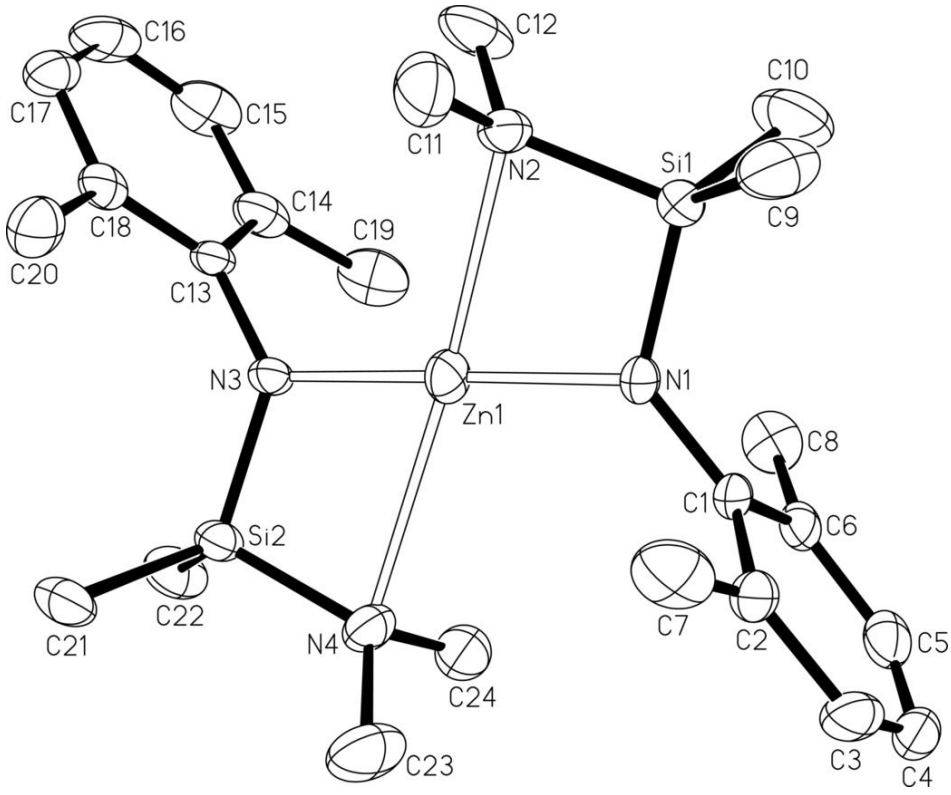
C21—H21C	0.9600	C46—Si4	1.867 (6)
C22—Si2	1.862 (6)	C46—H46A	0.9600
C22—H22A	0.9600	C46—H46B	0.9600
C22—H22B	0.9600	C46—H46C	0.9600
C22—H22C	0.9600	C47—N8	1.487 (6)
C23—N4	1.485 (7)	C47—H47A	0.9600
C23—H23A	0.9600	C47—H47B	0.9600
C23—H23B	0.9600	C47—H47C	0.9600
C23—H23C	0.9600	C48—N8	1.463 (7)
C24—N4	1.435 (7)	C48—H48A	0.9600
C24—H24A	0.9600	C48—H48B	0.9600
C24—H24B	0.9600	C48—H48C	0.9600
C24—H24C	0.9600	N5—Si3	1.701 (4)
N1—Si1	1.712 (4)	N5—Zn2	1.871 (4)
N1—Zn1	1.865 (4)	N6—Si3	1.757 (4)
N2—Si1	1.756 (5)	N6—Zn2	2.396 (4)
N2—Zn1	2.454 (4)	N7—Si4	1.696 (4)
N3—Si2	1.694 (4)	N7—Zn2	1.856 (4)
N3—Zn1	1.863 (4)	N8—Si4	1.735 (4)
N4—Si2	1.745 (5)	Si3—Zn2	2.806 (2)
C25—C30	1.404 (7)	Si4—Zn2	2.889 (2)
N1—C1—C6	121.2 (5)	C26—C25—N5	120.4 (5)
N1—C1—C2	120.4 (5)	C27—C26—C25	119.0 (6)
C6—C1—C2	118.3 (5)	C27—C26—C31	120.2 (6)
C3—C2—C1	117.9 (6)	C25—C26—C31	120.8 (5)
C3—C2—C7	121.6 (6)	C28—C27—C26	121.5 (6)
C1—C2—C7	120.5 (5)	C28—C27—H27A	119.2
C4—C3—C2	122.9 (7)	C26—C27—H27A	119.2
C4—C3—H3A	118.5	C29—C28—C27	119.4 (6)
C2—C3—H3A	118.5	C29—C28—H28A	120.3
C3—C4—C5	119.8 (7)	C27—C28—H28A	120.3
C3—C4—H4A	120.1	C28—C29—C30	121.5 (6)
C5—C4—H4A	120.1	C28—C29—H29A	119.2
C4—C5—C6	120.3 (7)	C30—C29—H29A	119.2
C4—C5—H5A	119.8	C29—C30—C25	119.7 (6)
C6—C5—H5A	119.8	C29—C30—C32	120.0 (5)
C5—C6—C1	120.7 (6)	C25—C30—C32	120.3 (5)
C5—C6—C8	118.4 (6)	C26—C31—H31A	109.5
C1—C6—C8	120.8 (5)	C26—C31—H31B	109.5
C2—C7—H7A	109.5	H31A—C31—H31B	109.5
C2—C7—H7B	109.5	C26—C31—H31C	109.5
H7A—C7—H7B	109.5	H31A—C31—H31C	109.5
C2—C7—H7C	109.5	H31B—C31—H31C	109.5
H7A—C7—H7C	109.5	C30—C32—H32A	109.5
H7B—C7—H7C	109.5	C30—C32—H32B	109.5
C6—C8—H8A	109.5	H32A—C32—H32B	109.5
C6—C8—H8B	109.5	C30—C32—H32C	109.5
