Sulphonamide Nitrogen-containing, Nitrogen-protected Amino Acids interacting with the Cd^{2+} Ion. A Cadmium-113 Nuclear Magnetic Resonance and Potentiometric Study. *X*-Ray Diffraction of $[Cd(ts\text{-}\beta\text{-}alaO)_2(H_2O)_4]$†

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α-Alanine and β-alanine, N-protected by a tosyl (toluene-*p*-sulphonyl) group, bind Cd^{2+} acting initially as a simple carboxylate at low pH, and, at increasing pH, as *N,O*-bidentate ligands, through the carboxylic oxygen and the deprotonated amide nitrogen atoms. In the latter case they give rise to five- and six-membered ring chelate species, respectively. Cadmium-113 n.m.r. and potentiometric measurements reveal that the stability of the complexes is almost unaffected by the chelate ring size. The five-membered ring chelate species has a more deshielded chemical shift and only a slightly greater stability than the six-membered species. The crystal and molecular structures of the $[Cd(ts\text{-}\beta\text{-}alaO)_2(H_2O)_4]$ (ts-β-alaO = *N*-tosyl-β-alaninate monoanion) complex have been solved. Crystal data are: monoclinic, space group $P2_1/c$, $a = 14.956(6)$, $b = 5.472(2)$, $c = 16.860(7)$ Å, $\beta = 107.36(3)°$, $Z = 2$, and $R = 0.039$ for 1 635 reflections. The amino acid molecule binds through the unidentate carboxylate group and the structure consists of discrete units in which the Cd^{2+} exhibits a nearly regular octahedral geometry.

The main co-ordinative property of amino acids bearing a sulphonic group as an N-protecting group is involvement of the deprotonated amide nitrogen in metal co-ordination at acidic or slightly alkaline pH in aqueous and alcoholic media.[1] The ions Pd^{2+}, Cu^{2+}, and Cd^{2+} [1–3] are the only metal ions that have hitherto been found effective in such a metal-promoted amide nitrogen deprotonation. In particular, the effectiveness of the Cd^{2+} has recently been demonstrated, mostly by ^{113}Cd n.m.r. measurements.[3] In the corresponding complexes the ligands show a chelate binding mode through the carboxylate group and the deprotonated amide nitrogen.

For a wide variety of metals and chelating ligands, including the Cd^{2+} ion interacting with simple amino acids, the stability of the complex decreases on increasing the chelate ring size.[4,5] The aim of this work is to investigate the conditions which allow the Cd^{2+} ion to promote amide-nitrogen deprotonation in sulphonic N-protected amino acids. To quantify this behaviour, in terms of amino acid side-chain length and sulphonyl group position, the stability constants of the corresponding complexes were evaluated. We have thus investigated the ^{113}Cd n.m.r. behaviour of the Cd^{2+}–*N*-tosyl-α-alanine and Cd^{2+}–*N*-tosyl-β-alanine systems in aqueous solution, and determined the stability constants of the complexes by potentiometric titrations. At the same time, the possibility of obtaining complexes with different ligand-binding modes (as simple carboxylate or as *N,O*-bidentate ligands) prompted us to investigate the solid-state behaviour of these systems.

Experimental

Reagents.—*N*-Tosyl-α-alanine and *N*-tosyl-β-alanine (Sigma) were twice recrystallized from methanol–water, 1:4 solution, and the concentration of the solutions was tested potentiometrically with at least four titration experiments. Carbonate-free sodium hydroxide (0.2 mol dm^{-3}) (C. Erba) was used as a titrant. Reagent grade $Cd(ClO_4)_2\cdot6H_2O$ (Alfa Chem.) was recrystallized twice and a stock solution was analysed by alkalimetric edta (ethylenediaminetetra-acetate) titrations. Cadmium-113 oxide (91.67 atom %, ^{113}Cd), obtained from Oak Ridge National Laboratory, was converted into the perchlorate for use in the n.m.r. study. Doubly distilled water was used throughout.

