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Metal halide coordination compounds with 4(3H)-quinazolinone

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Abstract

4(3H)-Quinazolinone may act as ligand for metal ions in different coordination modes – coordinating through nitrogen atom *para* to the quinazolinone oxygen atom (mode 1), or through nitrogen atom *ortho* to the quinazolinone oxygen atom (mode 2), after hydrogen atom migration (tautomerization). Earlier crystal structural investigations have shown that in the reaction of cadmium chloride or bromide with 4(3H)-quinazolinone, this ligand interacts with Cd(II) cations via *para* nitrogen atoms (mode 1), and the octahedral coordination around the metal is completed by two ligands in a *trans* axial geometry. New cadmium(II) and mercury(II) coordination polymers were obtained via reaction of 4(3H)-quinazolinone with $CdBr_2$ and $HgCl_2$, respectively. Single crystal X-ray structural analysis reveals that coordination compounds crystallize in monoclinic $P2_1/c$ and triclinic P-1 space groups, featuring halide-bridged 1D chain polymers based on momonuclear $[M(X)_2(L)]$ subunits ((M = Cd, Hg, X = halide ion and L = 4(1H)-quinazolinone). Each metal ion is coordinated to one quinazolinone ligand, via the nitrogen atom *ortho* to the quinazolinone oxygen atom, with similar coordination geometries for metal ions in both coordination polymers.

Keywords: 4(3H)-quinazolinone; crystal structure;
cadmium coordination polymer.

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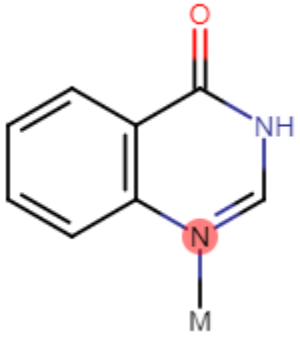
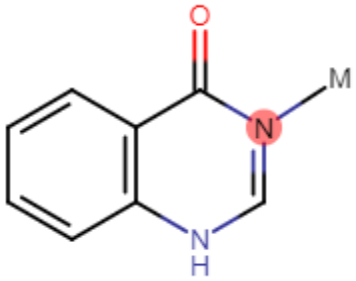
Introduction

Quinazolin-4-ones may act as ligands in different coordination modes as shown in the scheme. Earlier crystal structural investigations have shown that in the cadmium coordination polymer of 4(3H)-quinazolinone the ligand molecules interact with Cd(II) cations via nitrogen atoms at the position 1 (mode 1)[1]. In the case of the mononuclear copper(II) coordination compound the ligand molecules are bonded to Cu(II) cations by nitrogen atoms at the position 3 (mode 2) [2].



mode 1



mode 2

[1] K.Turgunov and U.Englert. *Acta Cryst*., 2010, **E66**, m1457.
[2] K.Turgunov et al., *Acta Cryst*., 2010, **E66**, m1680.

Synthesis and crystallization

Cadmium bromide complex with 4(3H)-quinazolinone. 70 mg (0.2 mmol) of cadmium bromide tetrahydrate was dissolved in a mixture of 4 ml of ethyl alcohol and 1 ml of water. 60 mg (0.4 mmol) of the ligand was dissolved in 5 ml of ethyl alcohol and it was added to the cadmium bromide solution. After 1-2 minutes, in the solution crystals began to appear. Within 2-3 hours prismatic crystals, suitable for X-ray diffraction were formed.

