Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(2-cyclobutyliminomethyl-4,6-dihydroselenophenolato)zinc(II)

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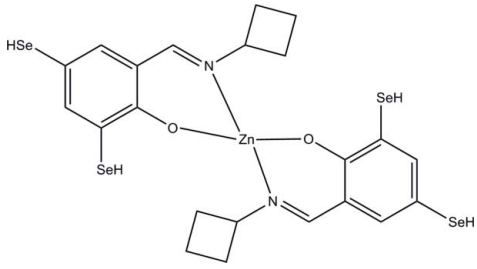
Received 10 August 2009; accepted 11 August 2009

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.010 Å; R factor = 0.046; wR factor = 0.130; data-to-parameter ratio = 14.7.

In the title complex, $[Zn(C_{11}H_{12}NOSe_2)_2]$, the Zn^{II} atom is four-coordinated by two *O*,*N*-bidentate Schiff base ligands in a distorted tetrahedral geometry.

Related literature

For background to Schiff bases, see: Shi *et al.* (2008); Xu *et al.* (2009). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Zn(C_{11}H_{12}NOSe_2)_2]$
M_r = 729.64
Triclinic, $P\overline{1}$
a = 8.0876 (6) Å
b = 12.2986 (16) Å
c = 12.7956 (16) Å
α = 93.166 (6)°
β = 108.216 (6)°
γ = 95.716 (6)°
V = 1197.9 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 7.12 mm^{-1}
T = 296 K
0.32 × 0.28 × 0.25 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968) T_{min} = 0.209, T_{max} = 0.269 (expected range = 0.131–0.168)
6184 measured reflections
4183 independent reflections
3165 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
3 standard reflections
every 200 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.130
S = 1.05
4183 reflections
284 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −1.48 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—N1	2.002 (5)	Zn1—O1	1.908 (4)
Zn1—N2	1.987 (5)	Zn1—O2	1.911 (4)

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The project was supported by the Scientific Research Foundation for Returned Overseas Chinese Scholars, State Education Ministry, Educational Commission of Hubei Province (D20091703) and the Natural Science Foundation of Hubei Province (2008CDB038).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5040).

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supplementary materials

Acta Cryst. (2009). E**65**, m1076 [**doi:10.1107/S1600536809031596**]

Bis(2-cyclobutyliminomethyl-4,6-dihydroselenophenolato)zinc(II)

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Comment

There has been much research interest in Schiff base metal complexes due to their molecular architectures and biological activities (Shi *et al.*, 2008; Xu *et al.*, 2009). In this work, we report here the crystal structure of the title compound, (I). In (I), all bond lengths are within normal ranges (Allen *et al.*, 1987) (Fig. 1). The Zn(II) is four-coordinated in a distorted tetrahedral coordination by two N atoms and two O atoms of the Schiff base ligands.

Experimental

A mixture of 3,5-dihydroseleno-2-hydroxybenzaldehyde (564 mg, 2 mmol), cyclobutanamine (142 mg, 2 mmol) and $ZnCl_2$ (1 mmol, 134 mg) in methanol (10 ml) was stirred for 1 h. After keeping the filtrate in air for 8 d, colorless blocks of (I) were formed.

Refinement

All H atoms were positioned geometrically (C—H = 0.93–0.96 Å, Se—H = 0.82Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(carrier).

Figures

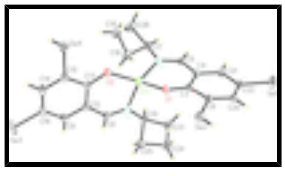


Fig. 1. The molecular structure of (I) showing 30% probability displacement ellipsoids.

Bis(2-cyclobutyliminomethyl-4,6-dihydroselenophenolato)zinc(II)

Crystal data

$[Zn(C_{11}H_{12}NOSe_2)_2]$	$Z = 2$
$M_r = 729.64$	$F_{000} = 704$
Triclinic, $P\overline{1}$	$D_x = 2.023$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 8.0876$ (6) Å	Cell parameters from 25 reflections
$b = 12.2986$ (16) Å	$\theta = 9$–12º
$c = 12.7956$ (16) Å	$\mu = 7.12$ mm^{-1}
$\alpha = 93.166$ (6)º	$T = 296$ K
$\beta = 108.216$ (6)º	Block, colorless

