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Synthesis, Crystal Structure, and Infrared Spectroscopy of a novel hydronium trihydrate hybrid compound: $(C_6H_{22}N_4)_2H_9O_4CdCl_6CdCl_5Cl_2$

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ABSTRACT

A 0-dimensional (0D) hybrid compound, $(C_6H_{22}N_4)_2H_9O_4CdCl_6CdCl_5Cl_2$ has been prepared by a facile conventional evaporation method. The crystal packing of discrete constituents of $[Cd(1)Cl_6]$ octahedra, $[Cd(2)Cl_5]$ trigonal bipyramids, Cl^- ions, protonated tris(2-aminoethyl)amine molecules ($[(C_2H_7N)_3NH]^{4+}$) and $H_9O_4^+$ ions, is stabilized by diverse hydrogen bonds of N-H···Cl, C-H···Cl and C-H···O. Uncommonly, an isolated chlorine ion (i.e. Cl(4)) is fixed at a special position at 12*c*(3.) by hydrogen bonds from four surrounding hydrogen atoms at a trigonal pyramidal configuration whereas other chlorine atoms Cl(1), Cl(2) and Cl(3) are stabilized by hydrogen bonds from 2, 2 and 3 hydrogen atoms at bifurcated, linear and trigonal configurations, respectively. The ordered arrangement of [Cl(4) [Cl(4)···H_4] trigonal pyramidal configuration upward or downward is responsible for the long *c*-axis of the title compound. Additionally, a $H_9O_4^+$ ion is entangled with symmetry restriction and half occupancy. All these features of the title compound add our new knowledge about hydrogen bonds.

Indexing terms/Keywords

X-ray diffraction; Crystal structure; IR spectroscopy; Trihydrated hydronium ion; trigonal pyramidal configuration of [Cl···H4]; DFT calculations.

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INTRODUCTION

The hydrogen bonded network of water plays an important role in many chemical and biological processes [1-4]. In fact, the water molecule has a complex structure due to its ability to act as a hydrogen bond donor and acceptor. In the solid hydrates of strong acids, the H atom has been found to be hydrated to form a series of cations which have been characterized as H_3O^+, $H_5O_2^+$, $H_7O_3^+$ and $H_9O_4^+$ depending upon the degree of hydration. In the last three ions, the extra proton inserted goes with one water molecule and forms hydronium ion (H_3O^+) which is solvated by one, two and three water molecules, respectively. The structure of the hydronium ion solvated by three water molecules in its first solvation shell is called as an Eigen ion $H_9O_4^+$.

Polynuclear d^{10}-metal complexes can exhibit important structural and photoluminescent properties [5]. Among the d^{10} metals, cadmium gives rise to structural flexibility with coordination numbers varying between 4 and 8 with often severely distorted coordination geometries [6-9]. Since they don't have unwanted d-d transitions in the visible region, Cd^{2+} ions are also used as connecting points in Metal-Organic Frameworks (MOFs) for second-order nonlinear optical applications [10]. A disadvantage of the use of Cd^{2+} in functional materials is its toxic effects, which are well established and documented [11]. The ions have been found to induce various pathological conditions, such as e.g. cardiovascular diseases [12], hypertension, and cancer [13]. It is also known, however, that most of cadmium ions in biological systems is not in the form of free Cd^{2+} ions, but is coordinated by the abundance of biological ligands therein [14-16]. Therefore, the coordination chemistry of Cd^{2+} ions with such ligands is of interest.

As a contribution to the investigation of the above materials, we report here the crystal structure of one such compound, $(C_6H_{22}N_4)_2H_9O_4CdCl_6CdCl_5Cl_2$, formed through the reaction of tris(2-aminoethyl)amine with cadmium chloride and hydrochloric acid in an aqueous medium.

2. Experiment

2.1. Chemical preparation

To a mixture of tris(2-aminoethyl)amine (0.27 g, 2 mmol) and cadmium chloride (0.36 g, 2 mmol) in water (30 mL) was added 20% of hydrochloric acid until the pH was 3. The resulting solution was slowly evaporated at room temperature for several days until single crystals formed. The compound chemical formula was determined when resolving the crystal structure by X-ray diffraction (yield: 57%).