H8A—C8—H8B	109.5	H32A—C32—H32C	109.5
C6—C8—H8C	109.5	H32B—C32—H32C	109.5

H8A—C8—H8C	109.5	Si3—C33—H33A	109.5
H8B—C8—H8C	109.5	Si3—C33—H33B	109.5
Si1—C9—H9A	109.5	H33A—C33—H33B	109.5
Si1—C9—H9B	109.5	Si3—C33—H33C	109.5
H9A—C9—H9B	109.5	H33A—C33—H33C	109.5
Si1—C9—H9C	109.5	H33B—C33—H33C	109.5
H9A—C9—H9C	109.5	Si3—C34—H34A	109.5
H9B—C9—H9C	109.5	Si3—C34—H34B	109.5
Si1—C10—H10A	109.5	H34A—C34—H34B	109.5
Si1—C10—H10B	109.5	Si3—C34—H34C	109.5
H10A—C10—H10B	109.5	H34A—C34—H34C	109.5
Si1—C10—H10C	109.5	H34B—C34—H34C	109.5
H10A—C10—H10C	109.5	N6—C35—H35A	109.5
H10B—C10—H10C	109.5	N6—C35—H35B	109.5
N2—C11—H11A	109.5	H35A—C35—H35B	109.5
N2—C11—H11B	109.5	N6—C35—H35C	109.5
H11A—C11—H11B	109.5	H35A—C35—H35C	109.5
N2—C11—H11C	109.5	H35B—C35—H35C	109.5
H11A—C11—H11C	109.5	N6—C36—H36A	109.5
H11B—C11—H11C	109.5	N6—C36—H36B	109.5
N2—C12—H12A	109.5	H36A—C36—H36B	109.5
N2—C12—H12B	109.5	N6—C36—H36C	109.5
H12A—C12—H12B	109.5	H36A—C36—H36C	109.5
N2—C12—H12C	109.5	H36B—C36—H36C	109.5
H12A—C12—H12C	109.5	C42—C37—C38	119.0 (5)
H12B—C12—H12C	109.5	C42—C37—N7	119.8 (5)
C18—C13—C14	118.5 (5)	C38—C37—N7	121.2 (5)
C18—C13—N3	121.1 (5)	C39—C38—C37	119.5 (5)
C14—C13—N3	120.4 (5)	C39—C38—C43	119.0 (5)
C15—C14—C13	118.8 (6)	C37—C38—C43	121.5 (5)
C15—C14—C19	120.6 (6)	C40—C39—C38	120.9 (6)
C13—C14—C19	120.5 (5)	C40—C39—H39A	119.5
C16—C15—C14	122.7 (7)	C38—C39—H39A	119.5
C16—C15—H15A	118.7	C41—C40—C39	120.3 (5)
C14—C15—H15A	118.7	C41—C40—H40A	119.9
C15—C16—C17	118.6 (6)	C39—C40—H40A	119.9
C15—C16—H16A	120.7	C40—C41—C42	120.4 (6)
C17—C16—H16A	120.7	C40—C41—H41A	119.8
C16—C17—C18	121.0 (7)	C42—C41—H41A	119.8
C16—C17—H17A	119.5	C37—C42—C41	119.8 (5)
C18—C17—H17A	119.5	C37—C42—C44	120.8 (5)
C17—C18—C13	120.4 (6)	C41—C42—C44	119.3 (5)
