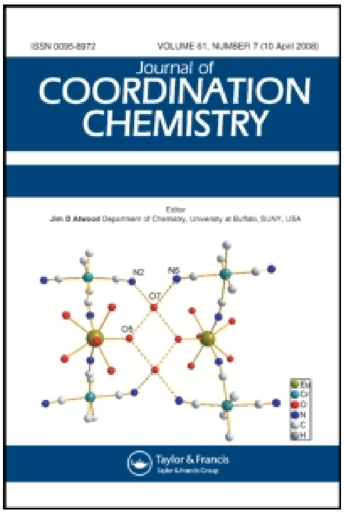

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Complexes of Zn(II) and Cd(II) with N-phthaloylglycinate (N-phthgly), imidazole (imi), 5-amino tetrazole (Atz) and 2,4,6-*tris*(2-pyridyl)-1,3,5-triazine (tptz) were synthesized and characterized by elemental analysis, IR and thermogravimetric analysis. The X-ray crystal structure of the cadmium complex $[Cd(imi)_3(N\text{-}phthgly)_2] \cdot 2H_2O$ is also reported. It crystallizes in the space group $P2_1/m$. The metal centre is hepta coordinated as a distorted pentagonal bipyramid. The cadmium atom is surrounded by five equatorial atoms (four oxygen atoms of two bidentate N-phthaloylglycinate moieties and a nitrogen atom of an imidazole ligand) and two axial nitrogens of two imidazole rings. In the crystal, the molecules are connected by H-bonds involving water molecules, the carboxylic oxygens of the N-phthaloylglycinate molecules and the imidazole nitrogens.

Keywords: Zinc; Cadmium; Phthaloylglycinate; Imidazole; Amino tetrazole; X-ray structure

1. Introduction

Interactions of metal ions with biologically important compounds such as amino acids and peptides are of interest [1]. Metal ions are of essential importance in many enzymes and interactions of metal ions with non-enzymatic proteins are numerous. For example, transport of zinc and copper in blood involves complexes with serum albumin and amino acids [2]. Furthermore, the interactions of small peptides such as glutathione with metal ions have generated considerable interest. In non-biological systems, the reactivity of amino acids and peptides is modified by metal ions in processes such as proton exchange, racemization and aldol condensation. Such modification occurs due to alteration of the electron distribution resulting from coordination of the amino group to a metal ion [3]. Studying changes in the electronic environments of nitrogen in metal complexes of amino acids or peptides is important [4].

Ternary complexes have importance in biological systems. Cadmium toxicity [7, 8] and N-phthaloylglycinate which possesses auxine-like properties and phthalimide

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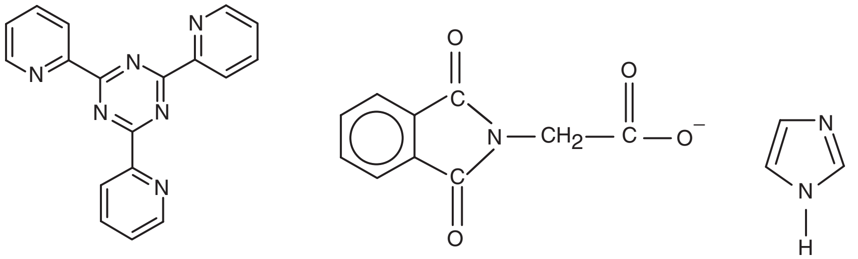
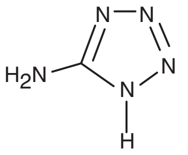


2,4,6-*tris*(2-Pyridyl)-1,3,5-triazine

N-Phthaloylglycinate (phthgly)

Imidazole (imi)



5-Amino tetrazole (Atz)

Scheme 1. Chemical structure of the ligands.

residue are of interest. Several phthalimide derivatives have importance in medicinal chemistry [9] and are used as antimicrobial reagents [10]. Therefore, as a continuation to our previous work on N-phthaloylglycinate (N-phthgly) ternary complexes [5, 6], we report here the structural features of N-phthaloylglycinate complexes of Zn(II) and Cd(II) with imidazole (imi), 5-amino tetrazole (Atz) and 2,4,6-*tris*(2-pyridyl)-1,3,5-triazine (tptz), scheme 1. The X-ray crystal structure of the ternary cadmium(II) complex was also investigated. To our knowledge, there are no cadmium ternary compounds with N-phthaloylglycinate described in the literature.