2.2. Investigation techniques

2.2.1. X-ray diffraction

Single-crystal X-ray diffraction data were collected at room temperature on a Bruker AXS SMART APEX CCD diffractometer equipped with graphite-monochromatized MoKα radiation (λ = 0.71073 Å). The structure was solved by direct methods using SHELXS-97 [17] and refinement was performed on F^2 by full-matrix least-squares techniques using SHELXL 2013 [18]. The non-hydrogen atoms were refined anisotropically, and hydrogen atoms isotropically. All hydrogen atoms except for those bonding oxygen atoms were generated geometrically. Both oxygen atoms of O(1) and O(2) were refined with half occupacy on the base of their unusually high displacement parameters if taking them as an entity. This treatment is consistent with the shorter distances between oxygen atoms and the principle of charge-neutrality. The drawings were made with Diamond [19]. The experimental conditions of data collection, the strategy followed for the structure determination and the final results are given in Table 1.

2.2.2. Infrared spectroscopy

IR spectra were recorded in the range 4000 - 400 cm^{-1} with a ''Perkin-Elmer FT-IR-1000'' spectrophotometer using samples dispersed in spectroscopically pure KBr pellets.

2.2.3. DFT calculations

The infrared spectrum was calculated with the Gaussian 09 software by taking into account three different entities, the two Cd atoms with their surrounding of five or six chlorine atoms and the organic cation. All calculations were made with the B3LYP method. For all atoms the 6-311++G** basis was chosen except for cadmium for which the LanL2DZ pseudopotential was used. In all cases the positions of the atoms were those determined by the X-ray diffraction study except for the hydrogen atoms which were first optimized at the above level of theory. The frequencies were then calculated and the absence of imaginary frequencies checked. Finally the spectrum was drawn by broadening the peaks with a lorentzian. The trihydrated hydronium ion was not studied as hydrogen bonds are often badly described by DFT methods.

Table 1.Experimental details

Crystal data	
Chemical formula	$(C_6H_{22}N_4)_2H_9O_4CdCl_6CdCl_5Cl_2$
M_r	1059.27
Crystal system, space group	Trigonal, *R*-3*c*:*H*
Temperature (K)	293
a, *c*(Å)	9.6544 (3), 73.571 (3)
V(Å^3)	5938.7 (4)
Z	6
Radiation type	Mo*K*α
μ (mm^{-1})	1.98
Crystal size (mm)	0.60×0.56×0.52
Data collection	
Diffractometer	Bruker APEXII CCD area-detector diffractometer
Absorption correction	Multi-scan
T_{min}, T_{max}	0.288, 0.354
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	34886, 1594, 1534
R_{int}	0.023
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.032, 0.098, 1.08
No. of reflections	1594
No. of parameters	74
No. of restraints	1
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.62, -0.66

3. Results and discussion

3.1. Structure description

In the title compound, $(C_6H_{22}N_4)_2H_9O_4CdCl_6CdCl_5Cl_2$, the two Cd atoms are located on special positions. The Cd^{II}(1) atom at 6*b*(-3.) has a six-coordinated octahedral geometry, while the Cd^{II}(2) cation at 6*a*(32) is five-coordinate with a perfectly regular trigonal bipyramidal geometry by chloride ions. Each discrete $[Cd(1)Cl_6]$ octahedron at the site of 6*b*(-3.) links to six surrounding $[HN(C_2H_7N)_3]^{4+}$ ions via hydrogen bonds while this is true for the $[Cd(2)Cl_5]$ trigonal bipyramid at the site of 6*a*(32). This compound is entangled with the $H_9O_4^+$ ion and an hydrogen atom, H(1), on an inversion center. In this trihydrated hydronium ion, the O(1) and O(2) oxygen atoms are a half occupancy. The O(1) and H(1) hydrogen atoms are located on special positions. The crystal structure is characterized by the presence of $[Cl\cdots H_4]$ trigonal pyramidal configuration. The crystal packing is stabilized by N-H⋯Cl, C-H⋯Cl and C-H⋯O hydrogen bonds, between which three are bifurcated.

