Powder diffraction data of novel complexes CdX_2-2(NH_2-PhY), part I

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Four new compounds with general formula CdI_2-2(NH_2-PhX) (Ph represents phenyl radical; X represents Cl or H atoms) were obtained and characterized. Two of them, bisaniline diiodidecadmium(II) — $CdI_2 \cdot 2[NH_2-C_6H_5]$ {1} and bis(2-chloroaniline) diiodidecadmium(II) — $CdI_2 \cdot 2[NH_2-C_6H_4Cl]$ {2}, crystallize in monoclinic system, whereas another two, bis(3-chloroaniline) diiodidecadmium(II) — $CdI_2 \cdot 2[NH_2-C_6H_4Cl]$ {3} and bis(4-chloroaniline) diiodidecadmium(II) hemi(4-chloroanilate) — $CdI_2 \cdot 2[NH_2-C_6H_4Cl]\frac{1}{2}[NH_2-C_6H_4Cl]$ {4}, crystallize in triclinic system. The investigated compounds, from chemical point of view, are similar to the so-called cisplatin—a compound used as a chemotherapy drug to treat many types of cancers. Their syntheses and results of X-ray powder diffraction studies at room and elevated temperatures are described in this paper. © *2010 International Centre for Diffraction Data.* [DOI: 10.1154/1.3503662]

Key words: X-ray powder diffraction, high-temperature X-ray diffraction, indexing of powder pattern

I. INTRODUCTION

The synthesis and structural studies of novel family of complexes MeX_2-2(NH_2-PhY) (Baldovino-Pantaleón *et al.*, 2007; Rademeyer, 2004), where Me—transition metal; X—I, Br, Cl; Ph—phenyl radical; and Y—H or Cl, were undertaken to understand the principles guiding the construction of complex compounds and their multidimensional architecture. General structural scheme for this kind of complexes is shown in Figure 1(a). Complexes with similar chemical structure are investigated due to their similarity to cisplatin; *cis*-Pt$(NH_3)_2Cl_2$ [Figure 1(b)], a compound which belongs to very important group of anticancer drugs (Thorn *et al.*, 2006).

The aim of our study is to replace Pt by other transition metals (e.g., Cd or Zn), Cl by other halogen atoms, and NH_3 by aromatic amines, to synthesize new compounds, and next to investigate their structural and other properties by many techniques including powder diffraction.

Some properties of these compounds, such as low solubility in water, imply a possibility of their applications in removing of toxic pollutants, for instance, cadmium or zinc salts and aromatic amines. Such compounds can also be used as a storage media for amines or cadmium compounds. Their application in crystal engineering (hybrid inorganic-organic materials with structures based on fragments of CdI_2 layers or blocs with rotational polymorphism) seems also quite interesting.

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In this paper we present results of first part of our studies for compounds with general formula CdI_2-2(NH_2-PhY). Results of further investigations will be subject of subsequent publications (Dobija *et al.*, in press).

II. SYNTHESIS

To obtain a series of aniline derivative complexes, aniline or chloroanilines were mixed with water (10 ml) and 2-propanol (5 ml) and slowly (drop wisely) added to warm solution of CdI_2 (1.83 g, 0.005 mol) in water (15 ml). To obtain $CdI_2 \cdot 2[NH_2-C_6H_5]$ 0.93 g (0.01 mol) of aniline was used whereas for syntheses bis(2-chloroaniline) diiodidecadmium(II), bis(3-chloroaniline) diiodidecadmium(II), and bis(4-chloroaniline) diiodidecadmium(II) hemi(4-chloroanilate), 2-, 3-, and 4-chloroaniline (1.27 g, 0.01 mol) were used, respectively. After one day obtained white precipitates were filtered off, washed with the mixture of water (12 ml) and 2-propanol (4 ml), and dried in air. Before the X-ray powder diffraction measurements the samples were thoroughly powdered.

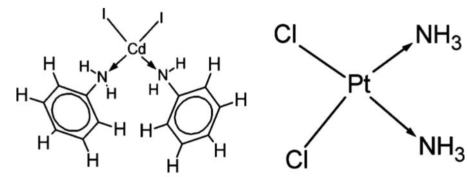

Figure 1. Structural scheme of complexes of formula CdI_2-2(NH_2-PhY) (a) and cisplatin (b).

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TABLE I. Crystallographic data of the investigated compounds.

Compound code and chemical name	{1} bisaniline diiodidecadmium(II)	{2} bis(2-chloroaniline) diiodidecadmium(II)	{3} bis(3-chloroaniline) diiodidecadmium(II)	{4} bis(4-chloroaniline) diiodidecadmium(II) hemi(4-chloroanilate)
Formula[a]	$CdI_2 \cdot 2[NH_2-C_6H_5]$	$CdI_2 \cdot 2[NH_2-C_6H_4Cl]$	$CdI_2 \cdot 2[NH_2-C_6H_4Cl]$	$CdI_2 \cdot 2[NH_2-C_6H_4Cl]\frac{1}{2}[NH_2-C_6H_4Cl]$
Formula weight (g/mol)	552.46	621.35	621.35	685.13
Crystal system	Monoclinic	Monoclinic	Triclinic	Triclinic
Space group	$C2/c$(15)	$C2/c$(15)	P-1(2)	P-1(2)
Cell parameters (Å, °)	a=25.378(4)	a=27.898(5)	a=8.088(2)	a=5.015(2)
	b=5.056(1)	b=4.484(1)	b=14.182(2)	b=13.987(4)
	c=13.714(3)	c=14.793(4)	c=7.026(1)	c=15.225(6)
	β=116.32(1)	β=114.72(2)	α=98.27(1)	α=105.15(3)
			β=99.93(2)	β=92.51(3)
			γ=90.32(2)	γ=98.00(5)
Volume ($Å^3$)	1577.1(4)	1680.9(5)	785.2(2)	1017.2(5)
Z	4	4	2	2
D_x (g/cm^3)	2.33	2.45	2.63	2.24
V/(non-H atom) (A^3)	23.2	22.1	20.7	18.8
$F30(\Delta,N)$[b]	57.99 (0.008, 66)	51.51 (0.009, 62)	30.00 (0.008, 127)	30.16 (0.01, 90)
$M30(\Delta,N)$[c]	28.37 (0.000 05, 66)	22.21 (0.000 06, 62)	13.03 (0.000 06, 127)	11.21 (0.000 06, 90)

[a]Determined by chemical analysis or single-crystal studies.
[b]Smith and Snyder, 1979.
[c]de Wolff, 1968.