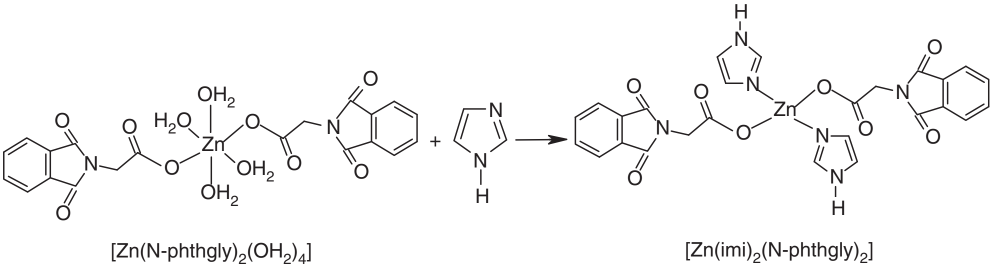
2. Experimental

Materials: All chemicals were reagent grade, purchased from Sigma and Janseen and used as received.

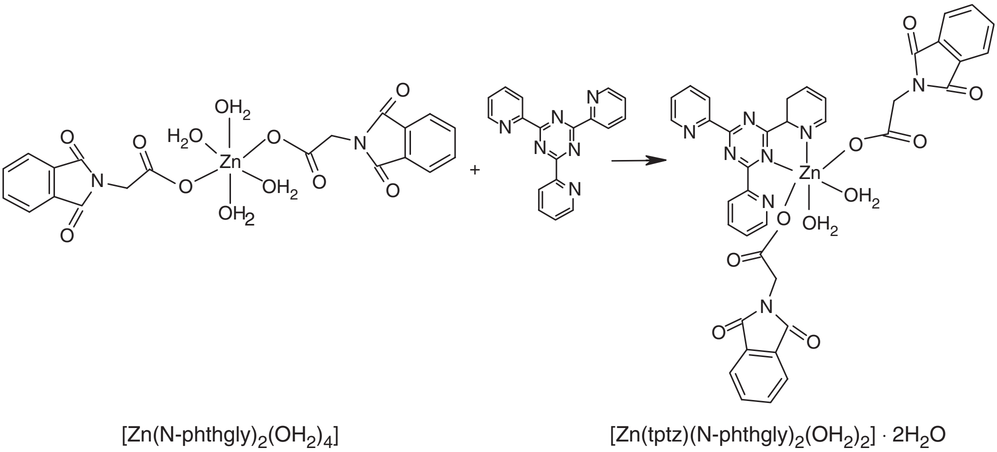
2.1. *Preparation of solid complexes*

2.1.1. [M(N-phthgly)$_2$(H$_2$O)$_4$] • 2H$_2$O (M = Zn(II) or Cd(II)). M(CH$_3$COO)$_2$ · xH$_2$O (M = Zn(II) 0.22 g, M = Cd(II) 0.27 g; 1.00 mmol) was dissolved in water (25 cm^3) and then added to 25 cm^3 of ethanolic solution of Hphthgly (0.41 g, 2.00 mmol). After 30 min of stirring, the solution was left covered and the solvent was slowly evaporated to give colourless crystalline compounds (yield 70%).

2.1.2. [Zn(imi)$_2$(N-phthgly)$_2$], [Cd(imi)$_3$(N-phthgly)$_2$] • 2H$_2$O and [Cd(Atz)$_3$(N-phthgly)$_2$] • 2H$_2$O. The corresponding binary complex (M = Zn(II) 0.58 g,



Scheme 2. Synthesis of $[Zn(imi)_2(N\text{-}phthgly)_2]$ ternary complex.



Scheme 3. Synthesis of $[Zn(tptz)(N\text{-}phthgly)_2(OH_2)_2] \cdot 2H_2O$ ternary complex.

M = Cd(II) 0.63 g, 1.00 mmol) was dissolved in C_2H_5OH (25 cm^3) and added to ethanolic solution (25 cm^3) of imidazole (0.14 g, 2.00 mmol, 1 : 2 molar ratio) for Zn complex and (0.21 g, 3.00 mmol, 1 : 3 molar ratio) for Cd. The reactions were allowed to proceed for 3 h with constant stirring. By slow evaporation of the solution at room temperature, prismatic, well-shaped, crystals of $[Cd(imi)_3(N\text{-}phthgly)_2] \cdot 2H_2O$, suitable for X-ray structure analysis, separated after two weeks. The $[Zn(imi)_2(N\text{-}phthgly)_2]$ complex was white powder and obtained after one week (scheme 2).

