The coordination of a multidentate N_xO_y-donor (x & y ≤ 2) oxazolidine-based ligand with Cd(II) and Hg(II)

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ABSTRACT

In this work, two binuclear complexes, *fac*-[Cd₂(AEPC)₂(μ-Cl)₂Cl₂] (**1**) and [Hg₂(AEPC)₂(μ-Cl)₂Cl₂] (**2**), of 2-(2-(pyridin-2-yl)oxazolidin-3-yl)ethanol (AEPC) were prepared and identified by elemental analysis, FT-IR, ¹H NMR spectroscopies and single-crystal X-ray diffraction. All coordination modes of 2-(pyridin-2-yl)oxazolidine derivatives were studied by analysis of the Cambridge Structural Database (CSD) for determination of coordination behaviors of the AEPC ligand with metals. In the crystal structure of **1**, the cadmium atom has a distorted octahedral geometry and CdN₂OCl₃ environment in which each ligand acts as

an NN'O-donor. In the crystal structure of **2**, the AEPC acts as NN'-donor toward the mercury atom to form a square-pyramidal geometry with three chloride ions. Each complex contains four chiral centers and *R,R,S,S* configuration with a center of inversion and C_i symmetry. In the crystal networks of the complexes, the alcoholic group of the ligands participate in hydrogen bonding and form $R_4^4(28)$ and $R_6^6(44)$ hydrogen bond motifs (observed for complex **1**). In addition to the hydrogen bonds, the crystal network is stabilized by π - π stacking interactions between pyridine rings of the AEPC ligands of adjacent complexes.

Keywords: Oxazolidine; Cadmium; Mercury; X-ray crystal structure; Binuclear complex; Chiral Center; *fac* isomer

1. Introduction

Several substituted oxazolidines have been investigated extensively because of their importance as pharmacological active compounds (such as antidiabetic [1], anticonvulsant [2], antitubercular [3], and aldose reductase inhibitors [4]), chiral auxiliaries in the synthesis of a variety of chiral compounds, chain-protecting groups for amino alcohols [5, 6], crosslinking agents [7] to stabilization of collagen [8, 9], linkers in solid-phase synthesis of peptide aldehydes process [10], optical probe applications [11] and fungicidal activities [12].

Usually, 1,3-oxazolidines are synthesized by the condensation of 1,2-amino alcohols with carbonyl compounds [13]. Some other approaches are found in literature by double-Michael reactions of acetylenes and β -amino alcohols [14], aza-Wacker type reaction of β -amino alcohols with alkenes [15], aziridines with vinyl arenes [16] and tandem ring-opening/closing reaction of aziridine itself [16]. One other methods is the ring formation process from α -hydroxyesters [17] or α -hydroxyamides [18] by treatment with a reagent already carrying the carbonyl function and α -hydroxycarboxylic acids with carbodiimide [19].

In order to extend the chemistry of oxazolidines, in this work, preparation, characterization of a new oxazolidine ligand (2-(2-(pyridin-2-yl)oxazolidin-3-yl)ethanol, Scheme 1) synthesized by condensation of 2,2'-azanediylbis(ethan-1-ol) with picolinaldehyde and its complexes, *fac*-[Cd₂(AEPC)₂(μ-Cl)₂Cl₂] (**1**) and [Hg₂(AEPC)₂(μ-Cl)₂Cl₂] (**2**), are described.

2. Experimental

2.1. Materials and Instrumentation

All starting chemicals and solvents were from Merck and were used as received without further purification. Infrared spectra (as KBr pellets) in the range 4000–400 cm⁻¹ were recorded with a FT-IR 8400-Shimadzu spectrometer. ¹H NMR spectra were recorded on a Bruker Aspect 3000 instrument; chemical shifts δ are given in parts per million, relative to TMS as internal standard. The carbon, hydrogen and nitrogen contents were determined using a Thermo Finnigan Flash Elemental Analyzer 1112 EA. The melting points were measured with a Barnsted Electrothermal 9200 electrically heated apparatus.