*Cadmium-*113 *N.M.R. Spectra.*—All measurements were made at 44.385 MHz on a Varian XL-200 spectrometer equipped with a multinuclear broad-band probe. Spectra were obtained using 10-mm outer diameter tubes and were externally referenced to 0.1 mol dm^{-3} aqueous $Cd(ClO_4)_2$ at 25 °C; positive chemical shift values correspond to lower shielding. Due to the high T_1 value for the ^{113}Cd nucleus in D_2O,[6] spectra were obtained with the minimum amount of D_2O required for an internal spectrometer lock. A ^{113}Cd-enriched perchlorate concentration of 4×10^{-3} mol dm^{-3} and a ligand-to-metal molar ratio of 2:1 were used throughout; the ionic strength was adjusted to 0.1 mol dm^{-3} with $NaClO_4$. Standard acquisition parameters were as follows: spectral width, 4 kHz; pulse delay, 6 s; pulse width, 10 μs (45° pulse); number of scans collected, 2 000—4 000. Due to the negative gyromagnetic ratio of the ^{113}Cd nucleus, all spectra were obtained without decoupling. No correction for diamagnetic susceptibility was applied. For each ligand the n.m.r. titrations were repeated three times. The accuracy of the observed shifts falls within ±0.1 p.p.m. up to pH 7, while at higher pH the accuracy decreases due to broadening of the signals. The highest uncertainty was found not to exceed ±0.4 p.p.m. All measurements were performed at 25.0 °C.

Potentiometric pH *Measurements.*—Potentiometric measurements were performed at 25.0 °C under a nitrogen atmosphere, and at an ionic strength of 0.1 mol dm^{-3} (adjusted with solid $NaClO_4$) using the fully automatic ORION 960 Autochemistry system, a Ross 8102 SC combined electrode, and a Centronics GLP II printer for recording e.m.f., pH readings, and titration

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† Tetra-aquabis(*N*-tosyl-β-alaninato-*O*)cadmium(II).

Supplementary data available: see Instructions for Authors, *J. Chem. Soc., Dalton Trans.*, 1989, Issue 1, pp. xvii—xx.

curves. The electrode was calibrated by the method of Irving *et al.*[7] The ionic product K_w (= 1.8×10^{-14} mol^2 dm^{-6}) was obtained in the alkaline region of each calibration curve. The ligand concentration in the titration cell was 8.0×10^{-3} mol dm^{-3} and the metal concentration ranged from 1.0×10^{-3} to 4.0×10^{-3} mol dm^{-3}. The stability constants (β_{pqr}), which are defined by equations (1) and (2), were refined by least squares

$$pL + qM + rH \rightleftharpoons L_pM_qH_r \qquad (1)$$

$$\beta_{pqr} = [L_pM_qH_r]/[L]^p[M]^q[H]^r \qquad (2)$$

using the computer program SUPERQUAD,[8] with $\sigma_E = 0.005$ (pH error) and $\sigma_V = 0.005$ (volume error). All calculations were performed on an IBM XT286 personal computer.

Preparation of Complexes.—The complexes were prepared by adding cadmium acetate (10 cm^3, 1.25×10^{-1} mol dm^{-3}) to a methanol–water solution (100 cm^3, 5×10^{-2} mol dm^{-3} 1:1, v/v) of *N*-tosyl- α- or β-alanine. By slow evaporation at room temperature (20 °C) white crystals separated out. Upon recrystallization from methanol–water (1:4), only crystals of the *N*-tosyl-β-alaninate compound were found to be suitable for *X*-ray diffractometry ([Cd(ts-α-alaO)$_2$(H$_2$O)$_4$]: Found: C, 35.70; H, 4.30; N, 4.00; S, 9.40. [Cd(ts-β-alaO)$_2$(H$_2$O)$_4$]: Found: C, 35.70; H, 4.80; N, 4.20; S, 9.60. Calc. for $C_{20}H_{32}CdN_2O_{12}S_2$: C, 35.90; H, 4.80; N, 4.20; S, 9.60%).

Sulphur, nitrogen, carbon, and hydrogen analyses were performed with a C. Erba model 1106 elemental analyser by Mr. G. Goldoni.

Crystallography.—A sample of dimensions $0.30 \times 0.45 \times 0.40$ mm was mounted in a random orientation on a Siemens AED single-crystal computer-controlled diffractometer, using Mo-K_α radiation. Cell dimensions were refined by least squares using $22 < \theta < 25$ values of 11 accurately measured reflections.