$[Cd(Atz)_3(N\text{-}phthgly)_2] \cdot 2H_2O$ was prepared by reacting $[Cd(N\text{-}phthgly)_2(H_2O)_4] \cdot 2H_2O$ (0.63 g, 1 mmol) in ethanol (25 cm^3) with (0.21 g, 2 mmol) of 5-amino tetrazole in 1 : 2 molar ratio, the reaction mixture was stirred at room temperature for 2 h and left undisturbed. A white precipitate was obtained after seven days by slow evaporation of the solution.

2.1.3. $[Zn(tptz)(N\text{-}phthgly)_2(H_2O)_2] \cdot 2H_2O$. The $[Zn(tptz)(N\text{-}phthgly)_2(H_2O)_2] \cdot 2H_2O$ complex was prepared in a similar way by reacting the corresponding binary complex $[Zn(N\text{-}phthgly)_2(H_2O)_4] \cdot 2H_2O$ (0.58 g, 1.00 mmol) dissolved in ethanol (25 cm^3) with (0.31 g, 1.00 mmol) of 2,4,6-*tris*(2-pyridyl)-1,3,5-triazine (25 cm^3). The solution was left covered for 10 days, and white powder, $[Zn(tptz)(N\text{-}phthgly)_2(H_2O)_2] \cdot 2H_2O$, formed (scheme 3). Table 1 gives elemental analyses, formula weights and melting points of the reported complexes.

Table 1. Elemental analyses, formula weights and melting point data for the zinc(II) and cadmium(II) complexes.

Complex	F.W.	Found (Calcd)%			M.p. (°C)
		C	H	N	
$[Zn(N\text{-phthgly})_2(OH_2)_4] \cdot 2H_2O$	581.75	41.4 (41.3)	4.2 (4.1)	4.9 (4.8)	283
$[Cd(N\text{-phthgly})_2(OH_2)_4] \cdot 2H_2O$	628.75	38.1 (38.2)	3.8 (3.8)	4.6 (4.5)	294
$[Zn(imi)_2(N\text{-phthgly})_2]$	607.39	51.2 (51.4)	3.2 (3.0)	13.8 (13.8)	250
$[Zn(tptz)(N\text{-phthgly})_2(OH_2)_2] \cdot 2H_2O$	857.39	53.0 (53.2)	3.9 (3.7)	13.0 (13.1)	259
$[Cd(imi)_3(N\text{-phthgly})_2] \cdot 2H_2O$	759.4	45.8 (45.9)	2.8 (2.6)	14.7 (14.8)	264
$[Cd(Atz)_3(N\text{-phthgly})_2] \cdot 2H_2O$	867.99	31.6 (31.8)	2.5 (2.6)	27.3 (27.4)	269

2.2. *Instrumentation*

Elemental CHN analyses were carried out on a Carlo-Erba CHNS-O EA1108 elemental analyzer. Infrared spectra (KBr pellets) were recorded on a Nicolet 5PC FT-IR spectrometer. Thermogravimetry (TG) studies were performed using a Stanton STA 1500 Thermo analyzer with a heating rate of 10°C min^{-1} under N_2.

2.3. *X-ray data collection and structure refinement*

The X-ray diffraction data were collected for the cadmium complex at room temperature on an Enraf-Nonius CAD 4 single crystal diffractometer using Mo-Kα radiation. A standard reflection was monitored every 100 reflections, during the data collection process, without significant variation. The data were corrected for Lorentz and for polarization effects during the data reduction procedures [11, 12] and, after the isotropic refinement, the data were also corrected for absorption following the method of Walker and Stuart [13] with a program written by Gluzinski [14].

The structure was solved with SIR97 [15] and the refinements were carried out with SHELX97 [16]. Most of the hydrogen atoms were found in a final ΔF map, the remaining were put in their theoretical positions and all refined automatically.

The crystal data and relevant details concerning data collection and refinements are summarized in table 2. The projection of the complex, in which the ellipsoids are at 30% probability level, is in figure 1 [17].

3. Results and discussion

3.1. *Infrared spectra*

Important IR data are given in table 3. The IR spectra of three complexes, $[Zn(tptz)(N\text{-phthgly})_2(OH_2)_2] \cdot 2H_2O$ $[Cd(imi)_3(N\text{-phthgly})_2] \cdot 2H_2O$ and $[Cd(Atz)_3(N\text{-phthgly})_2] \cdot 2H_2O$ displayed a broad band, due to the stretching vibration of the

Table 2. Crystallographic data and experimental information for $[Cd(imi)_3(N\text{-}phthgly)_2]\cdot 2H_2O$.