III. EXPERIMENTAL

Powder diffraction data were collected on a Philips X-pert PRO MPD diffractometer equipped with a X'celerator detector. The measurements were performed at room temperature, 2θ range from 5° to 90° 2θ, converted with 0.02° step. Other experimental details were as follows: radiation type—Cu $K\alpha$ (1.541 87 Å) at 40 kV, 30 mA; fixed divergence slit $\frac{1}{2}$, receiving slit of 0.1. Peak positions were determined by use of the second derivative method using program written by Sonneveld and Visser (1975); unit-cell parameters were determined using indexing programs of the PROSZKI package (Łasocha and Lewiński, 1994). High-temperature studies were carried out in air, on a Philips X-pert PRO MPD diffractometer, using XRK camera (Anthon Paar). Annealing temperatures of the samples were as follow: 25, 100, 200, 300, and 400 °C.

IV. RESULTS AND DISCUSSION

A. Powder diffraction

Crystallographic data for the investigated compounds are shown in Table I. The first two compounds {**1**, **2**} crystallize in the monoclinic crystal system with space group $C2/c$ and the last two {**3** and **4**} in the triclinic crystal system with space group P-1. Unit-cell parameters for the compounds {**1**, **2**, and **4**} were confirmed by structural studies on single-crystal samples. Complete structural data will be the subject of further publications, diffraction data are listed in Tables II–V. Compound {**3**} crystallizes only in the form of very fine powder, which makes it impossible to carry out classical structural single-crystal studies. At the same time, the small number of strong diffraction lines makes indexing problem extremely difficult. Obtaining reliable unit-cell parameters is also hampered because of a dominant zone problem. We used all indexing programs (Łasocha and Lewiński, 1994) to obtain solutions based on two periods: 14.183(1) Å, 7.0278(1) Å, and 98.25(1)°, while the third one is determined with lower reliability. Among dozens of plausible solutions we have selected one with the volume enabling accommodation in the unit-cell two formal molecules. To check lattice parameters for this compound additional efforts such as structural studies or recrystallization are necessary. Such studies as we mentioned above are in progress.

Compound {**4**} seems to be a very interesting sample. Despite of many attempts (synthesis with various amounts of the reactants) the compound with a formula CdI_2-2(NH_2-Ph)·1/2(NH_2-PhCl) was always obtained. Excess of amine is likely to stabilize the structure; it is also the reason for lower density in comparison to other compounds {**1**, **2**, and **3**}.

B. High-temperature X-ray diffraction

The obtained compounds become very unstable with increasing temperature. All the compounds decompose at temperature about 200 °C (Figures 2–5). Cadmium iodide is the final main product of thermal decomposition of the investigated compounds, PDF-4+ 00-033-0239 or PDF-4+ 01-089-3192 (ICDD, 2009). In the temperature of 400 °C, melting of the CdI_2 samples is observed and all diffraction lines disappear. The compound {**4**} also decomposes in a similar way, and structural changes connected with the loss of excess of amine were not observed (Figure 5). Compounds {**1**} and {**3**} appeared to be the most unstable (Figures 2 and 4). Lines from cadmium iodide appear in temperature of 100 °C, and the pure CdI_2 phase is observed in temperature of 200 °C. In the case of compounds {**2**} and {**4**} additional peaks (not listed on above mentioned PDF cards) are observed even in the temperatures above 200 °C. These maxima can be partially attributed to other polytypic modifications of cadmium iodide (Figures 3 and 5).

TABLE II. X-ray diffraction data of $CdI_2 \cdot 2[NH_2-C_6H_5]$ {1}.