2.1.1. Synthesis of 2-(2-(Pyridin-2-yl)oxazolidin-3-yl)ethanol, (AEPC)

A mixture of 2.10 g (20 mmol) of 2,2'-azanediylbis(ethan-1-ol) and 2.14 g (20 mmol) of picolinaldehyde were reacted in a 250 ml round bottom flask under reflux condition (without solvent) in an oil bath with stirring for 24 h by keeping the temperature at 90 °C. The redundant precursors were removed at the rotary evaporator. The product was dissolved in water (20 mL) and washed three times with 1,2-dichloroethane (20 mL). The isolated water layer was evaporated to dryness to give a thick brown oil. Several attempts to crystallize the compound were unsuccessful. Yield: 3.0 g, 77%. Anal. Calcd for C₁₀H₁₄N₂O₂ (%): C, 61.84; H, 7.27; N, 14.42. Found: C, 60.65; H, 7.02; N, 13.94. IR (KBr disk): 3363 (ν OH), 3010 (ν

CH)_{ar}, 2942 (ν CH), 1603 (ν C=N), 1400 (δ_{as} CH₂ and/or ν C=C), 1387 (δ_s CH₂), 1250 (ν C–O), 1040 (ν C–N), 753 and 702 (γ py) cm⁻¹. ¹H NMR (300 MHz, [D₆]DMSO): δ = 8.50–8.54 (d, 1 H, C¹⁰H), 7.68–7.74 (t, 1 H, C⁸H), 7.51–7.54 (d, 1 H, C⁷H), 7.21–7.28 (m, 1H, C⁹H), 5.29 (s, 1H, C⁵H), 5.07 (s, 1H, OH), 2.81–4.10 (m, 8H, C¹H₂–C⁴H₂) ppm.

2.1.2. Synthesis of di(μ -chloro)dichlorobis(2-(2-(pyridin-2-yl)oxazolidin-3-yl)ethanoldicadmium(II), *fac*-[Cd₂(AEPC)₂(μ -Cl)₂Cl₂] (1).

A solution of 0.47 g (2.39 mmol) of AEPC, dissolved in ethanol (10 mL), was added to a stirring solution of 0.49 g (2.39 mmol) of CdCl₂·H₂O in the same solvent (5 mL). The reaction mixture was heated under reflux for 24 hour, cooled and filtered. Colorless crystals suitable for X-ray diffraction studies were obtained by slow evaporation of the solution for three days and collected by filtration. Yield: 0.33 g, 72%; m.p. 123 °C. Anal. Calcd for C₁₀H₁₄CdCl₂N₂O₂ (%): C, 31.81; H, 3.74; N, 7.42. Found: C, 31.62; H, 3.70; N, 7.50. IR (KBr disk): 3393 (ν OH), 3069 (ν CH_{ar}), 2954 (ν CH), 1592 (ν C=N), 1441 (δ_{as} CH₂), 1441 (ν C=C), 1353 (δ_s CH₂), 1237 (ν C–O), 1065 (ν C–N), 771 and 634 (γ py), 527 (ν Cd–N), 470 (ν Cd–O) cm⁻¹. ¹H NMR (300 MHz, [D₆]DMSO): δ = 7.61–8.70 (m, 4H, C⁷H–C¹⁰H), 6.14 (s, 1H, OH), 5.33 (s, 1H, C⁵H), 2.69–3.96 (m, 8H, C¹H₂–C⁴H₂) ppm.

2.1.3. Synthesis of di(μ -chloro)dichlorobis(2-(2-(pyridin-2-yl)oxazolidin-3-yl)ethanoldimercury(II), [Hg₂(AEPC)₂(μ -Cl)₂Cl₂] (2).

The procedure for the synthesis of **2** was the same as that for **1** except that CdCl₂·H₂O was replaced by 0.65 g (2.39 mmol) of HgCl₂. Colorless crystals suitable for X-ray diffraction studies were obtained by slow evaporation of the solution for four days and collected by filtration. Yield: 0.15 g, 27%; m.p. 239 °C. Anal. Calcd for C₁₀H₁₄Cl₂HgN₂O₂ (%): C, 25.79; H, 3.03; N, 6.02. Found: C, 25.63; H, 3.03; N, 6.06. IR (KBr disk): 3373 (ν OH), 3071 (ν CH_{ar}), 2946 (ν CH), 1599 (ν C=N), 1456 (δ_{as} CH₂), 1456 (ν C=C), 1385 (δ_s CH₂), 1227 (ν

C–O), 1048 (ν C–N), 775 and 639 (γ py), 544 (ν Hg–N) cm^{-1} . ^1H NMR (300 MHz, $[\text{D}_6]\text{DMSO}$): δ = 8.63–8.64 (d, 1H, C^{10}H), 8.05–8.10 (t, 1H, C^8H), 7.73–7.76 (d, 1H, C^7H), 7.64–7.68 (t, 1H, C^9H), 5.46 (s, 2H, C^5H , OH), 2.69–4.02 (m, 8H, $\text{C}^1\text{H}_2\text{--C}^4\text{H}_2$) ppm.