Complex	$[Cd(imi)_3(N\text{-}phthgly)_2]\cdot 2H_2O$
Formula	$C_{29}H_{28}N_8O_{10}Cd$
MW	379.5
Crystal dimensions (mm^3)	$0.09 \times 0.19 \times 0.27$
Cell parameters (Å, °)	
a	8.133(2)
b	22.485(3)
c	8.874(3)
α	90
β	102.62(3)
γ	90
Cell determination	
n° of reflections	24
θ range (°)	7.8–15.3
Cell volume (Å^3)	1583.6
Symmetry	Monoclinic
Space group	$P2_1/m$
Collected reflections	2738
Unique reflections, *R* int.	2551, 0.03
Observed reflections $[F_o > 4\sigma(F_o)]$	2034
2θ max (°)	48.01
Indices range	
h	−9/9
k	0/25
l	0/10
No. of refined parameters	538
R_1	0.024
R_w	0.057
$w = 1/[(\sigma^2 F_o^2 + KP)^2 + YP]$	0.020
K, *Y*	0.0
GOF	1.04
$\Delta\rho_{min/max}$	−0.39/0.48
Diffractometer	Enraf-Nonius CAD 4
Radiation	Mo-Kα
Lambda (Å)	0.71069

water of hydration [18]. The IR spectra of the complexes $[Zn(imi)_2(N\text{-}phthgly)_2]$, $[Cd(imi)_3(N\text{-}phthgly)_2]\cdot 2H_2O$ and $[Cd(Atz)_3(N\text{-}phthgly)_2]\cdot 2H_2O$ also showed a strong band at 3384, 3208 and 3233 cm^{-1} respectively, which corresponded to the stretching vibration of the NH group of imidazole and tetrazole ring. The presence of a very strong band in the range of 1592–1626 cm^{-1} for all complexes, typical for asymmetric vibration of the coordinated carboxylate group, confirms the coordination of the N-phthaloylglycinate through the carboxylic oxygen [19]. In addition, bands in the range 1421–1424 cm^{-1} for all complexes can be ascribed to the symmetric vibration of the coordinated carboxylate group. The presence of two strong bands in the range 1768–1773 and 1704–1713 cm^{-1} in the spectra of all complexes, can be assigned to the stretching vibration of two uncoordinated ketonic carbonyl groups $\upsilon(CO)_{ket}$, in agreement with the results of X-ray crystal structures of the ternary complexes [19]. The coordination of a metal ion via O carboxylate is confirmed by the $\upsilon(M\text{–}O)$ bands at 558 (Zn) and 550 cm^{-1} (Cd).

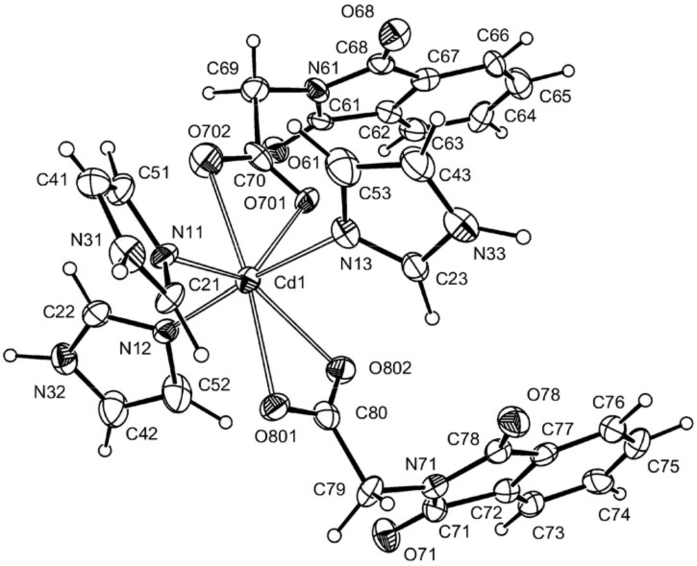


Figure 1. Projection of $[Cd(imi)_3(N\text{-}phthgly)_2] \cdot 2H_2O$ complex.

Table 3. Important IR data for the zinc(II) and cadmium(II) complexes.