γ = 95.716 (6)º	0.32 × 0.28 × 0.25 mm
V = 1197.9 (2) Å^3	

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.024
Radiation source: fine-focus sealed tube	θ_{max} = 25.0º
Monochromator: graphite	θ_{min} = 1.7º
T = 296 K	h = −9→9
ω/2θ scans	k = −11→14
Absorption correction: ψ scan (North *et al.*, 1968)	l = −15→14
T_{min} = 0.209, T_{max} = 0.269	3 standard reflections
6184 measured reflections	every 200 reflections
4183 independent reflections	intensity decay: 1%
3165 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
$R[F^2 > 2\sigma(F^2)]$ = 0.046	H-atom parameters constrained
$wR(F^2)$ = 0.130	$w = 1/[\sigma^2(F_o^2) + (0.0591P)^2 + 4.4413P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max} < 0.001$
4183 reflections	$\Delta\rho_{max}$ = 0.73 e Å^{-3}
284 parameters	$\Delta\rho_{min}$ = −1.48 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}
C3	−0.0178 (8)	0.4782 (5)	0.1563 (5)	0.0251 (13)

C4	−0.1460 (8)	0.5305 (5)	0.0777 (5)	0.0270 (14)
C5	−0.1629 (8)	0.6448 (5)	0.0877 (5)	0.0275 (14)
H5	−0.2448	0.6703	0.0285	0.033*
C6	−0.0144 (8)	0.3665 (5)	0.1286 (5)	0.0285 (14)
C8	0.2692 (9)	0.8003 (5)	0.6800 (5)	0.0334 (15)
H8	0.1939	0.7846	0.7206	0.040*
C9	0.0370 (9)	0.7100 (5)	0.5214 (5)	0.0333 (15)
H9	−0.0288	0.7034	0.5692	0.040*
C10	−0.2221 (9)	0.6202 (6)	0.3895 (6)	0.0351 (16)
H10	−0.2957	0.6743	0.3521	0.042*
C12	0.2138 (8)	0.7668 (5)	0.5674 (5)	0.0316 (15)
C13	0.3264 (8)	0.7890 (5)	0.5038 (5)	0.0301 (15)
C14	0.5457 (9)	0.8801 (6)	0.6732 (6)	0.0381 (17)
H14	0.6567	0.9177	0.7088	0.046*
C15	0.4932 (8)	0.8481 (5)	0.5614 (6)	0.0323 (15)
C16	0.4309 (9)	0.8554 (6)	0.7316 (6)	0.0394 (17)
C17	−0.1131 (9)	0.8311 (5)	0.1571 (6)	0.0381 (17)
H17	−0.2085	0.8365	0.0888	0.046*
C18	−0.1400 (11)	0.8977 (6)	0.2528 (8)	0.053 (2)
H18A	−0.2618	0.9052	0.2436	0.063*
H18B	−0.0817	0.8737	0.3246	0.063*
C19	−0.0413 (11)	0.9963 (6)	0.2242 (8)	0.059 (2)
H19A	0.0410	1.0404	0.2879	0.071*
H19B	−0.1158	1.0415	0.1747	0.071*
C20	−0.1314 (8)	0.3059 (5)	0.0389 (5)	0.0298 (14)
H20	−0.1264	0.2313	0.0265	0.036*
C21	−0.2633 (8)	0.4682 (5)	−0.0173 (5)	0.0314 (15)
H21	−0.3447	0.5025	−0.0692	0.038*
C22	−0.2581 (8)	0.3579 (5)	−0.0336 (5)	0.0313 (15)
C23	−0.2772 (10)	0.5116 (6)	0.3183 (7)	0.049 (2)
H23A	−0.1871	0.4629	0.3319	0.059*
H23B	−0.3285	0.5187	0.2400	0.059*
C24	−0.4130 (10)	0.4865 (7)	0.3787 (7)	0.048 (2)
H24A	−0.5283	0.5064	0.3405	0.058*
H24B	−0.4207	0.4121	0.3998	0.058*
C25	−0.3008 (10)	0.5711 (7)	0.4725 (6)	0.048 (2)
H25A	−0.3676	0.6196	0.5008	0.058*
H25B	−0.2175	0.5401	0.5320	0.058*
C26	0.0420 (13)	0.9166 (6)	0.1673 (9)	0.066 (3)
H26A	0.1535	0.8983	0.2142	0.079*
H26B	0.0501	0.9379	0.0970	0.079*
N1	−0.0797 (7)	0.7162 (4)	0.1679 (4)	0.0288 (12)
N2	−0.0372 (7)	0.6683 (4)	0.4224 (4)	0.0297 (12)
O1	0.0927 (6)	0.5283 (4)	0.2458 (4)	0.0331 (11)
O2	0.2880 (6)	0.7612 (4)	0.3987 (4)	0.0372 (11)
Se1	−0.41129 (11)	0.27481 (7)	−0.16339 (7)	0.0561 (3)
H1	−0.5133	0.2804	−0.1676	0.084*
Se2	0.16624 (10)	0.29622 (6)	0.22268 (6)	0.0406 (2)
H2	0.1451	0.2297	0.2068	0.061*