2θ exp (deg)	2θ cal (deg)	I/I_O(0.25–100)	d_{exp} (Å)	d_{cal} (Å)	h	k	l	$\Delta 2\theta$ (deg)
7.773	7.767	100	11.3644	11.3732	2	0	0	0.006
12.968	12.976	0.5	6.8211	6.8171	−2	0	2	−0.008
14.416	14.400	0.25	6.1392	6.1460	0	0	2	0.016
15.574	15.570	8.5	5.6851	5.6866	4	0	0	0.004
15.837	15.846	1	5.5913	5.5881	−4	0	2	−0.010
18.693	18.704	0.25	4.7431	4.7404	−1	1	1	−0.011
19.201	19.204	0.5	4.6186	4.6180	2	0	2	−0.003
20.547	20.550	0.25	4.3191	4.3185	−3	1	1	−0.003
21.369	21.381	3	4.1547	4.1526	−6	0	2	−0.012
21.984	21.968	0.25	4.0399	4.0427	−1	1	2	0.015
23.449	23.447	1	3.7906	3.7911	6	0	0	0.002
23.957	23.966	0.25	3.7115	3.7100	3	1	1	−0.010
24.182	24.170	0.25	3.6774	3.6792	1	1	2	0.012
24.883	24.879	0.25	3.5754	3.5760	−5	1	1	0.003
25.610	25.608	0.25	3.4755	3.4758	4	0	2	0.002
26.131	26.122	0.25	3.4074	3.4086	−4	0	4	0.009
26.345	26.333	0.25	3.3802	3.3818	−5	1	0	0.012
	26.348			3.3799	−3	1	3	−0.003
26.879	26.889	0.25	3.3142	3.3130	−1	1	3	−0.011
28.104	28.104	1	3.1725	3.1726	−6	0	4	0.00
	28.114			3.1715	−8	0	2	−0.01
	28.115			3.1713	−5	1	3	−0.011
28.483	28.487	0.25	3.1312	3.1308	3	1	2	−0.004
29.611	29.593	0.25	3.0143	3.0162	5	1	1	0.019
	29.623			3.0132	1	1	3	−0.011
31.439	31.438	2	2.8431	2.8433	8	0	0	0.001
32.759	32.735	0.25	2.7315	2.7336	7	1	0	0.025
	32.771			2.7306	6	0	2	−0.011
	32.789			2.7291	−1	1	4	−0.030
33.371	33.379	0.5	2.6828	2.6822	2	0	4	−0.008
34.185	34.190	0.25	2.6207	2.6204	5	1	2	−0.005
34.789	34.824	0.25	2.5766	2.5742	−7	1	4	−0.035
35.479	35.462	0.25	2.5280	2.5293	−10	0	2	0.017
	35.483			2.5279	0	2	0	−0.003
37.001	36.991	0.25	2.4275	2.4282	−9	1	3	0.010
37.289	37.295	0.25	2.4094	2.4091	−10	0	4	−0.006
38.968	38.957	0.5	2.3094	2.3101	−9	1	4	0.012
	38.959			2.3099	4	2	0	0.009
	38.976			2.3090	4	0	4	−0.008
39.579	39.567	0.25	2.2751	2.2759	−4	0	6	0.013
	39.589			2.2746	10	0	0	−0.010
39.829	39.844	0.25	2.2614	2.2606	9	1	0	−0.015
40.388	40.351	0.5	2.2314	2.2334	3	1	4	0.037
	40.397			2.2310	8	0	2	−0.009
41.129	41.128	0.25	2.1929	2.1930	−2	0	6	0.001
42.609	42.599	0.25	2.1201	2.1206	1	1	5	0.010
43.539	43.554	0.25	2.0769	2.0763	−12	0	4	−0.015
44.179	44.172	0.25	2.0483	2.0487	0	0	6	0.007
44.779	44.798	0.25	2.0222	2.0215	−11	1	1	−0.019
	44.801			2.0214	−2	2	4	−0.022
45.449	45.458	0.25	1.9940	1.9936	6	0	4	−0.009
	45.470			1.9932	6	2	1	−0.021
48.395	48.399	0.5	1.8793	1.8792	10	0	2	−0.004
52.599	52.620	0.25	1.7385	1.7379	8	0	4	−0.021
	52.625			1.7378	−13	1	1	−0.026
56.589	56.602	0.25	1.6250	1.6247	14	0	0	−0.013
56.749	56.714	0.25	1.6208	1.6218	−12	2	3	0.035
	56.744			1.6210	−2	0	8	0.005
	56.773			1.6203	12	0	2	−0.024
65.589	65.566	0.25	1.4222	1.4226	14	0	2	0.023
	65.617			1.4217	16	0	0	−0.028

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TABLE III. X-ray diffraction data of $CdI_2 \cdot 2[NH_2-C_6H_4Cl]$ {2}

2θ exp (deg)	2θ cal (deg)	I/I_O(0.25–100)	d_{exp} (Å)	d_{cal} (Å)	h	k	l	$\Delta 2\theta$ (deg)
6.981	6.976	100	12.6626	12.6712	2	0	0	0.005
12.056	12.057	3	7.3413	7.3407	−2	0	2	−0.001
13.177	13.178	1	6.7192	6.7188	0	0	2	−0.001
13.980	13.979	9	6.3350	6.3356	4	0	0	0.001
14.674	14.669	2	6.0369	6.0390	−4	0	2	0.005
17.332	17.333	1	5.1166	5.1162	2	0	2	−0.002
19.602	19.599	7	4.5289	4.5296	−6	0	2	0.003
21.033	21.034	11	4.2239	4.2237	6	0	0	−0.001
22.460	22.449	0.25	3.9587	3.9605	3	1	0	0.010
22.980	22.971	0.75	3.8703	3.8717	4	0	2	0.008
23.260	23.288	0.5	3.8243	3.8198	−1	1	2	−0.028
23.720	23.738	0.25	3.7512	3.7484	−3	1	2	−0.018
24.250	24.250	0.5	3.6704	3.6703	−4	0	4	−0.001
24.402	24.409	1	3.6478	3.6468	−2	0	4	−0.007
24.930	24.926	0.5	3.5718	3.5724	1	1	2	0.004
25.585	25.589	6	3.4818	3.4813	−8	0	2	−0.004
26.150	26.174	0.5	3.4079	3.4048	−5	1	2	−0.024
26.990	26.971	0.5	3.3037	3.3060	−3	1	3	0.019
27.320	27.311	0.5	3.2645	3.2656	−1	1	3	0.008
28.291	28.313	1	3.1546	3.1522	3	1	2	−0.022
29.304	29.308	3	3.0478	3.0475	6	0	2	−0.004
30.250	30.228	0.75	2.9547	2.9568	−7	1	1	0.022
	30.241			2.9555	2	0	4	0.008
31.380	31.360	0.5	2.8508	2.8526	−3	1	4	0.019
32.112	32.118	3	2.7874	2.7870	−10	0	2	−0.006
32.969	32.957	1	2.7169	2.7179	5	1	2	0.012
	32.997			2.7147	3	1	3	−0.028
34.279	34.251	0.75	2.6160	2.6181	−7	1	4	0.029
	34.276			2.6163	−10	0	4	0.004
34.619	34.597	0.75	2.5911	2.5927	7	1	1	0.022
34.689	34.713	0.75	2.5860	2.5843	1	1	4	−0.024
36.049	36.050	0.5	2.4915	2.4915	8	0	2	−0.001
37.716	37.726	1	2.3852	2.3846	−9	1	0	−0.010
	37.749			2.3832	−9	1	4	−0.033
	37.756			2.3828	−2	0	6	−0.040
38.426	38.385	0.5	2.3427	2.3451	3	1	4	0.041
	38.466			2.3404	7	1	2	−0.040
39.029	38.996	0.75	2.3079	2.3098	−12	0	2	0.034
40.269	40.226	0.75	2.2396	2.2419	0	2	0	0.043
	40.270			2.2396	0	0	6	−0.001
40.719	40.704	0.75	2.2159	2.2168	9	1	1	0.016
	40.714			2.2162	6	0	4	0.006
	40.736			2.2151	−9	1	5	−0.016
43.889	43.898	0.75	2.0629	2.0625	2	0	6	−0.009
44.219	44.200	0.75	2.0483	2.0492	11	1	0	0.019
44.559	44.530	1	2.0335	2.0347	−11	1	5	0.029
	44.596			2.0319	9	1	2	−0.037
46.149	46.162	0.5	1.9670	1.9665	−14	0	2	−0.013
46.928	46.937	0.75	1.9362	1.9359	8	0	4	−0.009
	46.948			1.9354	−13	1	3	−0.020
47.285	47.295	0.75	1.9224	1.9220	11	1	1	−0.010
48.419	48.446	0.5	1.8800	1.8791	4	0	6	−0.027
	48.462			1.8784	7	1	4	−0.043
51.169	51.141	0.75	1.7852	1.7862	2	2	4	0.029
	51.163			1.7855	−10	0	8	0.006
52.609	52.580	0.5	1.7397	1.7406	−16	0	4	0.029
	52.647			1.7386	−10	2	3	−0.037
53.649	53.613	0.75	1.7084	1.7095	−16	0	2	0.036
	53.643			1.7086	10	0	4	0.006
	53.675			1.7077	−12	0	8	−0.026
60.779	60.790	0.5	1.5240	1.5237	12	0	4	−0.011
65.979	65.960	0.5	1.4159	1.4163	3	3	2	0.018
	66.020			1.4151	16	0	2	−0.041