Complex	$\nu(OH)$	$\nu(NH)_{imi}$	$\nu(CO)_{ket}$	$\nu(COO)_a$	$\nu(COO)_s$
$[Zn(N\text{-}phthgly)_2(OH_2)_4] \cdot 2H_2O$	3485b	–	1774s 1714s	1604s	1431s
$[Cd(N\text{-}phthgly)_2(OH_2)_4] \cdot 2H_2O$	3486b	–	1768s 1712s	1596s	1429s
$[Zn(imi)_2(N\text{-}phthgly)_2]$	–	3384m	1772s 1713s	1658s 1625s	1421s
$[Zn(tptz)(N\text{-}phthgly)_2(OH_2)_2] \cdot 2H_2O$	3468s	–	1773s 1708s	1638s 1618m	1422s
$[Cd(imi)_3(N\text{-}phthgly)_2] \cdot 2H_2O$	3420s	3208s	1768s 1704s	1646s 1592s	1424s
$[Cd(Atz)_3(N\text{-}phthgly)_2] \cdot 2H_2O$	3433b	3233sh	1772s 1711s	1626s 1590s	1423s

3.2. *Thermogravimetric analysis*

Thermogravimetric (TG) analysis has been performed on the complexes to verify the amount of water of crystallization in these complexes. The thermogram of $[Zn(tptz)(N\text{-}phthgly)_2(OH_2)_2] \cdot 2H_2O$ displays weight loss in two steps. The first step occurs at 80–100°C, corresponding to 4.20% of the total weight. This loss of weight can be accounted for by loss of two water molecules. At 160–200°C the molecule loses the two coordinated water molecules, totaling to a loss of weight of 8.40% for four water molecules. The TG plot for $[Cd(imi)_3(N\text{-}phthgly)_2] \cdot 2H_2O$ (figure 3) displays an initial slow weight loss of 4.49% in the range 50–150°C, which is in accord with the loss of two water molecules of hydration. A second weight loss of 8.68% (theoretical 8.96%), in the temperature range 150–260°C, could probably be due to the loss of one imidazole molecule which lies in the equatorial plane, as the bond length between Cd–N11 is

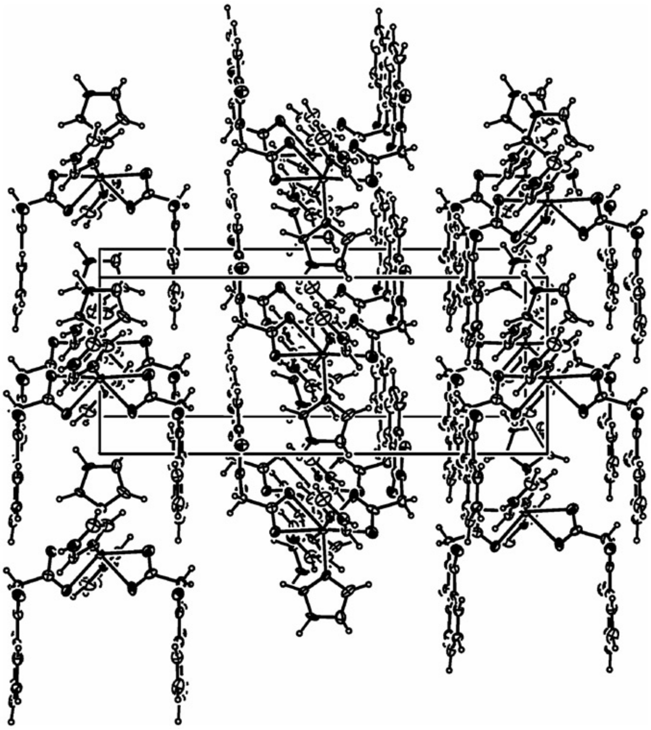


Figure 2. Packing of [Cd(imi)$_3$(N-phthgly)$_2$] · 2H$_2$O complex.