Crystal data. $C_{20}H_{32}CdN_2O_{12}S_2$, M = 669.0, monoclinic, space group $P2_1/c$, a = 14.956(6), b = 5.472(2), c = 16.860(7) Å, β = 107.36(3)°, U = 1 317.0 Å^3, D_m = 1.65 g cm^{-3}, Z = 2, D_c = 1.687 g cm^{-3}, F(000) = 684, λ = 0.710 69 Å, μ(Mo-K_α) = 10.381 cm^{-1}.

Intensity data were collected by the ω—2θ scan method with individual profiles analysed as described by Lehmann and Larsen.[9] One reflection (4 0 4) was measured every 50 scans as a check of alignment and instrument stability (intensity variation 3.6%). A total of 2 659 reflections, with $3 \leqslant \theta \leqslant 25$; $-17 \leqslant h \leqslant 17$, $0 \leqslant k \leqslant 6$, $0 \leqslant l \leqslant 19$, scan width (1.20 + 0.35 tan θ)°, and scan speed 3° min^{-1}, were measured. 1 635 reflections had $I > 2\sigma(I)$ and were considered observed. The structure amplitudes were obtained by the usual Lorentz and polarization reduction and put on an absolute scale by least squares. Absorption correction was considered unnecessary as the μR of 0.19 was very low and the absorption correction factor was invariant over the range 0 3—25° (A^* = 1.40) assuming a cylindrical shape for the crystal.

The structure was solved by the heavy-atom method and the refinements were carried out isotropically by several cycles of full-matrix least squares. The hydrogen atoms were located from a ΔF map, and refined isotropically in the last cycles: the final R values were R = 0.039 and R' = 0.042. The effects of anomalous dispersion were included in all structure calculations; the atomic scattering factors were taken from ref. 10. The function minimized was $\Sigma w|\Delta F^2|$, where $w = K/[\sigma^2(F_o) + gF_o^2]$ (K = 0.3407, $g = 5.05 \times 10^{-3}$). The final atomic co-ordinates are quoted in Table 1.

The calculations were performed using a CRAY-X/MP computer of the Centro di Calcolo dell'Italia Nord Orientale, Bologna, with financial support from the University of Parma, and a GOULD-SHELX 32/77 computer of the Centro di Studio per la Strutturistica Diffrattometrica del C.N.R. (Parma), using the SHELX system of programs,[11] ORTEP,[12] and PARST.[13]

Table 1. Final fractional co-ordinates ($\times 10^4$) of [Cd(ts-β-alaO)$_2$-(H$_2$O)$_4$] with estimated standard deviations (e.s.d.s) in parentheses

Atom	*X/a*	*Y/b*	*Z/c*
Cd	0(0)	0(0)	0(0)
S	2 684(1)	8 364(3)	4 130(1)
O(1)	234(3)	2 742(9)	1 065(3)
O(2)	1 498(4)	1 148(10)	1 946(3)
O(3)	2 743(3)	6 439(10)	4 712(3)
O(4)	2 491(3)	10 771(9)	4 362(3)
O(5)	−1 431(4)	1 678(12)	−0 653(4)
O(6)	643(4)	2 831(11)	−0 663(3)
N	1 880(4)	7 752(11)	3 286(4)
C(1)	891(5)	2 754(13)	1 729(4)
C(2)	921(5)	4 854(19)	2 313(5)
C(3)	1 888(5)	5 418(14)	2 874(5)
C(4)	3 774(5)	8 485(14)	3 925(4)
C(5)	4 417(9)	6 943(31)	4 189(12)
C(6)	5 276(10)	7 130(36)	4 019(13)
C(7)	5 497(6)	8 849(25)	3 640(6)
C(8)	6 461(8)	9 093(42)	3 515(11)
C(9)	4 905(16)	10 660(38)	3 457(20)
C(10)	3 971(12)	10 276(34)	3 515(17)

Additional material available from the Cambridge Crystallographic Data Centre comprises H-atom co-ordinates, thermal parameters, and remaining bond lengths and angles.