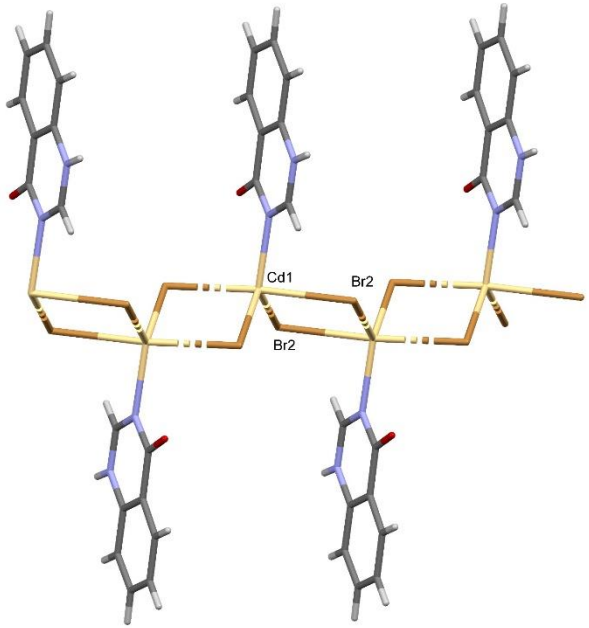
Mercury(II) chloride complex with 4(3H)-quinazolinone. 54.3 mg (0.2 mmol) of mercury (II) chloride was dissolved in a acetone. 30 mg (0.2 mmol) of the 4(3H)-quinazolinone was dissolved in 3 ml of acetone with little heating and ligand solution was added to the mercury (II) chloride solution. Within several seconds prismatic crystals, suitable for X-ray diffraction were formed.

Cadmium iodide complex with 4(3H)-quinazolinone. 73 mg (0.2 mmol) of cadmium iodide was dissolved in a ~1 ml of ethyl alcohol. 60 mg (0.4 mmol) of the ligand was dissolved in 4 ml of ethyl alcohol with little heating and it was added to the cadmium iodide solution. After several days single crystals suitable for X-ray diffraction were obtained by slow evaporation.

Results and Discussion
1. Structure of complex with $CdBr_2$.

The asymmetric unit of the compound crystal consists of one Cd^{2+} cation, two Br^- anions and one molecule of the 4(1H)-quinazolinone. The Cd^{2+} coordination environment ($CdBr_4N$) is a slightly distorted trigonal bipyramid supplemented by the nitrogen atom of 4(1H)-quinazolinone molecule. Two μ-bromide anions bridge Cd^{2+} cations, forming a one-dimensional polymer along the *b* axis. Two slightly different Cd…Cd distances of 3.867(1) Å and 3.905(1) Å are subtended.

P*2$_1$/*c	
Chemical formula	$[CdBr_2(C_8H_6N_2O)]$
Temperature (K)	100
a, (Å)	10.7967 (11)
b, (Å)	7.2041 (7)
c, (Å)	13.7643 (14)
β (°)	100.470 (2)
V (Å^3)	1052.77 (18)
R_1, wR_2	0.053, 0.139
CCDC	2041760



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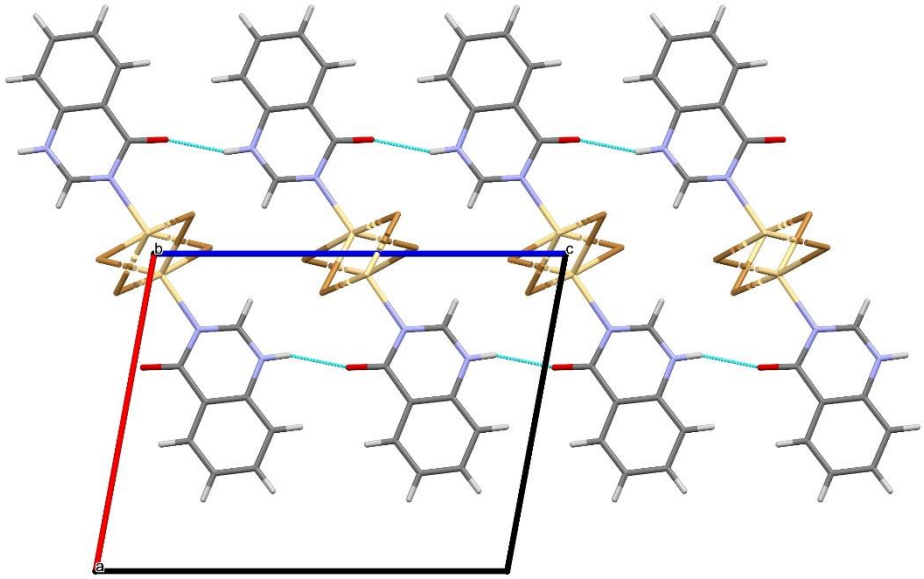
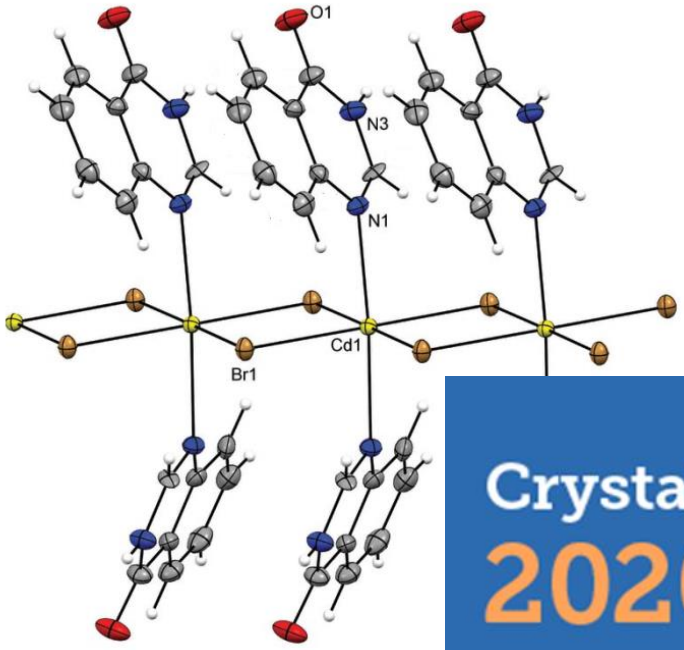