Se3	0.50639 (12)	0.89915 (10)	0.88567 (7)	0.0660 (3)
H3	0.4248	0.9208	0.9027	0.099*
Se4	0.64728 (10)	0.88355 (6)	0.48096 (7)	0.0435 (2)
H4	0.7125	0.9397	0.5105	0.065*
Zn1	0.08132 (11)	0.67103 (7)	0.30778 (7)	0.0407 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C3	0.025 (3)	0.026 (3)	0.022 (3)	−0.005 (3)	0.008 (3)	−0.002 (3)
C4	0.024 (3)	0.031 (3)	0.027 (3)	−0.002 (3)	0.010 (3)	0.001 (3)
C5	0.028 (3)	0.026 (3)	0.026 (3)	0.002 (3)	0.007 (3)	0.004 (3)
C6	0.028 (3)	0.032 (4)	0.027 (3)	0.002 (3)	0.012 (3)	0.002 (3)
C8	0.038 (4)	0.041 (4)	0.023 (3)	0.011 (3)	0.011 (3)	0.000 (3)
C9	0.036 (4)	0.037 (4)	0.029 (4)	−0.002 (3)	0.015 (3)	0.001 (3)
C10	0.028 (4)	0.039 (4)	0.035 (4)	−0.002 (3)	0.008 (3)	0.001 (3)
C12	0.029 (3)	0.031 (4)	0.030 (4)	0.003 (3)	0.004 (3)	−0.002 (3)
C13	0.029 (3)	0.026 (3)	0.030 (4)	0.002 (3)	0.003 (3)	−0.004 (3)
C14	0.028 (4)	0.040 (4)	0.037 (4)	0.008 (3)	−0.003 (3)	−0.009 (3)
C15	0.028 (3)	0.029 (4)	0.037 (4)	0.003 (3)	0.006 (3)	0.000 (3)
C16	0.033 (4)	0.046 (4)	0.029 (4)	0.006 (3)	−0.002 (3)	−0.012 (3)
C17	0.043 (4)	0.023 (3)	0.039 (4)	0.004 (3)	0.002 (3)	0.002 (3)
C18	0.050 (5)	0.035 (4)	0.076 (6)	0.009 (4)	0.023 (4)	0.002 (4)
C19	0.046 (5)	0.035 (4)	0.090 (7)	0.002 (4)	0.018 (5)	−0.009 (4)
C20	0.033 (4)	0.022 (3)	0.032 (4)	−0.005 (3)	0.012 (3)	−0.003 (3)
C21	0.026 (3)	0.035 (4)	0.030 (4)	0.002 (3)	0.004 (3)	−0.002 (3)
C22	0.026 (3)	0.032 (4)	0.030 (4)	−0.007 (3)	0.005 (3)	−0.005 (3)
C23	0.043 (5)	0.048 (5)	0.055 (5)	−0.011 (4)	0.021 (4)	−0.014 (4)
C24	0.039 (4)	0.047 (5)	0.060 (5)	−0.009 (3)	0.023 (4)	0.002 (4)
C25	0.037 (4)	0.066 (5)	0.041 (4)	−0.010 (4)	0.019 (3)	0.000 (4)
C26	0.076 (7)	0.038 (5)	0.100 (8)	0.006 (4)	0.052 (6)	0.008 (5)
N1	0.033 (3)	0.024 (3)	0.028 (3)	0.002 (2)	0.007 (2)	0.004 (2)
N2	0.031 (3)	0.030 (3)	0.025 (3)	−0.003 (2)	0.007 (2)	−0.002 (2)
O1	0.034 (3)	0.033 (3)	0.026 (2)	0.004 (2)	0.003 (2)	−0.005 (2)
O2	0.035 (3)	0.043 (3)	0.030 (3)	−0.009 (2)	0.011 (2)	−0.006 (2)
Se1	0.0466 (5)	0.0481 (5)	0.0492 (5)	−0.0046 (4)	−0.0123 (4)	−0.0193 (4)
Se2	0.0428 (4)	0.0318 (4)	0.0409 (4)	0.0097 (3)	0.0028 (3)	0.0024 (3)
Se3	0.0512 (5)	0.1048 (8)	0.0278 (4)	0.0108 (5)	−0.0035 (4)	−0.0202 (4)
Se4	0.0340 (4)	0.0438 (5)	0.0533 (5)	−0.0036 (3)	0.0181 (3)	0.0005 (4)
Zn1	0.0417 (5)	0.0415 (5)	0.0346 (5)	0.0002 (4)	0.0088 (4)	−0.0034 (4)