Results and Discussion

Solution Behaviour.—*Cadmium*-113 *n.m.r. data.* A recent ^{113}Cd n.m.r. and polarographic study[3] showed the ability of the Cd^{2+} ion in substituting for the nitrogen-bound hydrogen in amino acids N-protected by sulphonic groups, like the tosyl (toluene-*p*-sulphonyl) and dansyl (5-dimethylaminonaphthalene-1-sulphonyl) groups. The behaviour of the ^{113}Cd chemical shift on increasing pH for Cd^{2+} interacting with *N*-tosyl-α-alanine and *N*-tosyl-β-alanine (Figure 1) shows, like the previously investigated systems,[3] an initial shielding of the cadmium resonance under fast chemical exchange conditions, due to metal co-ordination of the carboxylate group of the ligands, followed by a sudden deshielding effect caused by bidentate co-ordination of the ligands through the carboxylate oxygen and the deprotonated amide nitrogen atoms. (It is known that oxygen donor atoms shield the ^{113}Cd resonance, while nitrogen atoms have an opposite effect.[14]) The metal binding of the deprotonated amide nitrogen of these ligands is unequivocally confirmed by the ^{113}Cd n.m.r. titrations performed in the presence of *N*-benzoylglycine, which is known not to undergo metal-promoted amide deprotonation,[3] and whose δ *vs.* pH profile is characterized only by the low frequency shift due to metal co-ordination of the carboxylate group (Figure 1). Furthermore, while over the whole pH range investigated no changes in the linewidths are found in the Cd^{2+}–*N*-benzoylglycine system, the *N*-tosyl-α- and -β alanine complexes, starting from about pH 6, show an increase of the linewidth which broadens the signal beyond detection at about pH 8. Compared to *N*-tosyl-α-alanine, the β derivative shows larger low-frequency shifts at low pH. This overall behaviour is qualitatively similar to that exhibited by glycine and β-alanine.[15] However, the difference between the chemical shift values of the two Cd^{2+}–ligand systems at the same pH is much smaller.

Table 2. Logarithms of cumulative protonation and complex-formation constants for Cd^{II}- ts-α- and β-alaninate systems at 25 °C and $I = 0.1$ mol dm^{-3} ($NaClO_4$). Standard deviations are given in parentheses

		Ligand	
Complex		ts-α-ala	ts-β-ala
Ligand	log β_{101}	11.236(12)	11.194(6)
	log β_{102}	14.684(14)	15.487(7)
CdL′	log β_{110}	5.45(2)	5.34(4)
CdL'_2	log β_{210}	9.45(9)	9.90(8)
CdL_2	log β_{212}	27.04(9)	28.14(7)
	log β'_{210}*	4.61(3)	5.21(4)

* log β'_{210} values were calculated considering the ligands as monoprotic, according to the reaction $Cd^{2+} + 2L^- \rightleftharpoons CdL_2$.

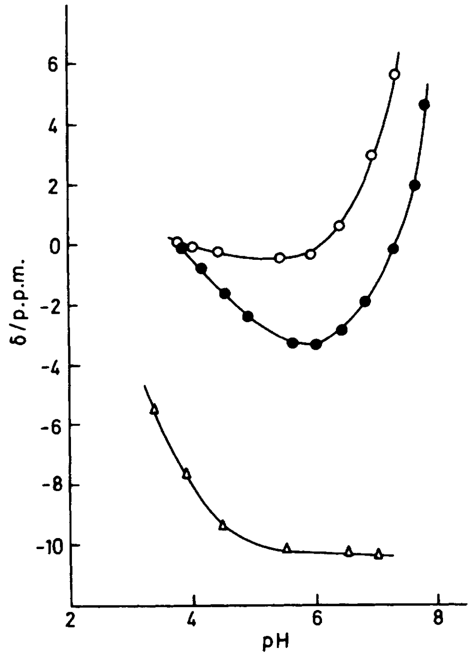

Figure 1. Cadmium-113 chemical shift of 4 × 10^{-3} mol dm^{-3} ^{113}Cd-enriched $Cd(ClO_4)_2$, with 8 × 10^{-3} mol dm^{-3} ligands, *vs.* pH in aqueous solution. (○) *N*-Tosyl-α-alaninate, (●) *N*-tosyl-β-alaninate, and (△) *N*-benzoylglycinate. 25 °C, $I = 0.1$ mol dm^{-3}