A classical N—H…O hydrogen bonds connects adjacent polymeric chains along the *c* axis.

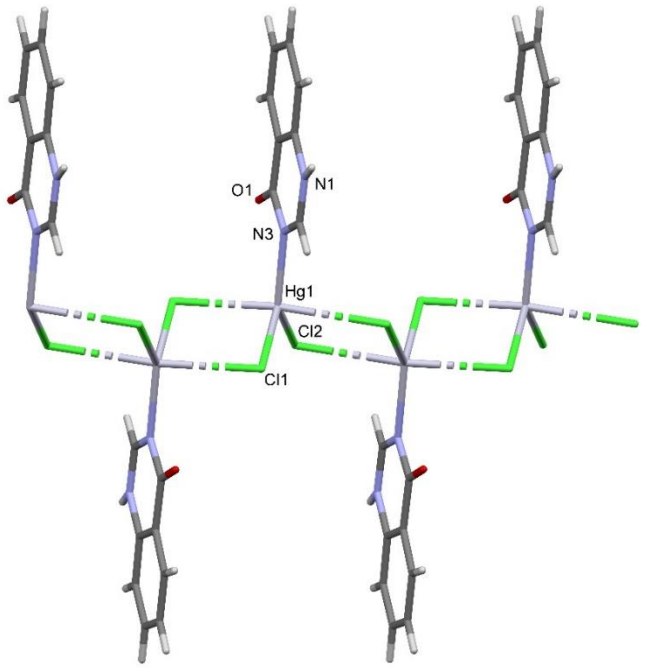
One-dimensional polymeric $CdBr_2$ complex with octahedral geometry around the cadmium(II) cations, including a *trans* arrangement of the two 4(3H)-quinazolinone ligands (coordinated via the nitrogen atom *para* to the quinazolinone oxygen atom) was obtained by another scientist [3].



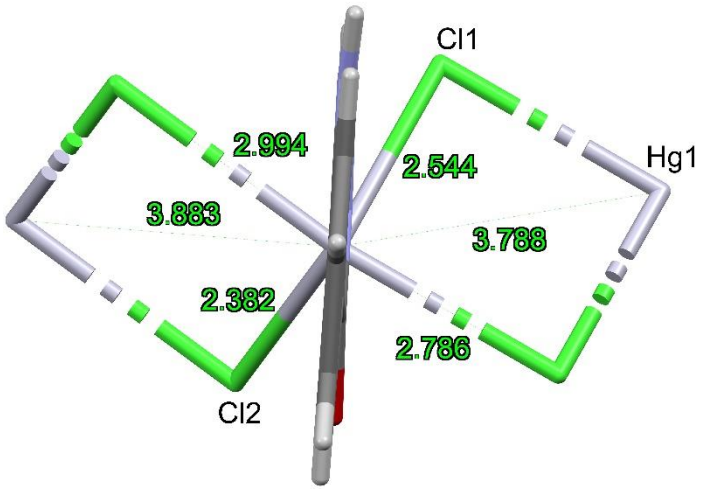
[3] M. Đakovic et al., *IUCrJ*, 2018, **5**, 13–21.

