

CRYSTAL STRUCTURE OF BIS(β -ALANINATO)ZINC(II)

Chew-Hee Ng^{*1}, Zhong-Yuan Zhou², Hoong-Kun Fun², Soon-Beng Teo³,
Siang-Guan Teoh³, Pance Naumov⁴ and Seik Weng Ng⁵

¹ School of Arts and Science, Tunku Abdul Rahman College, 53300 Kuala Lumpur, Malaysia

² X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 Penang, Malaysia

³ School of Chemical Sciences, Universiti Sains Malaysia, 11800 Penang, Malaysia

⁴ Institute of Chemistry, "Sv. Kiril i Metodij University", P.O. Box 162, MK-1001, Skopje, Macedonia

⁵ Institute of Postgraduate Studies, University of Malaya, 50603 Kuala Lumpur, Malaysia

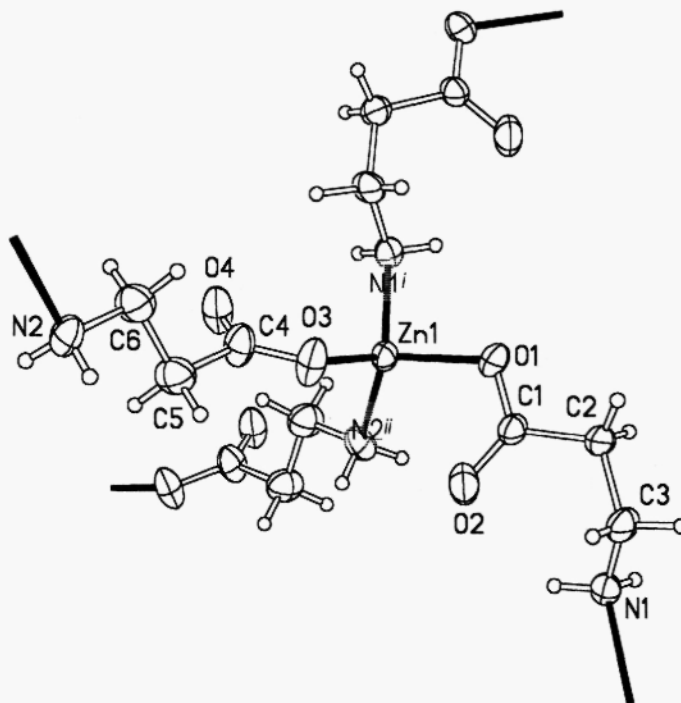


Figure 1. ORTEP plot of bis(β -alaninato)zinc(II) at the 50% probability level. Selected bond distances and angles: Zn1–O1 = 1.982(3), Zn1–O3 = 1.950(4), Zn1–N1ⁱ = 2.013(4), Zn1–N2ⁱⁱ = 2.013(4) Å; O1–Zn1–O3 = 109.8(2), O1–Zn1–N1ⁱ = 98.1(2), O1–Zn1–N2ⁱⁱ = 112.3(2), O3–Zn1–N1ⁱ = 113.7(2), O3–Zn1–N2ⁱⁱ = 106.7(2), N1ⁱ–Zn1–N2ⁱⁱ = 116.1(2)°. Symmetry transformation: $i = x - 1, -y, z - 1/2$; $ii = x - 1/2, -y + 1/2, z + 1/2$.

Comment

The zinc atom in bis(β -alaninato)zinc(II) is four-coordinate in a tetrahedral geometry, the atom being covalently bonded to the carboxyl oxygen atoms of the two β -alaninato entities and datively bonded to the nitrogen ends of two adjacent β -alaninato groups in a three-dimensional network structure. The related zinc aminoacetates are usually six- [1] and occasionally five-coordinate [2]. The bond distances in the compound are somewhat shorter than in these aminoacetates [1-3]. Unlike the copper [4], nickel and cobalt [5] analogs in which the β -alaninates are *N,O*-chelating, the carboxylato entities in bis(β -alaninato)zinc(II) exist in the *N,O*-bridging mode. The bridging nature of the β -alaninate in the present compound contrasts with the chelating mode exercised by the α -alaninato analog, $\text{Zn}[\text{O}_2\text{CCH}(\text{CH}_3)\text{NH}_2]_2$; in the latter, adjacent molecules are linked by a *O,O*-carboxylate bridge into chains [6]. The difference in coordination between the anionic α - and β -alaninate ligands in these two zinc(II) complexes may be due to differences in the synthetic route and reaction

condition. Such variation results in the parent acid, β -alanine, being zwitterionic and monodentate in the zinc nitrate adduct [7].