2.2. Crystal structure determination

1. Data were collected at 93.0 K using a Rigaku FRX (Mo- K , confocal optic) and Dectris P200. Intensity data were collected using ω steps accumulating area detector images spanning at least a hemisphere of reciprocal space. All data were corrected for Lorentz polarization effects. Absorption effects were corrected based on multiple equivalent reflections or by semi-empirical methods using CrystalClear.[new REF *CrystalClear-SM Expert* v3.1b27. Rigaku Americas, The Woodlands, Texas, USA, and Rigaku Corporation, Tokyo, Japan, 2013.

] Structures were solved by direct methods and refined by full-matrix least-squares against F^2 by using Shelxl [20]. Diagrams of the molecular structure and unit cell were created using Ortep-III [21, 22] and Diamond [23]. Crystallographic data and details of the data collection and structure refinement are listed in Table 1, selected bond lengths and angles in Table 2 and hydrogen bond geometries in Table 3. The structure of **2** has large residual electron density in the difference map; we examined several different crystals and the reported results came from the best dataset based on a very small crystal which is reflected in the quality of the outcome

3. Results and Discussion

2,2'-Azanediylbis(ethan-1-ol) in the reaction with picolinaldehyde under solvent free conditions gave AEPC *via* an oxazolidination reaction. Reaction of AEPC with an ethanolic solution of cadmium(II) or mercury(II) chlorides in a molar ratio of 1:1 resulted in the formation of **1** and **2**. The complexes are air-stable, and soluble in DMSO.

3.1. Spectroscopic characterization

The frequency of IR bands for the free ligand are different from those of the corresponding complexes providing significant indications of bonding sites of the AEPC. In the IR spectrum of AEPC, a broad peak at the 3363 cm^{-1} can be assigned to the $\nu(\text{OH})$ which is shifted to higher frequencies in the spectra of complexes by 30 and 10 cm^{-1} for **1** and **2**, respectively; the significant shift in the complex **1** confirming the coordination of alcoholic group toward cadmium atom. One of the important sites of the ligand in complexation is the nitrogen atom of the pyridine ring. The ring mode in the two IR spectra of complexes (about 1600 cm^{-1}) is slightly shifted to lower frequency than that of free ligand (11 and 4 cm^{-1} for **1** and **2**, respectively). Metal-ligand interactions can be studied at the below 600 cm^{-1} in the IR spectra. In this region, two bands at 527 and 470 cm^{-1} were assigned to the Cd–N and Cd–O stretching vibrations [24] and the $\nu\text{ Hg–N}$ was observed for **2** at 544 cm^{-1} .

In the ^1H NMR spectra (see scheme 1 for numbering) of the ligand and complexes, there are three set of signals including, 7–9 ppm for aromatic units, 5–6 ppm for the hydrogen on the chiral carbon and alcoholic group, 2.5–4 ppm for aliphatic moieties. After coordination, the signals in the aromatic region shifted by 0.1–0.5 ppm to lower magnetic field confirming the coordination of nitrogen atom of pyridine. A significant shift (1.07 ppm) to lower magnetic field of alcoholic proton in complex **1** revealed that the oxygen donation activity of the ligand.

3.2. Description of the crystal structures

The 2-(pyridin-2-yl)oxazolidine unit is a potentially tridentate ligand that can be bind to metal atoms through one O- and two N- atoms. A survey of the Cambridge Structural Database (CSD) [25] reveals that this unit has two different coordination modes, $\text{N}_{\text{py}}\text{N}_{\text{oxazolidine}}$ - and $\text{N}_{\text{py}}\text{O}_{\text{oxazolidine}}$ -donor (for more precise result, the examples containing cyclic moieties fused to oxazolidine ring, macrocycles and $\text{N}_{\text{oxazolidine}}$ -oxide compounds have

been omitted). Among the twelve examples similar to AEPC, the N_{py}N_{oxazolidine}-donor mode in which two coordinated nitrogen atoms form a five-membered chelate ring is the most common (92%) [13, 26-33]. There is only one example for N_{py}O_{oxazolidine}-donor mode (8%) [26] in which coordination of nitrogen atom of oxazolidine ring to metal center due to substitution of a phenyl ring on this atom is difficult.