2. Structure of complex with $HgCl_2$.

The complex displays essentially the same crystal structure as the one obtained with $CdBr_2$. As expected, the μ-Cl bridges are strongly asymmetric.



P-1	
Chemical formula	$[HgCl_2(C_8H_6N_2O)]$
Temperature (K)	100
a, (Å)	6.8205 (7)
b, (Å)	7.0742 (7)
c, (Å)	10.4689 (10)
α, (°)	85.717 (2)
β, (°)	80.789 (2)
γ, (°)	89.147 (2)
V, (Å^3)	497.21 (9)
R_1, wR_2	0.028, 0.070
CCDC	2041761



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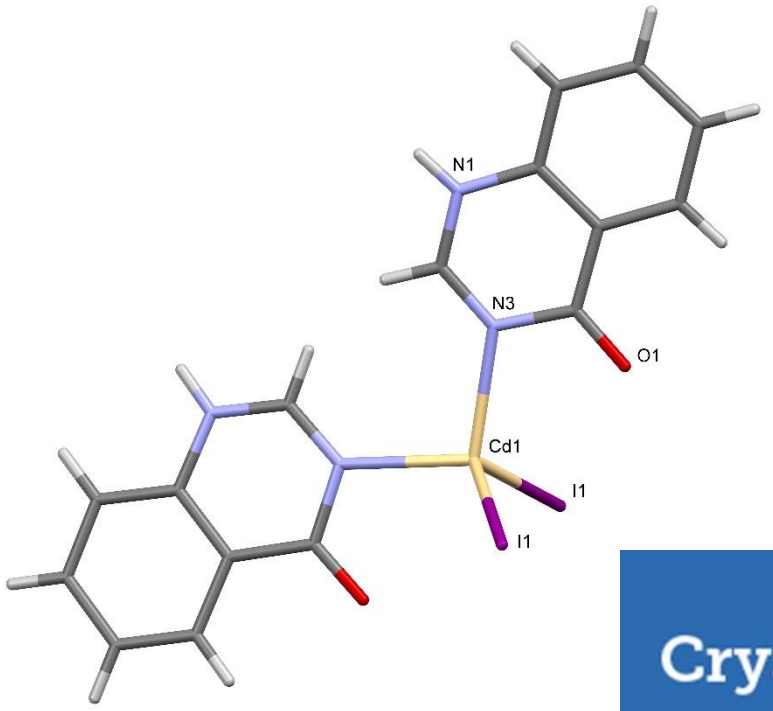
3. Structure of complex with CdI_2.

Finally, the structure determination of CdI_2 complex reveals a monomeric metal-containing building unit with a tetrahedral arrangement of two quinazolinone and two iodide ligands. The complex displays essentially the same crystal structure as that previously reported by other authors [3].

C2/c	
Chemical formula	$[CdI_2(C_8H_6N_2O)_2]$
Temperature (K)	100
a, (Å)	22.240 (3)
b, (Å)	6.8444 (10)
c, (Å)	13.369 (2)
β (°)	118.824 (2)
V (Å^3)	1783.0 (5)
R_1, wR_2	0.033, 0.085
CCDC	2041762



[3] M. Đakovic et al., *IUCrJ*, 2018, **5**, 13–21.

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Conclusions

4-Quinazolinone coordination to a metal ion may occur in two modes - with nitrogen atoms *para* or *ortho* to the quinazolinone oxygen atom.
In cadmium halide complexes with 4(3H)-quinazolinone, the Cd(II) ion may adopt trigonal bipyramidal, distorted octahedral or tetrahedral coordination geometry.

Acknowledgments

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