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TABLE IV. X-ray diffraction data of $CdI_2 \cdot 2[NH_2-C_6H_4Cl]$ {3}. Two lines $(2\theta, d, I)$: 30.537, 2.927 54, 0.5 and 37.782 00, 2.381 17, 0.25% were not indexed.

2θ exp (deg)	2θ cal (deg)	I/I_O(0.25–100)	d_{exp} (Å)	d_{cal} (Å)	h	k	l	$\Delta 2\theta$ (deg)
6.310	6.301	100	14.0077	14.0272	0	1	0	0.009
12.625	12.612	19	7.0117	7.0191	−1	1	0	0.013
	12.622			7.0136	0	2	0	0.003
12.927	12.932	1	6.8486	6.8459	0	0	1	−0.005
	12.955			6.8339	1	1	0	−0.028
13.530	13.533	1	6.5447	6.5432	0	−1	1	−0.003
16.711	16.714	1	5.3054	5.3044	0	−2	1	−0.003
18.981	18.981	5	4.6757	4.6757	0	3	0	0.000
19.400	19.406	0.25	4.5757	4.5743	0	2	1	−0.006
21.378	21.380	6	4.1565	4.1562	0	−3	1	−0.002
23.430	23.417	0.25	3.7970	3.7990	2	1	0	0.012
23.810	23.807	0.25	3.7372	3.7378	−2	0	1	0.003
24.333	24.330	0.25	3.6581	3.6585	−2	−1	1	0.003
24.578	24.586	1	3.6221	3.6211	0	3	1	−0.008
25.800	25.813	1	3.4533	3.4515	−1	3	1	−0.014
26.032	26.033	0.5	3.4230	3.4229	0	0	2	−0.001
26.400	26.408	0.5	3.3761	3.3751	−1	−1	2	−0.009
	26.443			3.3708	−2	−2	1	−0.043
26.810	26.806	2	3.3254	3.3259	0	−4	1	0.003
27.856	27.827	0.25	3.2028	3.2062	2	0	1	0.030
	27.854			3.2031	−1	−2	2	0.002
28.499	28.505	0.5	3.1321	3.1314	−1	−4	1	−0.007
29.829	29.832	0.5	2.9953	2.9951	−2	−3	1	−0.003
30.007	30.001	0.5	2.9779	2.9786	0	−3	2	0.006
31.398	31.395	0.75	2.8492	2.8495	−2	3	1	0.002
32.678	32.665	1	2.7404	2.7416	−2	−2	2	0.014
	32.669			2.7412	0	−5	1	0.010
33.459	33.449	0.25	2.6782	2.6790	1	4	1	0.010
	33.491			2.6758	1	−3	2	−0.031
33.779	33.772	0.5	2.6535	2.6542	3	0	0	0.007
	33.798			2.6522	0	−4	2	−0.018
34.074	34.024	0.5	2.6312	2.6351	−3	0	1	0.051
34.688	34.682	0.5	2.5861	2.5866	0	3	2	0.007
35.116	35.113	0.5	2.5555	2.5558	−2	2	2	0.003
	35.156			2.5528	−2	−3	2	−0.039
36.553	36.572	0.5	2.4583	2.4572	3	2	0	−0.018
38.489	38.466	0.75	2.3390	2.3404	3	0	1	0.023
	38.478			2.3397	−3	3	0	0.011
	38.504			2.3382	3	−1	1	−0.015
38.799	38.795	0.5	2.3210	2.3213	−3	−3	1	0.004
	38.832			2.3192	0	−6	1	−0.032
39.417	39.398	0.5	2.2860	2.2871	0	4	2	0.019
	39.445			2.2845	−1	−2	3	−0.027
39.909	39.884	0.25	2.2590	2.2604	2	5	0	0.025
40.739	40.698	0.25	2.2148	2.2170	2	−5	1	0.041
40.829	40.837	0.25	2.2102	2.2098	1	−6	1	−0.007
42.219	42.194	0.5	2.1406	2.1418	−3	2	2	0.025
43.504	43.472	0.5	2.0803	2.0818	0	2	3	0.032
	43.487			2.0811	−3	4	1	0.017
44.656	44.625	0.5	2.0293	2.0306	3	3	1	0.031
	44.658			2.0292	−2	−6	1	−0.002
	44.675			2.0285	0	5	2	−0.019
46.355	46.357	0.25	1.9588	1.9587	−3	5	0	−0.002
	46.381			1.9578	−1	7	0	−0.026
46.783	46.765	0.5	1.9418	1.9426	2	−5	2	0.018
	46.797			1.9413	0	3	3	−0.014
	46.821			1.9404	−2	−4	3	−0.038
47.472	47.457	0.25	1.9152	1.9159	−1	−5	3	0.015
49.207	49.172	0.5	1.8517	1.8530	−4	−3	1	0.035
	49.187			1.8524	−4	3	0	0.020
	49.195			1.8522	0	−7	2	0.012
50.383	50.343	0.5	1.8112	1.8126	−1	4	3	0.040
	50.367			1.8118	−1	6	2	0.016
	50.381			1.8113	4	3	0	0.002
53.104	53.068	0.25	1.7247	1.7258	−2	6	2	0.036
	53.080			1.7254	−1	−8	1	0.024
	53.137			1.7237	−1	8	0	−0.033
54.529	54.530	0.25	1.6829	1.6829	−2	0	4	−0.001
55.242	55.240	0.25	1.6629	1.6630	0	−8	2	0.002
63.048	63.018	0.25	1.4745	1.4751	−1	4	4	0.030
	63.018			1.4751	−4	−5	3	0.030
	63.022			1.4750	0	8	2	0.026