Experimental

The compound was synthesized by heating a mixture of β -alanine (35.6 g, 0.4 mol) and zinc oxide (16.6 g, >0.2 mol) in about 200 mL water for several hours. The unchanged oxide was removed by filtration and the filtrate concentrated. The compound was obtained in about 10 % yield. Diffraction measurements were carried out on a Siemens P4 diffractometer. The absolute structure parameter [8] refined to 0.01(2).

Table 1. Crystal data for bis(β -alaninato)zinc(II)

Empirical formula	C ₆ H ₁₂ N ₂ O ₄ Zn	Formula weight	241.55
Crystal system	Monoclinic	Space group	Cc
Unit cell dimensions	$a = 5.561(2) \text{ \AA}$ $b = 18.278(5) \text{ \AA}$, $\beta = 103.39(2)^\circ$ $c = 8.993(3) \text{ \AA}$	Volume	889.2(5) \AA^3
μ , mm ⁻¹	2.746	Density, g cm ⁻³	1.804
θ range of data	2.23 – 29.00°	Z	4
Independent reflections	1518 ($R_{\text{int}} = 0.024$)	$F(000)$	496
Refinement method	Full-matrix least-squares on F^2	Completeness of data	100%
Goodness-of-fit on F^2	1.074	Reflections collected	1615
R (all data)	0.038	Reflections with $I > 2\sigma(I)$	1496
Programs	SHELXS-97, SHELXL-97, ORTEP [9-11]	Parameters refined	118
		Final $R [I > 2\sigma(I)]$	0.037
		Diff. peak and hole, e \AA^{-3}	-0.77 – 0.95
		CCDC deposition no.	164870

Acknowledgments

We thank Tunku Abdul Rahman College, Universiti Sains Malaysia (IRPA 305/PFIZIK/610961) and the University of Malaya (F0758/2001A) for supporting this work.

References

- 1 H. Freeman, *Adv. Protein Chem.*, **22** (1976) 257.
- 2 C.H. Ng, H.K. Fun, S.B. Teo, S.G. Teoh and K. Chinnakali, *Acta Cryst.*, **C51** (1995) 244.
- 3 D. van der Helm, A.F. Nicholas and C.G. Fisher, *Acta Cryst.*, **B26** (1970) 1172.
- 4 Y. Mitsui, Y. Iitaka and H. Sakaguchi, *Acta Cryst.*, **B32** (1976) 1634.
- 5 P. Jose, L.M. Pant and A.B. Biswas, *Adv. Protein Chem.*, **22** (1976) 311.
- 6 S.D. Dalosto, M.G. Ferreyra, R. Calvo, O.E. Piro and E.E. Castellano, *J. Inorg. Biochem.*, **75** (1999) 151.
- 7 F. Dejehet, R. Debuyst, B. Ledieu, J.P. Declercq, G. Germain and M. van Meerssche, *Inorg. Chim. Acta*, **30** (1978) 197.
- 8 H.D. Flack and D. Schwarzenbach, *Acta Cryst.*, **A44** (1988) 499.
- 9 G.M. Sheldrick, *SHELXS-97*. Program for Crystal Structure Solution. University of Göttingen, Germany (1997).
- 10 G.M. Sheldrick, *SHELXL-97*. Program for Crystal Structure Refinement. University of Göttingen, Germany (1997).
- 11 C.K. Johnson, *ORTEP-II*. Report ORNL-5138. Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA (1976).

**Received: June 12, 2001 - Accepted: July 6, 2001 –
Accepted in publishable format: July 27, 2001**