When chemical exchange is fast on the n.m.r. time-scale, the chemical shifts of the time-averaged resonance ($\delta_{obs.}$) and a knowledge of the stability constants of the complexes allow the chemical shifts of the individual species to be obtained. The potentiometric analysis showed the presence of the species CdL_2, CdL′, and CdL'_2 (L = ligand co-ordinating through the carboxylate group; L′ = ligand acting as an *N*,*O*-bidentate ligand): their stability constants are reported in Table 2 and will be discussed in detail in the next section. The single chemical shift observed is taken to be the average of the chemical shifts of the individual complexes (δ_i) weighted according to their molar fractions (x_i): so, the various shifts, δ_i, can be calculated by

$$\delta_{obs.} = \Sigma_i x_i \delta_i \qquad (3)$$

means of a least-squares procedure. Some factors limit the accuracy of this determination: (1) the accuracy of the calculated equilibrium constants; (2) the accuracy of the observed chemical shifts (especially in the case of broad signals); (3) it is important to take into account the fact that the reliability of the calculated δ_i value for a given species is proportional to its molar fraction. In order to reduce errors arising from calculated equilibrium constants, potentiometric measurements and ^{113}Cd n.mr. titrations were performed on solutions having the same ionic strength (0.1 mol dm^{-3}) and Cd^{2+} concentration.

Table 3. Calculated ^{113}Cd chemical shifts[a] for the various Cd^{2+}–tosylalaninate complexes in aqueous solution at ionic strength 0.1 mol dm^{-3} [b]

	δ	
Ligand	CdL_2	CdL′
Tosyl-α-alaninate	−8.0	50
Tosyl-β-alaninate	−7.0	35

[a] Referred to aqueous 0.1 mol dm^{-3} $Cd(ClO_4)_2$ at 25 °C. [b] The chemical shift of the aquated Cd^{2+} ion is set at +1.02 p.p.m. (see text).

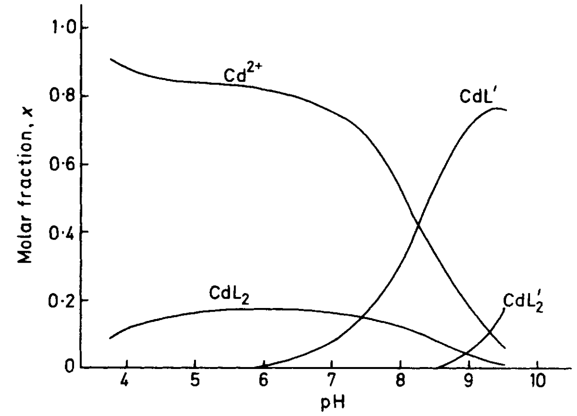

Figure 2. Species distribution curves for the complexes given by *N*-tosyl-α-alaninate. x = molar fraction. $c_{Cd} = 4 \times 10^{-3}$ mol dm^{-3}; ligand-to-metal molar ratio = 2:1; 25 °C; $I = 0.1$ mol dm^{-3}

Using the x_i values obtained from the computer program SUPERQUAD (reported in Figure 2 for *N*-tosyl-α-ala) and the observed chemical shifts,* a least-squares treatment of equation (3) gives the individual chemical shifts reported in Table 3. In the data analysis the chemical shift of the uncomplexed Cd^{2+} ion is fixed to its initial value in the absence of ligand (+1.02 p.p.m.), since the ^{113}Cd chemical shift of aqueous $Cd(ClO_4)_2$ is not very concentration dependent.[6,16]

The $\delta(CdL_2)$ values are negative, as expected for cadmium co-ordination by oxygen atoms, and fall into the range generally found for the Cd^{2+}–carboxylate complexes.[4] The small molar fraction of the CdL′ species in the ^{113}Cd n.m.r. data range ($x_{max.} \approx 0.2$), and the uncertainty which affects the observed chemical shifts (due to broadening of the signals), suggests that the δ(CdL′) values should be considered as estimated values. Indeed, they are less deshielded with respect to the δ value of the $[Cd(glycine)]^+$ species (+63 p.p.m.) determined in a supercooled aqueous solution at pH 7,[17] while more deshielded values should be expected owing to the higher basicity of the deprotonated nitrogen of these ligands compared to the amino nitrogen of glycine.[4] A disagreement between observed δ values in supercooled aqueous solution and calculated δ values under fast chemical exchange conditions, for species with small molar

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* The maximum linewidth of the signals used in the calculations was 80—100 Hz, *i.e.*, only signals up to pH 7.2 and 7.8 for *N*-tosyl-α- and -β-alanine, respectively, were used.