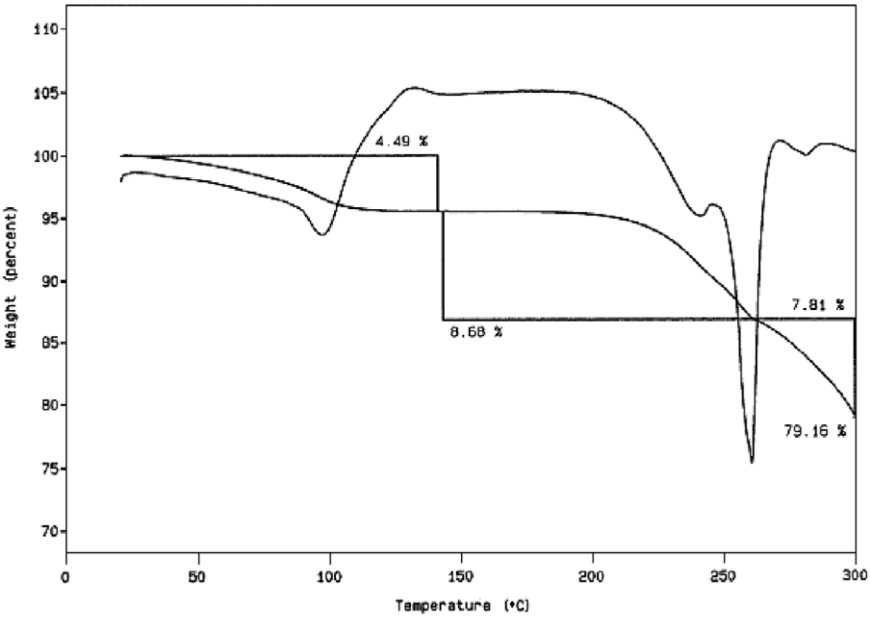


Figure 3. TG plot of [Cd(imi)$_3$(N-phthgly)$_2$] · 2H$_2$O complex.

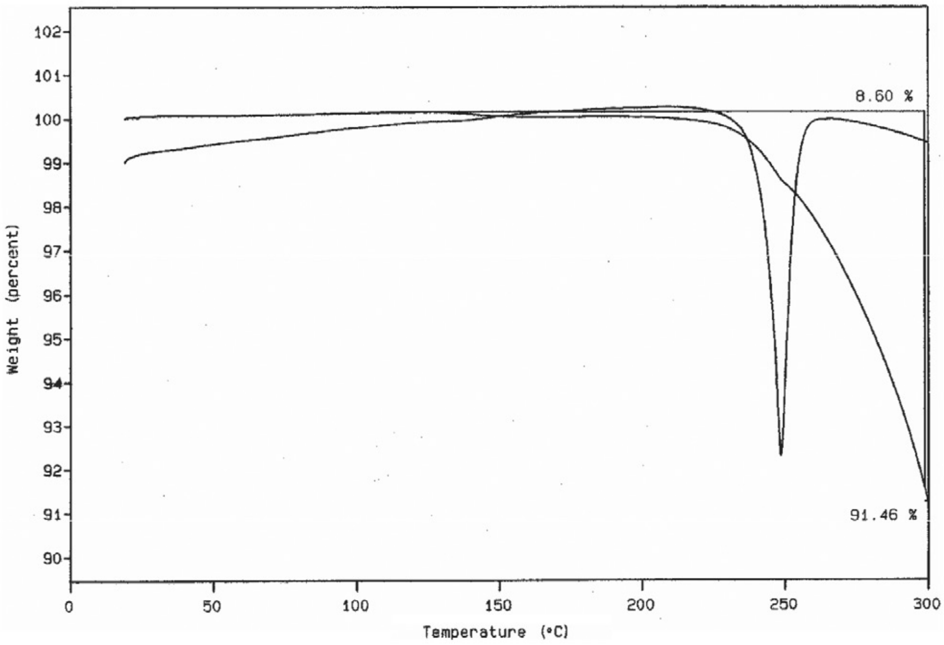


Figure 4. TG plot of $[Zn(imi)_2(N\text{-}phthgly)_2]$ complex.

longer than the other two bonds of the two axial imidazole groups, Cd–N12 and Cd–N13. This loss of imidazole would relieve steric congestion, which is a thermodynamically favourable process, in agreement with the results of the X-ray crystal structure. The compound loses a further 79.16% (theoretical 83.09%) of its weight from the parent composition in the region 260–300°C, corresponding to transformation to CdO. The thermogram of $[Zn(imi)_2(N\text{-}phthgly)_2]$ complex (figure 4), does not show any weight loss in the temperature range 50–200°C, in accord with the results of elemental analysis and IR spectra, which showed that the complex does not possess lattice water molecules and suggests the tetrahedral coordination geometry of Zn(II), ZnN_2O_2, as found for similar zinc adduct of imidazole and oxydiacetate [20]. A weight loss of 8.60% has been observed in the temperature range of 220–260°C, which could be ascribed to the loss of CH_2COO group (theoretical 9.50%). In the temperature range 260–300°C, the molecule transforms to ZnO by losing 91.40% of its weight.

