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Bis(L-prolinato-*N*,*O*)zinc(II)

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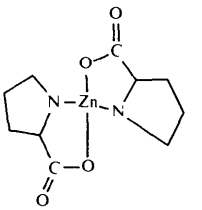
Abstract

The title *trans* complex, [$Zn(C_5H_7NO_2)_2$], forms a polymer and shows a helical structure along the 2_1 direction with atoms O4($2-x$, $y-\frac{1}{2}$, $-z$), Zn, N(2), C(7) and C(6) forming the repeating unit. The Zn atom has trigonal bipyramidal geometry and the pyrrolidine rings adopt envelope conformations.

Comment

The title complex results from the reaction of zinc oxide with L-proline. The two L-proline molecules in the complex are coordinated to the Zn atom *via* their N and carboxylic O atoms. The two bidentate ligands are *trans* with respect to each other, as in the case of the hexacoordinate complex bis(L-prolinato)copper(II) dihydrate (Mathieson & Welsh, 1952). The two pyrrolidine rings adopt envelope conformations with best mirror planes bisecting the N(1)—C(2) and N(2)—C(7) bonds, and passing through the C(4) and C(9) atoms, respectively.



(I)

The Zn atom is pentacoordinate, the fifth coordination site being occupied by the symmetry related atom O(4^i) [symmetry code: (i) $2-x$, $y-\frac{1}{2}$, $-z$] of a neighbouring proline molecule so that an infinite polymeric chain is generated. The polymer shows a helical structure along the 2_1 direction. The zinc coordination here is unique, as most zinc–amino acid complexes are hexacoordinate (Freeman, 1976).

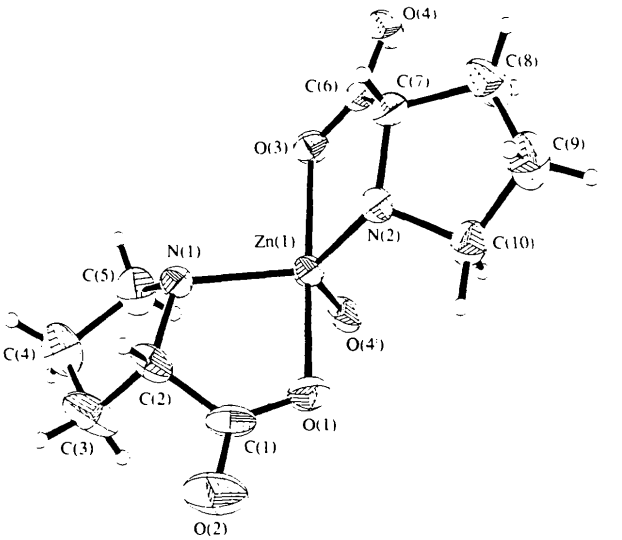


Fig. 1. View of the title molecule showing the labelling of the non-H atoms. Displacement ellipsoids are shown at the 50% probability level.

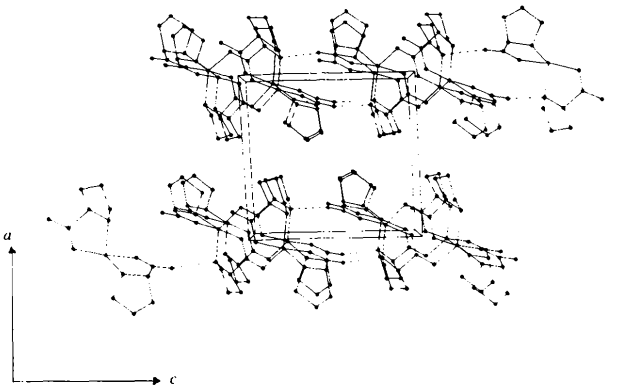


Fig. 2. Projection of the unit cell along the *b* axis.

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The geometry about the Zn atom is trigonal bipyramidal with atoms N(1), N(2) and O(4^{i}) forming the trigonal plane, and atoms O(3) and O(1) in axial positions. The observed bond angles approximate those of an ideal trigonal bipyramid. The O(3)—Zn(1)—O(1) axis is nearly linear with a bond angle of 173.8 (1)°.

The Zn—O and Zn—N distances and all bond lengths of the proline molecules are comparable and are normal for metal-coordinated amino acids (Freeman, 1976; Alcock, Berry & Moore, 1992; Kratochvíl, Ondráček, Novotný & Haber, 1991; Bell, Shearer & Spencer, 1984).

Experimental

Crystal data

$[Zn(C_5H_7NO_2)_2]$	Mo $K\alpha$ radiation
M_r = 291.6	λ = 0.71069 Å
Monoclinic	Cell parameters from 50 reflections
$P2_1$	θ = 7.5–17.5°
a = 9.609 (5) Å	μ = 2.162 mm^{-1}
b = 5.648 (3) Å	T = 298 K
c = 10.491 (5) Å	Plate
β = 91.63 (4)°	0.5 × 0.2 × 0.1 mm
V = 569.1 (5) Å^3	Colourless
Z = 2	
D_x = 1.702 Mg m^{-3}	
D_m = 1.695 Mg m^{-3}	

Data collection

Siemens $P4$ diffractometer	R_{int} = 0.015
$2\theta/\theta$ scans	θ_{max} = 27.5°
Absorption correction: empirical	h = 0 → 12
	k = 0 → 7
T_{min} = 0.69, T_{max} = 0.95	l = −13 → 13
1428 measured reflections	2 standard reflections
1347 independent reflections	monitored every 100 reflections
1262 observed reflections [$F > 4.0\sigma(F)$]	intensity decay: none