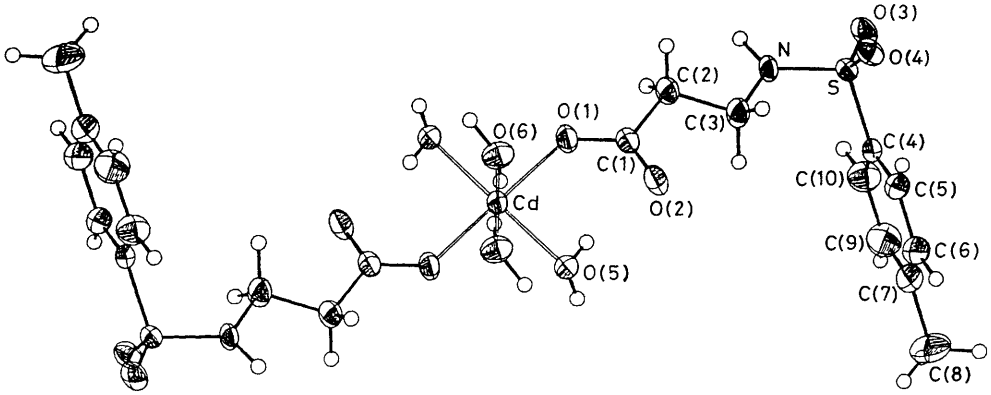

Figure 3. ORTEP view of the $[Cd(ts\text{-}\beta\text{-}alaO)_2(H_2O)_4]$ complex showing the atom numbering and the thermal motion ellipsoids (40%). The spheres corresponding to the hydrogen atoms are on an arbitrary scale

fractions, has been observed for other systems.[18,19] However, at the same time, it has been demonstrated[15,19] that the relationships between δ values belonging to each class are the same. Consequently, the 'internal' comparison between our two δ(CdL′) values is allowed, and the more deshielded value of δ(CdL′) (by 15 p.p.m.) for *N*-tosyl-α-alanine with respect to that of *N*-tosyl-β-alanine may be considered to have chemical significance. Actually, these chemical shifts follow the same trend observed for complexes of Cd^{2+} with diamines, dicarboxylates, and dithiolates; the five-membered ring chelate species having a more deshielded δ value with respect to the six-membered one.[4] The comparison between the δ values of the CdL'_2 species cannot be made since both the complexes begin to form at pH values higher than 8 (Figure 2), *i.e.* beyond the ^{113}Cd n.m.r. experimental data range.

Potentiometric data. Complexes in which the ligands act as simple carboxylates (L) and as *N,O*-bidentate ligands through the carboxylic oxygen and the deprotonated suphonamide nitrogen (L′) were detected. The calculated stability constants (β) are reported in Table 2. Mixed hydroxy–carboxylate complexes are absent and no evidence of their formation has been obtained in an analogous investigation on the Cd^{2+}–tosylglycinate system.[20] Consequently, the previously proposed involvement of the metal-bound hydroxy group in the mechanism of metal-promoted amide deprotonation is supported by reliable experimental data only in alcoholic solution, where direct evidence of the formation of such mixed hydroxy species has been obtained.[3] The greater stability of the CdL_2 species as compared to that of simple Cd^{2+}–carboxylates[5] is worthy of note. This pronounced ability of the carboxylate group to behave as an 'anchoring group'[2] for the Cd^{2+} ion modifies the N–H dissociation equilibrium, making its protonation constant similar to those of the corresponding toluenesulphonamides (pK_{NH} range 9—10).[21]

The stability constants of the complexes in which the ligands act as *N,O*-bidentate ligands are higher than those of the Cd^{2+} complexes with simple amino acids,[5] in agreement with the stronger donor ability of the deprotonated amide nitrogen as compared to the amino nitrogen. The CdL′ species given by ts-α-ala (five-membered chelate ring) is only slightly more stable than that of ts-β-ala (six-membered ring). In particular, the difference between the stability constants ($\Delta \log \beta = 0.11$) is much smaller compared to that observed between the five- and six-membered chelate ring species of Cd^{2+} complexes with diamines ($\Delta \log \beta = 0.95$)[4] and much smaller compared to that of simple amino acids ($\Delta \log \beta = 1.3$).[5] The lack of influence of the chelate-ring size on the stability of Cd^{2+}–*N*-tosylalaninate complexes can reasonably be said to be due to the strong donor ability of the deprotonated sulphonamide nitrogen which overcomes the unfavourable effect of the higher strain of a six-membered chelate ring as compared to a five-membered one.[4]