3.3. *Crystal structure of* $[Cd(imi)_3(N\text{-}phthgly)_2] \cdot 2H_2O$

Crystal structure analysis of $[Cd(imi)_3(N\text{-}phthgly)_2] \cdot 2H_2O$ showed that the complex crystallizes in $P2_1/m$ space group. The ORTEP representation is shown in figure 1. Selected bond lengths and bond angles are summarized in table 4. In the complex each cadmium is surrounded by five equatorial atoms and two axial nitrogens in a distorted pentagonal bipyramidal conformation, figure 1. The equatorial plane is formed by O701, O702 and O801, O802 atoms of two bidentate N-phthaloylglycinate moieties and by N11 of an imidazole ligand. At the vertices of the bipyramid, there are N12 and N13 of the two remaining imidazole rings. The constraints imposed

Table 4. Selected bond distances (Å) and bond angles (°) for the complex $[Cd(imi)_3(N\text{-}phthgly)_2] \cdot 2H_2O$.

Cd1–O701	2.549(7)	N71–C78	1.359(11)
Cd1–O702	2.480(10)	N71–C79	1.452(15)
Cd1–O801	2.450(8)	C42–C52	1.344(12)
Cd1–O802	2.498(7)	C43–C53	1.324(15)
Cd1–N12	2.284(5)	C61–C62	1.484(14)
Cd1–N13	2.284(6)	C62–C63	1.390(14)
Cd1–N11	2.325(5)	C62–C67	1.378(11)
O61–C61	1.201(10)	C63–C64	1.377(16)
O68–C68	1.213(11)	C64–C65	1.380(15)
O71–C71	1.186(10)	C65–C66	1.368(19)
O78–C78	1.220(11)	C66–C67	1.371(16)
O701–C70	1.242(12)	C67–C68	1.501(15)
O702–C70	1.269(13)	C69–C70	1.517(15)
O801–C80	1.249(13)	C71–C72	1.494(14)
O802–C80	1.245(12)	C72–C73	1.383(13)
N13–Cd1–N11	86.5(2)	N61–C61–C62	105.6(8)
N12–Cd1–N11	98.2(2)	O61–C61–C62	129.7(9)
N12–Cd1–N13	174.2(2)	C61–C62–C67	108.7(8)
O802–Cd1–N11	140.7(2)	C61–C62–C63	130.4(8)
O802–Cd1–N13	85.5(2)	C63–C62–C67	120.9(9)
O802–Cd1–N12	88.7(2)	C62–C63–C64	116.4(9)
O801–Cd1–N11	88.6(2)	C63–C64–C65	122.6(11)
O801–Cd1–N13	87.9(2)	C64–C65–C66	120.2(11)
O801–Cd1–N12	88.8(2)	C65–C66–C67	118.2(11)
O801–Cd1–O802	52.7(2)	C62–C67–C66	121.5(9)
O702–Cd1–N11	84.8(2)	C66–C67–C68	131.0(9)
O702–Cd1–N13	96.2(2)	C62–C67–C68	107.4(8)
O702–Cd1–N12	87.7(2)	N61–C68–C67	106.2(8)
O702–Cd1–O802	134.3(2)	O68–C68–C67	129.0(9)
O702–Cd1–O801	172.0(2)	O68–C68–N61	124.7(9)
O701–Cd1–N11	134.1(2)	N61–C69–C70	112.1(8)
O701–Cd1–N13	82.8(2)	O702–C70–C69	114.7(8)
O701–Cd1–N12	96.2(2)	O701–C70–C69	120.8(8)
O701–Cd1–O802	82.8(2)	O701–C70–O702	124.6(9)
O701–Cd1–O801	135.2(2)	O71–C71–N71	124.8(9)
O701–Cd1–O702	52.5(2)	N71–C71–C72	104.1(8)
Cd1–O701–C70	90.2(5)	O71–C71–C72	131.1(9)
Cd1–O702–C70	92.7(6)	C71–C72–C77	109.3(7)
Cd1–O801–C80	93.0(6)	C71–C72–C73	129.2(8)
Cd1–O802–C80	90.8(5)	C73–C72–C77	121.5(8)
Cd1–N12–C52	128.6(6)	C72–C73–C74	116.8(8)
Cd1–N12–C22	126.3(5)	C73–C74–C75	121.9(10)

by steric hindrance of the five ligands cause distortions in bond distances: the Cd–O bonds range from 2.450(8) to 2.549(7) Å, while the angles around Cd are in the range 134.3(2)–172.0(2)°. Comparable values were found for similar complexes analyzed by Baggio *et al.* [20, 21] and Chotalia *et al.* [22]. All the rings are planar within error; the two N-phthaloylglycinate molecules are quasi-parallel with 171.2(3) for the dihedral angles formed by their respective mean planes. The five-membered rings (N11–C51, N12–C52 and N13–C53) form dihedral angles of 107.0(5), 117.7(4), 169.2(4)°, respectively. In the crystal, the molecules are connected by H-bonds involving the water molecules, the carboxylic oxygens of the N-phthaloylglycinate molecules and the imidazole nitrogens, table 5. There are two types of hydrogen bonds, the first type is the intra-molecular hydrogen bonds resulting from interaction between the lattice water molecules and the coordinated carboxylate oxygen

Table 5. Possible intra- and inter-molecular H-bonds. (D = donor; A = acceptor, H = hydrogen) for $[Cd(imi)_3(N\text{-phthgly})_2] \cdot 2H_2O$ complex.