C17—C18—C20	118.2 (6)	C38—C43—H43A	109.5
C13—C18—C20	121.4 (5)	C38—C43—H43B	109.5
C14—C19—H19A	109.5	H43A—C43—H43B	109.5
C14—C19—H19B	109.5	C38—C43—H43C	109.5
H19A—C19—H19B	109.5	H43A—C43—H43C	109.5
C14—C19—H19C	109.5	H43B—C43—H43C	109.5
H19A—C19—H19C	109.5	C42—C44—H44A	109.5

H19B—C19—H19C	109.5	C42—C44—H44B	109.5
C18—C20—H20A	109.5	H44A—C44—H44B	109.5
C18—C20—H20B	109.5	C42—C44—H44C	109.5
H20A—C20—H20B	109.5	H44A—C44—H44C	109.5
C18—C20—H20C	109.5	H44B—C44—H44C	109.5
H20A—C20—H20C	109.5	Si4—C45—H45A	109.5
H20B—C20—H20C	109.5	Si4—C45—H45B	109.5
Si2—C21—H21A	109.5	H45A—C45—H45B	109.5
Si2—C21—H21B	109.5	Si4—C45—H45C	109.5
H21A—C21—H21B	109.5	H45A—C45—H45C	109.5
Si2—C21—H21C	109.5	H45B—C45—H45C	109.5
H21A—C21—H21C	109.5	Si4—C46—H46A	109.5
H21B—C21—H21C	109.5	Si4—C46—H46B	109.5
Si2—C22—H22A	109.5	H46A—C46—H46B	109.5
Si2—C22—H22B	109.5	Si4—C46—H46C	109.5
H22A—C22—H22B	109.5	H46A—C46—H46C	109.5
Si2—C22—H22C	109.5	H46B—C46—H46C	109.5
H22A—C22—H22C	109.5	N8—C47—H47A	109.5
H22B—C22—H22C	109.5	N8—C47—H47B	109.5
N4—C23—H23A	109.5	H47A—C47—H47B	109.5
N4—C23—H23B	109.5	N8—C47—H47C	109.5
H23A—C23—H23B	109.5	H47A—C47—H47C	109.5
N4—C23—H23C	109.5	H47B—C47—H47C	109.5
H23A—C23—H23C	109.5	N8—C48—H48A	109.5
H23B—C23—H23C	109.5	N8—C48—H48B	109.5
N4—C24—H24A	109.5	H48A—C48—H48B	109.5
N4—C24—H24B	109.5	N8—C48—H48C	109.5
H24A—C24—H24B	109.5	H48A—C48—H48C	109.5
N4—C24—H24C	109.5	H48B—C48—H48C	109.5
H24A—C24—H24C	109.5	C25—N5—Si3	129.3 (3)
H24B—C24—H24C	109.5	C25—N5—Zn2	126.4 (3)
C1—N1—Si1	127.7 (4)	Si3—N5—Zn2	103.5 (2)
C1—N1—Zn1	128.2 (3)	C36—N6—C35	110.2 (5)
Si1—N1—Zn1	104.2 (2)	C36—N6—Si3	120.8 (4)
C11—N2—C12	111.4 (5)	C35—N6—Si3	117.8 (4)
C11—N2—Si1	118.2 (4)	C36—N6—Zn2	118.6 (4)
C12—N2—Si1	119.0 (4)	C35—N6—Zn2	102.2 (3)
C11—N2—Zn1	108.7 (4)	Si3—N6—Zn2	83.50 (17)