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TABLE V. X-ray diffraction data of $\{CdI_2 \cdot 2[NH_2-C_6H_4Cl]\}1/2NH_2-C_6H_4Cl$ {4}.

2θ exp (deg)	2θ cal (deg)	I/I_O(0.25–100)	d_{exp} (Å)	d_{cal} (Å)	h	k	l	$\Delta 2\theta$ (deg)
6.028	6.036	21	14.6624	14.6436	0	0	1	−0.008
6.632	6.628	100	13.3281	13.3355	0	1	0	0.004
10.099	10.107	2	8.7590	8.7522	0	1	1	−0.008
12.097	12.088	5	7.3164	7.3218	0	0	2	0.009
	12.117			7.3048	0	−1	2	−0.020
13.284	13.279	28	6.6652	6.6677	0	2	0	0.005
15.356	15.367	6	5.7702	5.7664	0	−2	2	−0.011
16.025	16.026	2	5.5308	5.5307	0	2	1	−0.001
17.600	17.580	0.5	5.0393	5.0450	0	−1	3	0.020
18.167	18.175	1	4.8832	4.8812	0	0	3	−0.008
18.416	18.438	3	4.8178	4.8122	−1	0	1	−0.022
19.040	19.021	0.5	4.6613	4.6659	1	−1	1	0.019
19.228	19.210	2	4.6161	4.6206	−1	1	1	0.018
	19.236			4.6142	0	−3	1	−0.008
19.988	19.975	4	4.4423	4.4452	0	3	0	0.013
	20.008			4.4379	−1	−1	1	−0.020
20.374	20.379	9	4.3590	4.3580	0	−3	2	−0.005
21.005	21.004	1	4.2294	4.2296	0	1	3	0.001
21.687	21.673	0.5	4.0980	4.1006	1	−1	2	0.014
	21.712			4.0934	−1	−1	2	−0.026
21.971	21.943	1	4.0456	4.0508	1	1	1	0.028
	22.005			4.0395	−1	1	2	−0.034
22.428	22.418	5	3.9642	3.9660	0	3	1	0.010
23.433	23.396	3	3.7964	3.8024	0	−1	4	0.037
	23.473			3.7902	−1	−2	1	−0.040
24.478	24.501	1	3.6367	3.6333	−1	−2	2	−0.023
	24.519			3.6307	−1	0	3	−0.041
24.867	24.854	0.5	3.5807	3.5825	−1	−1	3	0.012
25.760	25.754	2	3.4585	3.4594	0	−4	1	0.006
26.019	25.987	3	3.4247	3.4289	−1	1	3	0.032
	26.027			3.4236	1	2	1	−0.008
26.193	26.159	8	3.4023	3.4068	1	−2	3	0.034
	26.208			3.4005	0	−4	2	−0.015
26.702	26.708	1	3.3386	3.3380	1	0	3	−0.006
	26.741			3.3339	0	4	0	−0.039
28.186	28.178	0.5	3.1662	3.1671	−1	−3	1	0.008
29.009	29.000	3	3.0781	3.0791	−1	−1	4	0.009
	29.002			3.0789	−1	2	3	0.007
	29.025			3.0765	1	3	0	−0.016
29.341	29.321	3	3.0440	3.0462	1	−4	1	0.020
	29.335			3.0448	−1	3	2	0.006
30.396	30.390	0.5	2.9408	2.9414	1	−2	4	0.005
	30.414			2.9391	−1	−3	3	−0.019
30.728	30.734	0.5	2.9097	2.9093	−1	1	4	−0.005
30.895	30.880	0.25	2.8944	2.8958	0	2	4	0.014
31.668	31.671	0.5	2.8255	2.8252	−1	4	1	−0.004
31.751	31.722	0.5	2.8182	2.8209	0	−3	5	0.030
32.476	32.457	1	2.7570	2.7587	0	−5	1	0.019
	32.476			2.7571	0	−5	2	0.001
33.038	33.042	3	2.7114	2.7111	0	1	5	−0.004
33.687	33.658	0.5	2.6606	2.6629	−1	−4	1	0.029
	33.659			2.6628	0	−5	3	0.029
	33.699			2.6598	−1	2	4	−0.011
34.901	34.888	0.75	2.5708	2.5718	0	−4	5	0.013
	34.918			2.5696	1	−4	4	−0.017
	34.931			2.5687	−1	−4	3	−0.030
35.861	35.864	2	2.5041	2.5040	−2	1	0	−0.003
	35.904			2.5013	0	−5	4	−0.043
36.691	36.701	1	2.4494	2.4488	0	2	5	−0.010
	36.715			2.4479	−2	2	0	−0.025
36.817	36.819	2	2.4413	2.4412	1	4	1	−0.002
	36.828			2.4406	0	0	6	−0.012
37.476	37.510	0.5	2.3998	2.3978	−1	5	1	−0.033
39.770	39.763	0.5	2.2666	2.2670	0	−6	3	0.007
	39.789			2.2656	−1	0	6	−0.019
41.248	41.245	1	2.1887	2.1889	0	3	5	0.003