3.2.1. *Crystal structure of fac-[Cd₂(AEPC)₂(μ-Cl)₂Cl₂] (1)*

The single crystal X-ray analysis of complex **1** reveals that a binuclear complex of cadmium containing two chloro bridges. The geometry around the cadmium atom is distorted octahedral (Fig. 1) formed by coordination of two nitrogen atoms and one oxygen atom of AEPC and three chloro ligands. The Cd–N_{py} bond length (2.374(3) Å) is shorter than the Cd–N_{oxazolidine} (2.453(3) Å); similar result has been reported for the only one similar structure (cadmium complexes containing 2-(pyridin-2-yl)oxazolidine unit) [13]. There are two types of chloro ligands in the crystal structure of **1**, asymmetrically-bound bridging and terminal. Bridging chloro ligands and cadmium atoms are co-planar (with no r.m.s. deviation). The two Cd–Cl_{bridging} bond lengths are similar to other complexes of the type [Cd₂(L)₂(μ-Cl)₂Cl₂] (L is any “NN’O-donor” ligand) as is the terminal Cd–Cl bond length (Table 4).

Each ligand acts as tridentate NN'O-donor and forms two five-membered non-planar chelate rings. The angle between the mean planes through the two chelate rings of each AEPC ligand is 70.13°, showing the ligand binds to cadmium atom tending to the *fac* form. The C5 carbon atom of ligand (Scheme 1) has four different substituents and is chiral but two chiral carbon atoms of complex. In addition a new chiral center is formed (nitrogen atom of oxazolidine ring) upon coordination. Thus two metal centers are associated with two C-chiral and two N-chiral centers. The formula of complex can be written as *R,R,S,S-fac-*

[Cd₂(AEPC)₂(μ-Cl)₂Cl₂]. The complex has one center of inversion on the center of Cd1/Cl2/Cd1ⁱ/Cl2ⁱ plane and C_i symmetry.

3.2.2. Crystal structure of [Hg₂(AEPC)₂(μ-Cl)₂Cl₂] (**2**)

In the crystal structure of complex **2** (Fig. 2), the mercury atom is coordinated by two nitrogen atoms of the AEPC and three chloride ions with total coordination number five. A pentacoordinate geometry may adopt either a square pyramidal or a trigonal bipyramidal structure. To determine the geometry for such complexes, the formula of Addison *et al.* [34, 35] was applied. The angular structural parameter (τ) value for **2** was calculated to be 5.17% indicating an almost square-pyramidal geometry around the metal atoms. Studying the CSD database revealed that there is no example for coordination of 2-(pyridin-2-yl)oxazolidine unit toward mercury atom that would allow us to compare the geometric parameter with complex **2**. Similarly to complex **1**, in this complex the Hg–N_{py} bond length (2.277 Å) is shorter than the Hg–N_{oxazolidine} (2.526 Å). Two types of Hg–Cl bonds in the crystal structure of **2** were compared with CSD average for complexes of the type [Hg₂(L)₂(μ-Cl)₂Cl₂] (L is any “NN’-donor” ligand) and the results listed in Table 4. In all complexes the Hg–Cl_{terminal} bond length is shorter than the bridging one and two bridged chlorides and two mercury atoms lie on a plane. The distance of all Hg–Cl bonds are in range of reported for similar structures (Table 4).

In addition to one chiral carbon atom of AEPC ligand, after coordination of the ligand to the mercury atom, the nitrogen atom of the oxazolidine ring becomes a chiral atom and the complex has *R,R,S,S* configuration (similar to **1**). The complex has one center of inversion on the center of Hg1/Cl2/Hg1ⁱ/Cl2ⁱ plane and C_i symmetry.