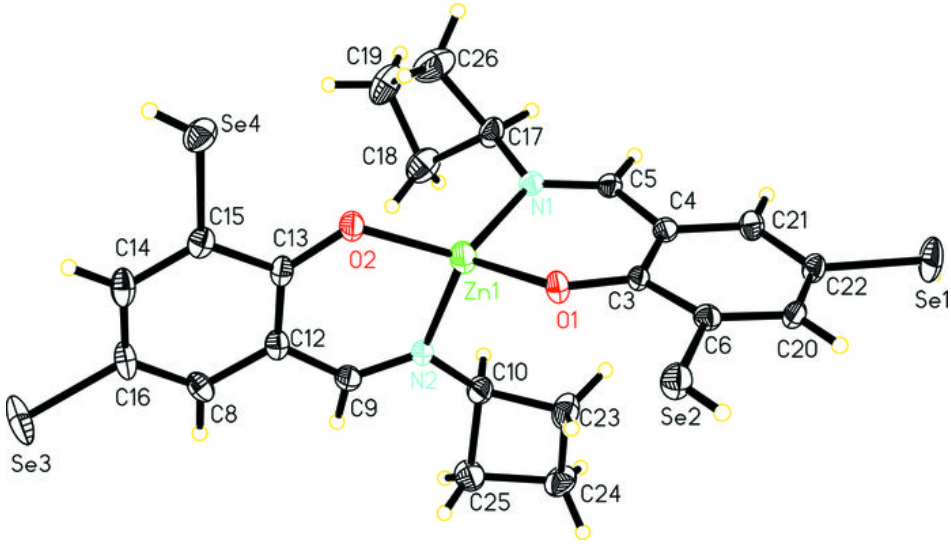
Geometric parameters (Å, °)

C3—O1	1.290 (7)	C17—H17	0.9800
C3—C6	1.405 (9)	C18—C19	1.509 (12)
C3—C4	1.432 (9)	C18—H18A	0.9700
C4—C21	1.413 (9)	C18—H18B	0.9700
C4—C5	1.429 (9)	C19—C26	1.518 (12)
C5—N1	1.276 (8)	C19—H19A	0.9700