TABLE V. (*Continued.*)

2θ exp (deg)	2θ cal (deg)	I/I_O(0.25–100)	d_{exp} (Å)	d_{cal} (Å)	h	k	l	$\Delta 2\theta$ (deg)
	41.262			2.1880	0	4	4	−0.014
41.843	41.865	1	2.1590	2.1579	0	−1	7	−0.022
	41.875			2.1574	−1	6	0	−0.033
42.815	42.771	1	2.1122	2.1143	0	6	1	0.044
	42.777			2.1140	−1	3	5	0.038
	42.808			2.1125	0	5	3	0.007
43.600	43.585	1	2.0759	2.0767	1	4	3	0.015
	43.625			2.0748	1	−6	4	−0.025
46.030	45.992	0.5	1.9718	1.9734	−2	0	5	0.039
	45.993			1.9734	2	−5	2	0.037
	46.002			1.9730	−1	−6	3	0.028
46.479	46.477	0.5	1.9538	1.9540	0	4	5	0.003
	46.493			1.9533	−1	6	2	−0.014
49.462	49.440	0.5	1.8428	1.8436	0	6	3	0.022
	49.445			1.8434	−2	−3	5	0.017
	49.449			1.8432	2	−5	4	0.013
52.354	52.325	0.5	1.7476	1.7485	2	−5	5	0.029
	52.331			1.7483	0	−7	6	0.023
	52.384			1.7467	1	−3	8	−0.030
52.802	52.771	0.25	1.7338	1.7348	−1	4	6	0.031
	52.789			1.7342	−1	−7	1	0.013
	52.801			1.7338	−2	−3	6	0.001
56.459	56.455	0.25	1.6299	1.6300	−1	7	3	0.004
57.370	57.340	0.25	1.6061	1.6069	−1	−7	6	0.031
	57.345			1.6068	−1	8	1	0.025
	57.347			1.6068	3	1	0	0.023

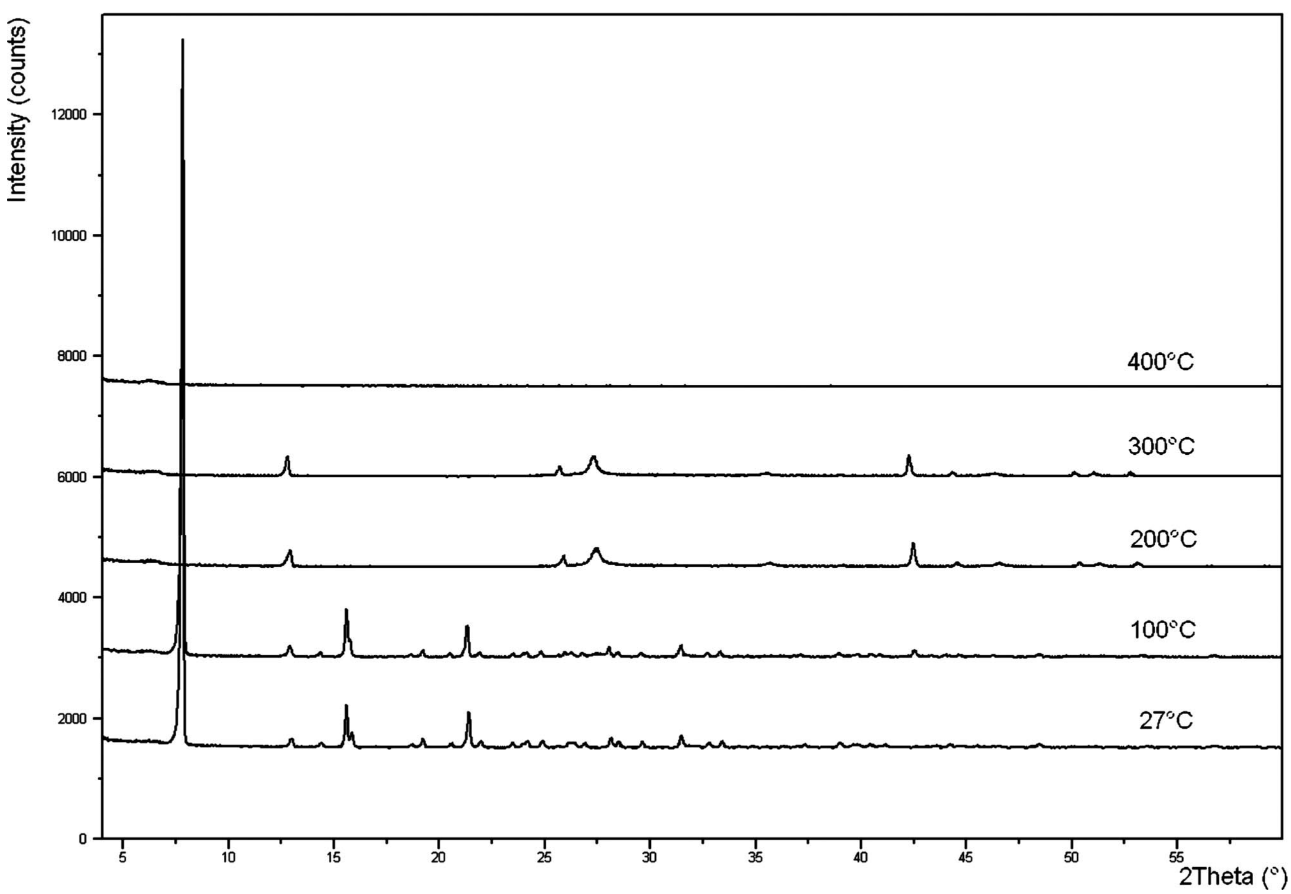

Figure 2. Powder diffraction patterns of $CdI_2 \cdot 2[NH_2-C_6H_5]$ {1} in various temperatures.