The angle between two mean planes through the pyridine and oxazolidine rings in complexes of **1** and **2** is 73.49 and 78.90° respectively, proving these rings are almost

perpendicular to each other but the direction of rings in two complexes are different. In the complex **1** (Fig. 3a), the pyridine and oxazolidine rings are “face to face” perpendicular while the complex **2** (Fig. 3b) shows “face to side” perpendicular rings. It seems that this is the important ability which can help to AEPC to bind the metal centers in different coordination modes. Converting from “face to face” to “face to side” mode is accompanied by increasing the bond angle for chiral carbon atom of the chelate ring (Fig 3).

3.2.3 *Crystal network interactions*

In the crystal network of **1** and **2**, there are intermolecular strong O–H···O, and relatively strong intramolecular O–H···Cl [36] hydrogen bonds, respectively, together with weak interactions (Table 3) . In this way, the chloride ions act as proton acceptors whereas the oxygen atoms of the ligands participate in hydrogen bonding as proton donors and acceptors. In addition to the hydrogen bonds, the crystal network is stabilized by π – π stacking interactions between pyridine rings of the AEPC ligands of the adjacent complexes. The nitrogen atom of a pyridine ring has *trans* position with respect to the nitrogen atom on the other pyridine ring connected by π – π stacking (Fig. 4). Centroid–centroid distance of two parallel pyridine rings in the crystal network of **2** (the angle between planes through two pyridine rings, 0°) and the perpendicular distance between the pyridine planes is 3.733 and 3.541 Å, respectively. Thus the slippage of pyridine rings was calculated to be 0.620 Å (Fig. 4).

In the crystal packing of **1**, the O–H···O hydrogen bonds participate in the formation of R₄⁴(28) hydrogen bond motifs (four proton acceptors, four proton donors with degree of 28) [37, 38] between four complexes (Fig. 5) and R₆⁶(44) between six complexes.

4. Conclusions

In this work, two new complexes of 2-(2-(pyridin-2-yl)oxazolidin-3-yl)ethanol (AEPC) *fac*-[Cd₂(AEPC)₂(μ-Cl)₂Cl₂] (**1**) and [Hg₂(AEPC)₂(μ-Cl)₂Cl₂] (**2**) were synthesized and their spectral (IR, ¹H NMR) and structural properties were investigated. These complexes revealed that the AEPC ligand can coordinate either NN'O or NN'. In these binuclear complexes, the cadmium atom has distorted octahedral geometry (**1**), CdN₂OCl₃, while the geometry around the mercury atom is square-pyramidal (**2**), HgN₂Cl₃. A structural study of 2-(pyridin-2-yl)oxazolidine-based ligands revealed that this type of ligand is commonly coordinated to metal centers as N_{py}N_{oxazolidine}-donor (92%) while the another mode (N_{py}O_{oxazolidine}-donor) is rare (8%). Each complex contains four chiral centers (two nitrogen and two carbon atoms) and *R,R,S,S* configuration. Also the complexes contain a center of inversion and C_i symmetry. In the crystal networks of the complexes, the O–H and C–H bonds and chloride ions have important roles in the hydrogen bonding map. The O–H⋯O hydrogen bonds form R₄⁴(28) and R₆⁶(44) hydrogen bond motifs (complex **1**). In addition to the hydrogen bonds, the crystal network is more stabilized by π–π stacking interactions between pyridine rings of the AEPC ligands on the adjacent complexes.

Appendix A. Supplementary data

CCDC 1559606 and 1559605 respectively for complexes of **1** and **2** contain the supplementary crystallographic data for this paper. These data can be obtained free of charge via <http://www.ccdc.cam.ac.uk/conts/retrieving.html>, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; or e-mail: deposit@ccdc.cam.ac.uk.

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Table 1. Crystal data and structure refinement for complexes of **1** and **2**.