C5—H5	0.9300	C19—H19B	0.9700
C6—C20	1.361 (9)	C20—C22	1.386 (9)
C6—Se2	1.896 (6)	C20—H20	0.9300
C8—C16	1.356 (10)	C21—C22	1.368 (9)
C8—C12	1.393 (9)	C21—H21	0.9300
C8—H8	0.9300	C22—Se1	1.900 (6)
C9—N2	1.272 (8)	C23—C24	1.545 (10)
C9—C12	1.452 (9)	C23—H23A	0.9700
C9—H9	0.9300	C23—H23B	0.9700
C10—N2	1.472 (8)	C24—C25	1.530 (11)
C10—C23	1.518 (10)	C24—H24A	0.9700
C10—C25	1.522 (10)	C24—H24B	0.9700
C10—H10	0.9800	C25—H25A	0.9700
C12—C13	1.416 (9)	C25—H25B	0.9700
C13—O2	1.299 (8)	C26—H26A	0.9700
C13—C15	1.420 (9)	C26—H26B	0.9700
C14—C15	1.380 (9)	Zn1—N1	2.002 (5)
C14—C16	1.384 (11)	Zn1—N2	1.987 (5)
C14—H14	0.9300	Zn1—O1	1.908 (4)
C15—Se4	1.883 (7)	Zn1—O2	1.911 (4)
C16—Se3	1.902 (7)	Se1—H1	0.8200
C17—N1	1.470 (8)	Se2—H2	0.8200
C17—C18	1.519 (11)	Se3—H3	0.8200
C17—C26	1.522 (11)	Se4—H4	0.8200
O1—C3—C6	120.5 (6)	C18—C19—H19B	114.1
O1—C3—C4	123.8 (6)	C26—C19—H19B	114.1
C6—C3—C4	115.6 (5)	H19A—C19—H19B	111.3
C21—C4—C5	116.3 (6)	C6—C20—C22	118.6 (6)
C21—C4—C3	119.7 (6)	C6—C20—H20	120.7
C5—C4—C3	124.0 (6)	C22—C20—H20	120.7
N1—C5—C4	128.0 (6)	C22—C21—C4	120.6 (6)
N1—C5—H5	116.0	C22—C21—H21	119.7
C4—C5—H5	116.0	C4—C21—H21	119.7
C20—C6—C3	124.4 (6)	C21—C22—C20	120.9 (6)
C20—C6—Se2	118.2 (5)	C21—C22—Se1	120.6 (5)
C3—C6—Se2	117.5 (5)	C20—C22—Se1	118.3 (5)
C16—C8—C12	121.3 (7)	C10—C23—C24	86.9 (6)
C16—C8—H8	119.3	C10—C23—H23A	114.2
C12—C8—H8	119.3	C24—C23—H23A	114.2
N2—C9—C12	126.8 (6)	C10—C23—H23B	114.2
N2—C9—H9	116.6	C24—C23—H23B	114.2
C12—C9—H9	116.6	H23A—C23—H23B	111.3
N2—C10—C23	118.6 (6)	C25—C24—C23	88.1 (5)
N2—C10—C25	121.4 (6)	C25—C24—H24A	114.0
C23—C10—C25	89.4 (6)	C23—C24—H24A	114.0
N2—C10—H10	108.6	C25—C24—H24B	114.0
C23—C10—H10	108.6	C23—C24—H24B	114.0
C25—C10—H10	108.6	H24A—C24—H24B	111.2
C8—C12—C13	120.5 (6)	C10—C25—C24	87.4 (6)

C8—C12—C9	116.2 (6)	C10—C25—H25A	114.1
C13—C12—C9	123.3 (6)	C24—C25—H25A	114.1
O2—C13—C12	125.4 (6)	C10—C25—H25B	114.1
O2—C13—C15	118.6 (6)	C24—C25—H25B	114.1
C12—C13—C15	116.0 (6)	H25A—C25—H25B	111.3
C15—C14—C16	119.1 (6)	C19—C26—C17	88.0 (6)
C15—C14—H14	120.5	C19—C26—H26A	114.0
C16—C14—H14	120.5	C17—C26—H26A	114.0
C14—C15—C13	122.6 (6)	C19—C26—H26B	114.0
C14—C15—Se4	119.3 (5)	C17—C26—H26B	114.0
C13—C15—Se4	118.1 (5)	H26A—C26—H26B	111.2
C8—C16—C14	120.6 (6)	C5—N1—C17	118.3 (5)
C8—C16—Se3	121.0 (6)	C5—N1—Zn1	120.5 (4)
C14—C16—Se3	118.4 (5)	C17—N1—Zn1	121.0 (4)
N1—C17—C18	119.7 (6)	C9—N2—C10	118.7 (6)
N1—C17—C26	117.8 (6)	C9—N2—Zn1	123.1 (5)
C18—C17—C26	87.0 (6)	C10—N2—Zn1	118.2 (4)
N1—C17—H17	110.1	C3—O1—Zn1	125.6 (4)
C18—C17—H17	110.1	C13—O2—Zn1	125.8 (4)
C26—C17—H17	110.1	C22—Se1—H1	109.5
C19—C18—C17	88.5 (7)	C6—Se2—H2	109.5
C19—C18—H18A	113.9	C16—Se3—H3	109.5
C17—C18—H18A	113.9	C15—Se4—H4	109.5
C19—C18—H18B	113.9	O1—Zn1—O2	121.3 (2)
C17—C18—H18B	113.9	O1—Zn1—N2	113.3 (2)
H18A—C18—H18B	111.1	O2—Zn1—N2	94.9 (2)
C18—C19—C26	87.5 (6)	O1—Zn1—N1	94.9 (2)
C18—C19—H19A	114.1	O2—Zn1—N1	123.5 (2)
C26—C19—H19A	114.1	N2—Zn1—N1	109.6 (2)

Fig. 1


C19
C26
Se4
C17
C18
N1
C5
C4
C21
C15
C13
C14
O2
Zn1
C22
Se1
O1
C3
C12
C6
C20
N2
C10
C16
C8
C9
C23
Se2
Se3
C25
C24