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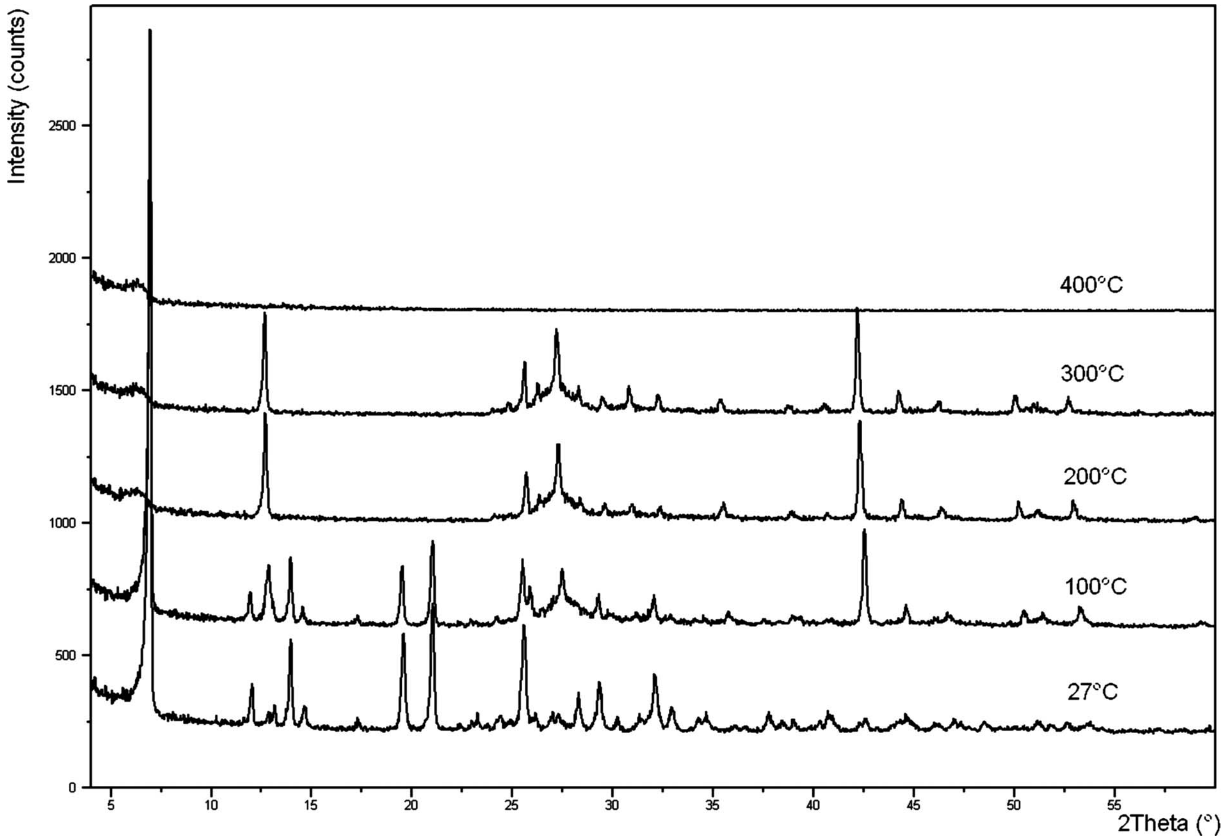

Figure 3. Powder diffraction patterns of $CdI_2 \cdot 2[NH_2-C_6H_4Cl]$ {2} in various temperatures.