	1	2
Empirical formula	C ₁₀ H ₁₄ CdCl ₂ N ₂ O ₂	C ₁₀ H ₁₄ Cl ₂ HgN ₂ O ₂
Formula weight, g mol ⁻¹	377.55	465.73
Crystal size, mm ³	0.10 × 0.10 × 0.10	0.10 × 0.06 × 0.03
Temperature, K	93	93
Crystal system	monoclinic	monoclinic
Space group	<i>C2/c</i>	<i>C2/c</i>
Unit cell dimensions (Å, °)		
<i>a</i>	15.828 (4)	16.595(6)
<i>b</i>	9.8509 (19)	9.989(3)
<i>c</i>	17.919 (4)	16.548(6)
β	110.624	110.366(10)
Volume, Å ³	2614.9 (10)	2571.6(15)
<i>Z</i>	8	8
Calculated density, g cm ⁻³	1.918	2.406
Absorption coefficient, mm ⁻¹	2.07	12.41
<i>F</i> (000), e	1488.00	1744
2 θ range for data collection (°)	4.8–55.0	4.8–54.8
<i>h</i> , <i>k</i> , <i>l</i> ranges	–9 ≤ <i>h</i> ≤ 19, –11 ≤ <i>k</i> ≤ 11, –21 ≤ <i>l</i> ≤ 21	–19 ≤ <i>h</i> ≤ 19, –9 ≤ <i>k</i> ≤ 2, –19 ≤ <i>l</i> ≤ 14
Reflections collected / independent / <i>R</i> _{int}	15974 / 2392 / 0.067	8112 / 2341 / 0.076
Data / ref. parameters	2392 / 158	2341 / 157
Goodness-of-fit on <i>F</i> ²	1.01	1.00
Final <i>R</i> indexes [<i>I</i> ≥ 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0399, <i>wR</i> ₂ = 0.1041	<i>R</i> ₁ = 0.0399, <i>wR</i> ₂ = 0.1041
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0452, <i>wR</i> ₂ = 0.1087	<i>R</i> ₁ = 0.0452, <i>wR</i> ₂ = 0.1087
Largest diff. peak / hole, e Å ⁻³	0.79 / –0.77	3.37 / –3.03

Table 2. Selected bond lengths (Å) and angles (°) for complexes of **1** and **2** with estimated standard deviations in parentheses.

Bond lengths (Å)		Angles (°)	
1			
Cd(1)–N(1)	2.374(3)	N(1)–Cd(1)–N(8)	70.4(1)
Cd(1)–N(8)	2.453(3)	N(8)–Cd(1)–O(14)	70.46(9)
Cd(1)–Cl(1)	2.497(1)	O(14)–Cd(1)–Cl(2)	85.04(7)
Cd(1)–Cl(2)	2.594(1)	Cl(2)–Cd(1)–Cl(1)	106.95(3)
Cd(1)–Cl(2) ⁱ	2.653(1)	Cl(2)–Cd(1)–N(1)	84.39(8)
Cd(1)–O(14)	2.381(3)	Cl(2)–Cd(1)–Cl(2) ⁱ	85.37(3)
		Cd(1)–Cl(2)–Cd(1) ⁱ	94.64(3)
2			
Hg(1)–N(1)	2.28(1)	N(1)–Hg(1)–N(8)	72.3(3)
Hg(1)–N(8)	2.526(9)	N(1)–Hg(1)–Cl(2)	83.2(2)
Hg(1)–Cl(1)	2.397(3)	N(1)–Hg(1)–Cl(1)	147.3(2)
Hg(1)–Cl(2)	3.021(3)	Cl(1)–Hg(1)–Cl(2)	87.01(9)
Hg(1)–Cl(2) ⁱⁱ	2.526(3)	Cl(2)–Hg(1)–Cl(2) ⁱⁱ	88.36(9)
		Hg(1)–Cl(2)–Hg(1) ⁱⁱ	91.64(9)

i: 1–*x*, 1–*y*, 1–*z*; *ii*: 0.5–*x*, 1.5–*y*, 1–*z*

i: 1–*x*, 1–*y*, 1–*z*; *ii*: 0.5–*x*, 1.5–*y*, 1–*z*

Table 3. Hydrogen bonds dimensions (Å and °) in complexes of **1** and **2**.

D–H···A	<i>d</i> (D–H)	<i>d</i> (H···A)	∠(DHA)	<i>d</i> (D···A)	Symmetry code on A atom
1					
O(14)–H(14)···O(11)	0.98	1.79	166	2.752(3)	$-1/2 + x, 1/2 - y, -1/2 + z$
O(14)–H(14)···C(7)	0.98	2.89	157	3.812(4)	$-1/2 + x, 1/2 - y, -1/2 + z$
O(14)–H(14)···C(10)	0.98	2.86	145	3.708(4)	$-1/2 + x, 1/2 - y, -1/2 +$
C(4)–H(4)···Cl(1)	0.951	2.677	140.6	3.464(5)	x, y, z
C(7)–H(7)···Cl(1)	1.000	2.6774	150	3.578(3)	$1 - x, 1 - y, 1 - z$
C(10)–H(10A)···Cl(1)	0.991	2.820	168.4	3.795(4)	$x, -1 + y, z$
2					
O(14)–H(14)···Cl(2)	0.99	2.3	147	3.18(2)	x, y, z
C(5)–H(5)···Cl(1)	0.95	2.910	155	3.79(1)	x, y, z
C(10)–H(10A)···O(11)	0.99	2.708	151.2	3.61(2)	x, y, z