D–H (Å)		D···A (Å)		H···A (Å)		D–H···A (°)	
O1W–H1W	0.88(10)	O1W···O702	2.784(12)	H1W···O702	2.92(10)	O1W–H1W···O702	169(9)
O2W–H2W	0.58(9)	O2W···O801	2.769(12)	H2W···O801	2.21(10)	O2W–H2W···O801	163(11)
N32–H32	0.89(8)	N32···O701i	2.932(9)	H32···O701i	2.08(9)	N32–H32···O701i	133(5)
C65–H65	0.98(8)	C65···O61ii	3.241(12)	H65···O61ii	2.49(7)	C65–H65···O61ii	133(5)
N33–H33	1.01(11)	N33···O2Wii	2.970(13)	H33···O2Wii	2.05(11)	N33–H33···O2Wii	151(8)
N31–H31	1.18(10)	N31···O802iii	2.939(11)	H31···O802iii	1.93(9)	N31–H31···O802iii	141(7)

Equivalent positions: (i) $+x-1$, $+y$, $+z$; (ii) $+x+1$, $+y$, $+z$; (iii) $+x$, $+y$, $+z+1$.

atoms (O1W···O702 = 2.84(12) Å, H1W···O702 = 2.92(10) Å; O1W–H1W···O702 = 169(9)°). The second type is the inter-molecular hydrogen bonds which involve the NH group of the coordinated imidazole and oxygen atoms of the coordinated carboxylate group of adjacent molecules (N32···O701i = 2.932(9) Å, H32···O701i = 2.08(9) Å; N32–H32···O701i = 133(5)°) ($i = +x-1$, $+y$, $+z$) and N31···O802iii = 2.939(11) Å, H31···O802iii = 1.93(9) Å; N31–H31···O802iii = 141(7)°)(iii = $+x$, $+y$, $+z+1$).

The bipolar arrangement of the phthalimide group results in additional inter-molecular hydrogen bonds between the carbon of the phthalimide group C65 and the uncoordinated carbonyl groups of adjacent molecules (C65···O61ii = 3.241(12) Å, H65···O61ii = 2.49(7) Å; C65–H65···O61ii = 133(5)°) (ii = $+x+1$, $+y$, $+z$). Figure 2 shows these interactions.

4. Conclusions

In conclusion, the phthaloylglycinate complexes of Zn(II) possess a monodentate N-phthaloylglycinate ligand. The carbonyl groups in the N-phthaloyl moiety as well as the glycinato part provide the anchor to form intra- and inter-molecular H-bonds. The study of Cd(II) ternary compounds, revealed some relevant features. Cadmium(II) is coordinated to a large number of oxygen donors. Martin recently reported [23] that the softness of cadmium is not clearly correlated to equilibrium constants with oxygen donors. In this sense, a far better correlation between acetate equilibrium constant ($\log k = 1.56$) and electron affinity of Cd(II) (16.91 eV), which is similar to that of Mn(II) was established. This correlation is in agreement with coordination of the carboxyl groups which are active binding sites. The preference of Cd(II) toward high coordination numbers leads to bidentate coordination of N-phthaloylglycinate, compared with the monodentate carboxylic coordination towards Cu(II) [5], Co(II), Ni(II) [6] and Zn(II). The bidentate coordination of the carboxylate group of the N-protected amino acids was also observed by Corradi *et al.* [24] for the cadmium(II) complex of N-*p*-tolylsulfonyl-l-glutamic acid and 2,2′-bipyridine, and by Capllonch *et al.* [25], for the dimeric ternary cadmium(II)-hippurate-cytosine complex.

The structure of the ternary cadmium complexes, showing oxygen donor coordination offers additional reasons for the toxicity of cadmium, not only that for sulfur or other soft biological donors. This conclusion is in agreement with the results obtained from similar structures [25].

Supplementary data

Supplementary crystallographic data are available from the CCDC, 12 Union Road, Cambridge CB2 IEZ, UK on request, deposition number: CCDC 604419.

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