Refinement

Refinement on F	$w = 1/[\sigma^2(F) + 0.0011F^2]$
R = 0.0269	$(\Delta/\sigma)_{max}$ = 0.243
wR = 0.0362	$\Delta\rho_{max}$ = 0.55 e Å^{-3}
S = 0.96	$\Delta\rho_{min}$ = −0.54 e Å^{-3}
1262 reflections	Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)
162 parameters	
All H-atom parameters refined	

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$$U_{eq} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Zn(1)	0.9411 (1)	0.0000	0.1929 (1)	0.027 (1)
O(1)	0.9046 (4)	−0.2379 (7)	0.3395 (3)	0.041 (1)
O(2)	0.8329 (5)	−0.2522 (10)	0.5383 (3)	0.068 (1)
O(3)	1.0008 (3)	0.2513 (6)	0.0506 (2)	0.031 (1)
O(4)	1.1840 (3)	0.3411 (6)	−0.0641 (2)	0.036 (1)
N(1)	0.8368 (4)	0.2287 (7)	0.3091 (3)	0.029 (1)
N(2)	1.1544 (3)	−0.0080 (9)	0.2226 (2)	0.026 (1)
C(1)	0.8518 (5)	−0.1479 (9)	0.4387 (4)	0.037 (1)
C(2)	0.8094 (5)	0.1101 (10)	0.4325 (4)	0.036 (1)
C(3)	0.6520 (5)	0.1323 (14)	0.4500 (5)	0.064 (2)
C(4)	0.6050 (5)	0.3295 (13)	0.3635 (5)	0.059 (2)
C(5)	0.7010 (5)	0.3066 (11)	0.2539 (4)	0.049 (1)
C(6)	1.1276 (4)	0.2517 (7)	0.0320 (3)	0.025 (1)
C(7)	1.2270 (4)	0.1518 (8)	0.1352 (3)	0.029 (1)
C(8)	1.3508 (4)	0.0170 (16)	0.0847 (4)	0.053 (1)
C(9)	1.3659 (5)	−0.1982 (11)	0.1720 (4)	0.054 (2)
C(10)	1.2160 (4)	−0.2459 (9)	0.2079 (4)	0.039 (1)

Table 2. *Selected geometric parameters* (Å, °)

Zn(1)—O(1)	2.079 (4)	Zn(1)—O(3)	2.150 (3)
Zn(1)—N(1)	2.056 (4)	Zn(1)—N(2)	2.065 (3)
Zn(1)—O(4^{i})	1.996 (3)	O(1)—C(1)	1.276 (6)
O(2)—C(1)	1.218 (6)	O(3)—C(6)	1.239 (5)
O(4)—C(6)	1.263 (4)	O(4)—Zn(1^{i})	1.996 (3)
N(1)—C(2)	1.488 (5)	N(1)—C(5)	1.479 (6)
N(2)—C(7)	1.476 (5)	N(2)—C(10)	1.478 (7)
C(1)—C(2)	1.514 (8)	C(2)—C(3)	1.534 (7)
C(3)—C(4)	1.498 (10)	C(4)—C(5)	1.500 (7)
C(6)—C(7)	1.531 (5)	C(7)—C(8)	1.520 (7)
C(8)—C(9)	1.527 (9)	C(9)—C(10)	1.523 (7)
O(1)—Zn(1)—O(3)	173.8 (1)	C(2)—N(1)—C(5)	107.4 (3)
O(3)—Zn(1)—N(1)	98.1 (1)	Zn(1)—N(2)—C(10)	113.8 (3)
O(3)—Zn(1)—N(2)	80.5 (1)	O(1)—C(1)—O(2)	125.4 (5)
O(1)—Zn(1)—O(4^{i})	95.7 (1)	(2)—C(1)—C(2)	117.1 (4)
N(1)—Zn(1)—O(4^{i})	112.9 (1)	N(1)—C(2)—C(3)	105.5 (4)
Zn(1)—O(1)—C(1)	115.1 (3)	C(1)—C(2)—C(3)	109.8 (5)
C(6)—O(4)—Zn(1^{i})	117.2 (2)	C(3)—C(4)—C(5)	102.6 (5)
Zn(1)—N(1)—C(5)	113.3 (3)	O(3)—C(6)—O(4)	124.9 (3)
Zn(1)—N(2)—C(7)	112.2 (2)	O(4)—C(6)—C(7)	116.0 (3)
C(7)—N(2)—C(10)	107.1 (3)	N(2)—C(7)—C(8)	107.4 (4)
O(1)—C(1)—C(2)	117.5 (4)	C(7)—C(8)—C(9)	104.6 (4)
N(1)—C(2)—C(1)	114.6 (4)	N(2)—C(10)—C(9)	104.4 (4)
O(1)—Zn(1)—N(1)	82.7 (1)	C(2)—C(3)—C(4)	105.6 (5)
O(1)—Zn(1)—N(2)	93.6 (1)	N(1)—C(5)—C(4)	106.3 (3)
N(1)—Zn(1)—N(2)	115.0 (1)	O(3)—C(6)—C(7)	119.0 (3)
O(3)—Zn(1)—O(4^{i})	89.6 (1)	N(2)—C(7)—C(6)	111.6 (3)
N(2)—Zn(1)—O(4^{i})	131.9 (1)	C(6)—C(7)—C(8)	114.6 (3)
Zn(1)—O(3)—C(6)	113.2 (2)	C(8)—C(9)—C(10)	102.4 (4)
Zn(1)—N(1)—C(2)	109.5 (3)		

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

The structure was solved by direct methods and refined using full-matrix least squares. *SHELXTL/PC* (Sheldrick, 1990) was used for all calculations.

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Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: LI1042). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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