C12—N2—Zn1	113.3 (3)	C37—N7—Si4	127.4 (3)
Si1—N2—Zn1	82.41 (17)	C37—N7—Zn2	123.0 (3)
C13—N3—Si2	128.7 (3)	Si4—N7—Zn2	108.8 (2)
C13—N3—Zn1	122.6 (3)	C48—N8—C47	109.6 (4)
Si2—N3—Zn1	107.9 (2)	C48—N8—Si4	118.9 (4)
C24—N4—C23	109.9 (5)	C47—N8—Si4	122.0 (4)
C24—N4—Si2	117.7 (4)	N5—Si3—N6	98.4 (2)
C23—N4—Si2	120.8 (4)	N5—Si3—C33	112.3 (2)
N1—Si1—N2	99.1 (2)	N6—Si3—C33	113.5 (3)
N1—Si1—C10	115.3 (3)	N5—Si3—C34	116.7 (3)
N2—Si1—C10	110.4 (3)	N6—Si3—C34	108.6 (3)

N1—Si1—C9	113.4 (3)	C33—Si3—C34	107.3 (3)
N2—Si1—C9	111.9 (3)	N5—Si3—Zn2	40.42 (13)
C10—Si1—C9	106.6 (4)	N6—Si3—Zn2	58.04 (15)
N3—Si2—N4	99.7 (2)	C33—Si3—Zn2	127.5 (2)
N3—Si2—C21	115.4 (3)	C34—Si3—Zn2	124.8 (2)
N4—Si2—C21	109.0 (3)	N7—Si4—N8	100.7 (2)
N3—Si2—C22	112.5 (2)	N7—Si4—C46	111.7 (2)
N4—Si2—C22	113.1 (3)	N8—Si4—C46	113.9 (3)
C21—Si2—C22	107.2 (3)	N7—Si4—C45	115.6 (3)
N3—Si2—Zn1	38.03 (14)	N8—Si4—C45	107.4 (3)
N4—Si2—Zn1	61.91 (16)	C46—Si4—C45	107.6 (3)
C21—Si2—Zn1	121.8 (2)	N7—Si4—Zn2	37.46 (13)
C22—Si2—Zn1	129.9 (2)	N8—Si4—Zn2	63.91 (16)
N3—Zn1—N1	172.83 (18)	C46—Si4—Zn2	132.3 (2)
N3—Zn1—N2	108.62 (17)	C45—Si4—Zn2	118.6 (2)
N1—Zn1—N2	73.96 (17)	N7—Zn2—N5	175.11 (18)
N3—Zn1—Si1	145.60 (13)	N7—Zn2—N6	110.30 (16)
N1—Zn1—Si1	36.01 (13)	N5—Zn2—N6	74.56 (16)
N2—Zn1—Si1	38.08 (11)	N7—Zn2—Si3	148.71 (13)
N3—Zn1—Si2	34.06 (12)	N5—Zn2—Si3	36.13 (13)
N1—Zn1—Si2	144.76 (14)	N6—Zn2—Si3	38.46 (10)
N2—Zn1—Si2	140.86 (11)	N7—Zn2—Si4	33.75 (12)
Si1—Zn1—Si2	177.91 (6)	N5—Zn2—Si4	141.55 (13)
C30—C25—C26	118.9 (5)	N6—Zn2—Si4	143.08 (11)
C30—C25—N5	120.6 (5)	Si3—Zn2—Si4	174.78 (5)

Fig. 1


C16
C17
C15
C12
C11
C10
N2
Si1
C9
C14
C18
C19
C20
C13
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N1
Zn1
C8
C1
C6
Si2
C22
C21
N4
C24
C7
C2
C5
C23
C3
C4