Table 4. Selected bond distances (Å) and angles (°), with e.s.d.s in parentheses

(a) In the co-ordination polyhedron			
Cd–O(1)	2.285(5)	O(5)–Cd–O(6)	87.8(2)
Cd–O(5)	2.287(6)	O(1)–Cd–O(6)	87.2(2)
Cd–O(6)	2.283(6)	O(1)–Cd–O(5)	90.9(2)
(b) In the ligand			
O(1)–C(1)	1.250(8)	O(1)–C(1)–O(2)	124.9(7)
O(2)–C(1)	1.238(9)	O(1)–C(1)–C(2)	116.8(7)
C(1)–C(2)	1.506(12)	O(2)–C(1)–C(2)	118.2(7)
C(2)–C(3)	1.505(10)	C(1)–C(2)–C(3)	113.7(7)
N–C(3)	1.457(10)	C(2)–C(3)–N	109.7(7)
N–S	1.600(6)	C(3)–N–S	119.8(5)
S–O(3)	1.424(6)	N–S–C(4)	109.0(3)
S–O(4)	1.428(6)	N–S–O(4)	106.0(4)
S–C(4)	1.765(8)	N–S–O(3)	109.5(3)
		O(3)–S–O(4)	118.0(3)
		O(3)–S–C(4)	107.0(4)
		O(4)–S–C(4)	107.1(4)

Solid State Behaviour.—We tried to obtain solid complexes from solutions at different pH values. Both ligands gave a crystalline compound of formula $[CdL''_2(H_2O)_4]$ (L″-*N*-tosyl-α- or -β-alaninate) from aqueous methanolic solution at pH <7.5.* At higher pH values no solid complexes separated, owing to competitive precipitation of cadmium hydroxide which, having a stability[22] comparable to that of the cadmium complexes at these pH values, separates in the course of a few hours. Only crystals of the *N*-tosyl-β-alaninate compound were found suitable for *X*-ray crystallographic analysis.

An illustration of the structural unit showing the atom numbering scheme is given in Figure 3. Bond distances and angles are listed in Table 4. The structure consists of discrete molecular units of $[Cd(ts\text{-}\beta\text{-}alaO)_2(H_2O)_4]$ linked into three-

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* The pH measurements in mixed aqueous methanolic solution, up to a methanol–water ratio of 1:1, were performed with a pH combined electrode standardized in aqueous solution.

dimensional chains through hydrogen bonds. The Cd atom lies at the centre of symmetry, exhibiting an ideal octahedral geometry arising from co-ordination by the carboxylate oxygens of two centrosymmetrically related *N*-tosyl-β-alaninate ions and four water molecules. The same metal arrangement has been found in the analogous zinc compound[23] and the two complexes are isomorphous and isostructural.

This structure shows some unusual features with respect to the known cadmium–carboxylate complexes. The carboxylate ligands normally act as bidentate ligands towards Cd^{2+} forming chelates and/or bridges, which lead to the formation of dimeric units and, more often, polymeric structures.[24] Moreover, Cd^{2+} generally exhibits distorted pentagonal-bipyramidal (seven) co-ordination and, less frequently, octahedral co-ordinations. In our complex, the carboxylate group acts as an unidentate ligand and the structure consists of monomeric units. These features, the latter being reasonable due to the high hydration of the complex, are uncommon[25] and, up to now, have never been observed in the same complex.

In the ligand molecule the C^{α}–COO group is planar with C^{β} and N 0.616(8) and 0.813(6) Å out of the plane, respectively; it forms dihedral angles of 120.9(3)° with the SO_2 group and 76.9(4)° with the phenyl group. The conformation of the *N*-tosyl-β-alaninate moiety can be described using torsion angles around the C'–C^{α} [$-153.8(7)°$] and C^{α}–C^{β} [168.2(6)°] bonds.

The structure is characterized by the presence of hydrophobic and hydrophilic regions. The metal ion lies in the hydrophilic region, while the phenyl rings lie in the hydrophobic region with contacts; the shortest of which involve C(5) and $C(5^{I})$ (I $1 - x$, $1 - y$, $1 - z$) [3.49(2) Å], and C(6) and $C(9^{II})$ (II x, $y - 1$, z) [3.66(3) Å]. The crystal packing is determined by a network of hydrogen bonds.

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