Table 4. Bond lengths for different types of M–Cl bonds (M: Cd and Hg, respectively for **1** and **2**) in complexes containing $[M_2(L)_2(\mu\text{-Cl})_2Cl_2]$ unit (for **1**, M: Cd and L is any “NN’O-donor” ligand, for **2**, M: Hg and L is any “NN’-donor” ligand).

	CCDC Numbers	M–Cl _{bridging}			M–Cl _{terminal}
		d_1	d_2	δd	
Cadmium Complexes	Complex 1	2.594	2.653	0.059	2.497
	1403454	2.609	2.647	0.038	2.543
	824895	2.637	2.642	0.005	2.466
	1422673	2.575	2.631	0.056	2.474
	1042576	2.586	2.791	0.205	2.544
	113669	2.614	2.618	0.004	2.603
	737385	2.621	2.626	0.005	2.619
	776439	2.488	2.929	0.441	2.550
	1001915	2.557	2.638	0.081	2.464
	1402318	2.500	2.738	0.238	2.452
	732063	2.478	2.935	0.457	2.549
	694024	2.652	2.707	0.055	2.570
	850085	2.513	2.819	0.306	2.575
	663562	2.535	2.674	0.139	2.498
	663562	2.582	2.656	0.074	2.490
Mercury Complexes	Complex 2	2.526	3.021	0.495	2.397
	845202	2.600	2.706	0.106	2.411
	907536	2.628	2.893	0.265	2.356
	902220	2.337	3.126	0.789	2.316
	807748	2.526	2.896	0.370	2.396
	839151	2.490	2.878	0.388	2.395
	744178	2.494	2.880	0.386	2.380
	194788	2.579	2.797	0.218	2.344
	194789	2.403	2.944	0.542	2.361
	230005	2.428	2.910	0.482	2.368
	990959	2.378	3.127	0.749	2.779
	892207	2.451	3.005	0.554	2.396
	892208	2.408	3.134	0.726	2.382
	892209	2.421	2.984	0.563	2.438
	892210	2.423	3.011	0.588	2.355
	926083	2.462	2.974	0.512	2.369
	807236	2.533	2.843	0.310	2.434
	1420119	2.447	3.031	0.584	2.407
	815449	2.516	2.807	0.291	2.394
	612971	2.558	2.880	0.322	2.430
	827007	2.399	3.046	0.647	2.447
	YIZTUW*	2.499	2.742	0.243	2.387
	1531593	2.459	2.999	0.540	2.402

*for this structure the CCDC number has not been assigned, thus CCDC number was replaced by refcode.

Figure Captions

Scheme 1. The synthetic route of 2-(2-(pyridin-2-yl)oxazolidin-3-yl)ethanol (AEPC).

Figure 1. The ortep diagram of the molecular structure of $[\text{Cd}_2(\text{AEPC})_2(\mu\text{-Cl})_2\text{Cl}_2]$. The ellipsoids are drawn at the 25% probability level.

Figure 2. The ortep diagram of the molecular structure of $[\text{Hg}_2(\text{AEPC})_2(\mu\text{-Cl})_2\text{Cl}_2]$. The ellipsoids are drawn at the 25% probability level.

Figure 3. “face to face” and “face to side” arrangement for the perpendicular pyridine and oxazolidine rings.

Figure 4. Packing of complex **2**, showing the hydrogen bonds. Only the hydrogen atoms involved in hydrogen bonding are shown. Each HgN_2Cl_3 unit is shown as square pyramid.

Figure 5. $R_4^4(28)$ hydrogen bond motifs between four complexes of **1**.

Scheme 1.

Figure 1.

Figure 2.

Figure 3.

Figure 4.

Figure 5.