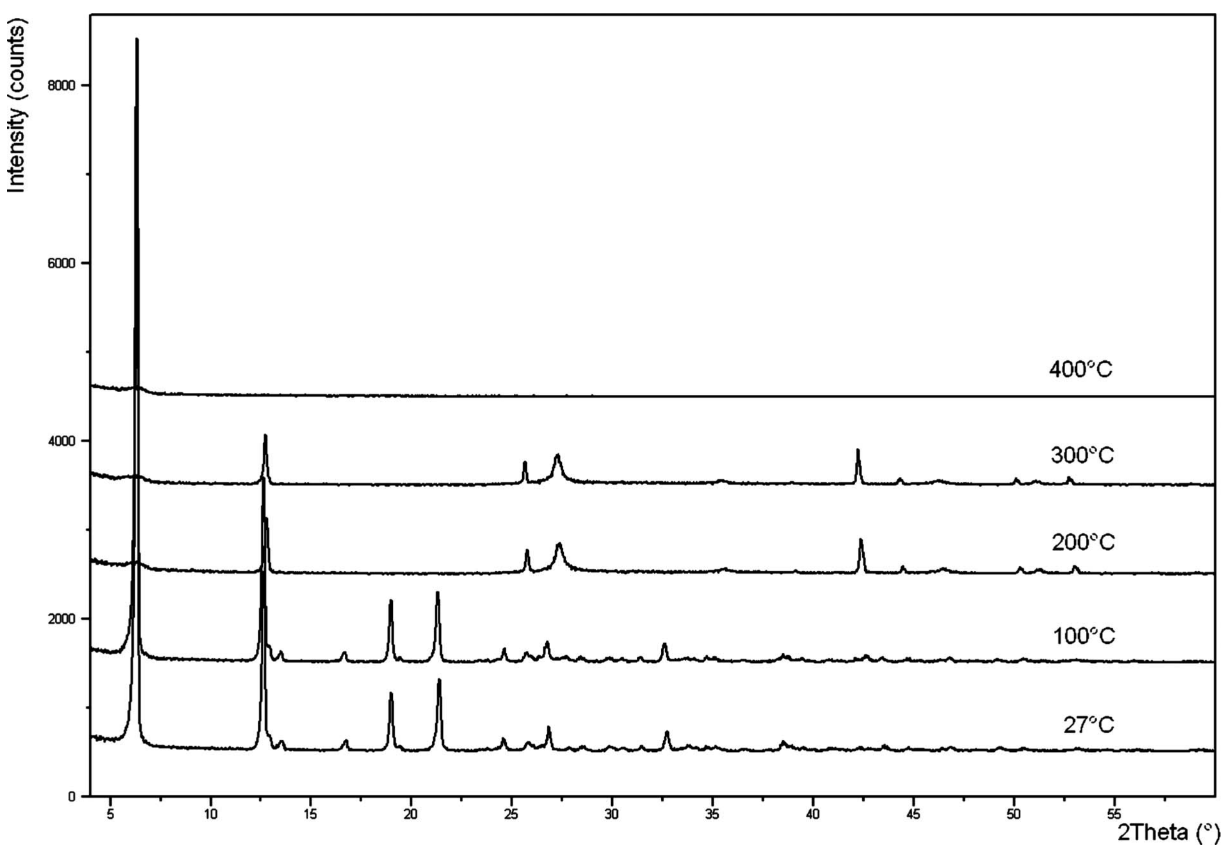

Figure 4. The X-ray patterns of the compound $CdI_2 \cdot 2[NH_2-C_6H_4Cl]$ {3} in various temperatures.

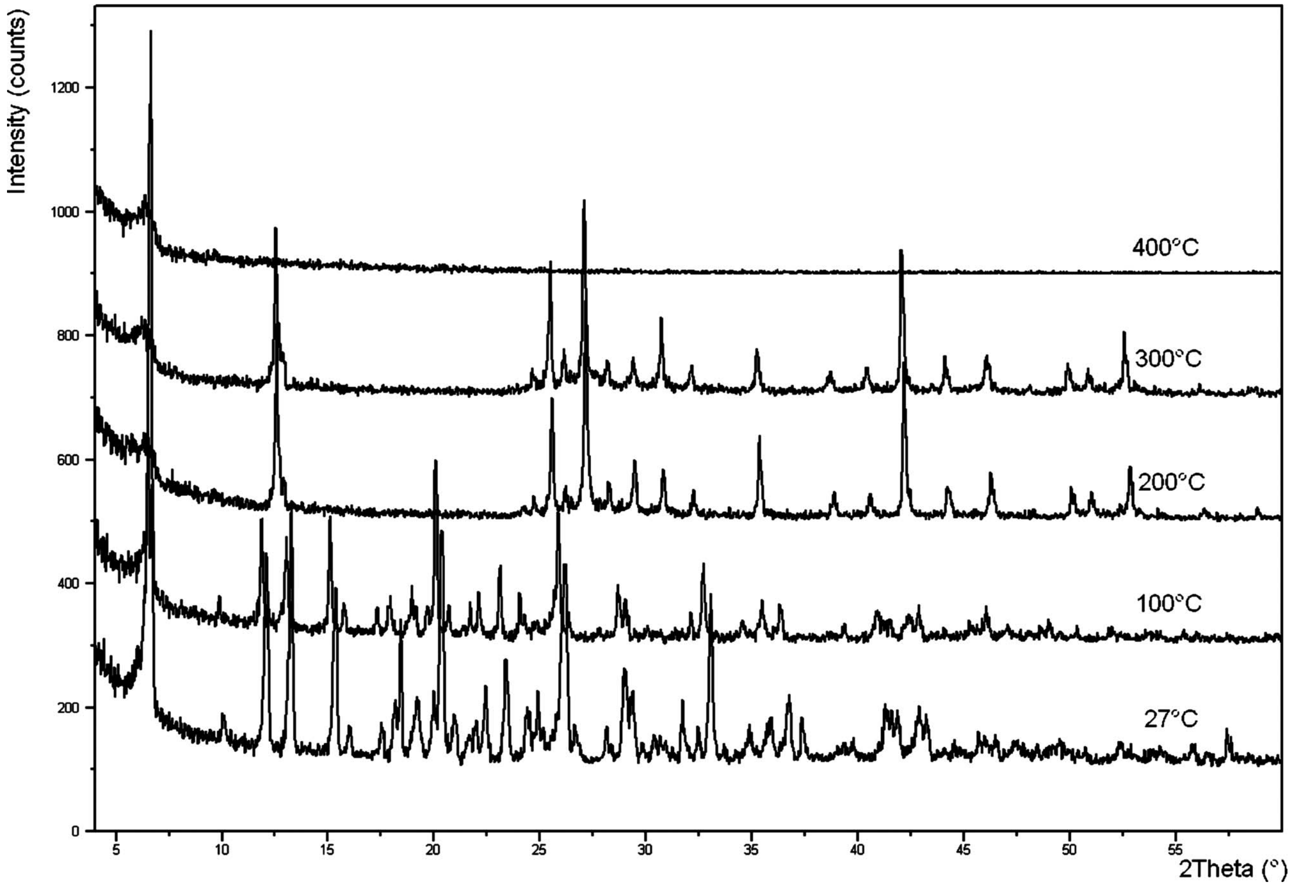

Figure 5. The powder diffraction patterns of the compound $\{CdI_2 \cdot 2[NH_2-C_6H_4Cl]\}1/2NH_2-C_6H_4Cl$ {4} in various temperatures.

V. CONCLUSION

Four new complexes of cadmium iodide with aniline and its derivatives were obtained. Crystallographic parameters (e.g., a, b, c, α, β, γ, Z, D_x, and space group) of these compounds were determined, and stability of these compounds as a function of increased temperature was examined. More detailed crystal structure studies, tests for the presence of rotational polymorphism, and initial pharmaceutical investigations will be the subject of our further research. The investigations were carried out due to the fact that obtained compounds can be of interest in environmental chemistry to remove or neutralize cadmium ion contaminants. In controlled conditions, these compounds may also serve as depository of amines or heavy atoms.

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