The final refinement model revealed the following structural features. As shown in Figure. 1, the structure of the title inorganic-organic hybrid material contains one hexachloridocadmate(II) anion, one pentachloridocadmate(II) anion, two chlorine anions, two tris(2-aminioethyl)aminium tetracations and one hydronium ion-3H_2O hydrogen bonded cationic complex. The overall composition can be best described as $(C_6H_{22}N_4)_2H_9O_4CdCl_6CdCl_5Cl_2$. An examination of the structure clearly shows four kinds of layers arranged parallel to (a, b) planes. The first one is composed of H_2O and H_3O^+ entities interconnected by O-H⋯O hydrogen bonds forming thirty-six-membered rings with an $R_2^{18}(36)$ motif (Figure. 2)

[20]. The second one is formed by $[HN(C_6H_{21}N_3)]^{4+}$ cations and $Cl(4)^-$ anions associated via N-H···Cl hydrogen bonds giving rise to thirty-membered rings with an $R_2^6(30)$ motif (Figure. 3). The third layer contains the $CdCl_6$ anions, which alternate with the firth one constituted of $CdCl_5$ anions (Figure. 4). All these layers are interconnected via N-H···Cl, C-H···Cl and C-H···O hydrogen bonds (Figure. 4, Table 3). Among these hydrogen bonds, three are bifurcated: N2-H2A…(Cl1, Cl1$^{\mathrm{i}}$), N2-H2B…(Cl2, Cl4$^{\mathrm{xi}}$) and C1-H1B…(Cl1, O2).

Table 2. Selected geometric parameters (Å, º)

Cd1 - Cl1	2.6440 (9)	Cd2 - Cl2$^{\mathrm{VI}}$	2.4487 (13)
Cd1 - Cl1$^{\mathrm{I}}$	2.6440 (9)	Cd2 - Cl2	2.4487 (13)
Cd1 - Cl1$^{\mathrm{II}}$	2.6441 (9)	Cd2 - Cl2$^{\mathrm{VII}}$	2.4487 (13)
Cd1 - Cl1$^{\mathrm{III}}$	2.6441 (9)	Cd2 - Cl3$^{\mathrm{VIII}}$	2.7489 (18)
Cd1 - Cl1$^{\mathrm{IV}}$	2.6441 (9)	Cd2 - Cl3	2.7490 (18)
Cd1 - Cl1$^{\mathrm{V}}$	2.6441 (9)		
Cl1 - Cd1 - Cl1$^{\mathrm{i}}$	89.06 (3)	Cl1$^{\mathrm{III}}$ - Cd1 - Cl1$^{\mathrm{V}}$	89.06 (3)
Cl1 - Cd1 - Cl1$^{\mathrm{II}}$	180.0	Cl1$^{\mathrm{IV}}$ - Cd1 - Cl1$^{\mathrm{V}}$	180.00 (8)
Cl1$^{\mathrm{i}}$ - Cd1 - Cl1$^{\mathrm{ii}}$	90.94 (3)	Cl2$^{\mathrm{vi}}$ - Cd2 - Cl2	120.0
Cl1 - Cd1 - Cl1$^{\mathrm{III}}$	90.94 (3)	Cl2$^{\mathrm{VI}}$ - Cd2 - Cl2$^{\mathrm{VII}}$	120.0
Cl1$^{\mathrm{i}}$ - Cd1 - Cl1$^{\mathrm{iii}}$	180.0	Cl2 - Cd2 - Cl2$^{\mathrm{vii}}$	120.0
Cl1$^{\mathrm{II}}$ - Cd1 - Cl1$^{\mathrm{III}}$	89.06 (3)	Cl2$^{\mathrm{VI}}$ - Cd2 - Cl3$^{\mathrm{VIII}}$	90.0
Cl1 - Cd1 - Cl1$^{\mathrm{IV}}$	89.06 (3)	Cl2 - Cd2 - Cl3$^{\mathrm{VIII}}$	90.0
Cl1$^{\mathrm{i}}$ - Cd1 - Cl1$^{\mathrm{iv}}$	89.06 (3)	Cl2$^{\mathrm{vii}}$ - Cd2 - Cl3$^{\mathrm{viii}}$	90.0
Cl1$^{\mathrm{II}}$ - Cd1 - Cl1$^{\mathrm{IV}}$	90.94 (3)	Cl2$^{\mathrm{VI}}$ - Cd2 - Cl3	90.0
Cl1$^{\mathrm{iii}}$ - Cd1 - Cl1$^{\mathrm{iv}}$	90.94 (3)	Cl2 - Cd2 - Cl3	90.0
Cl1 - Cd1 - Cl1$^{\mathrm{V}}$	90.94 (3)	Cl2$^{\mathrm{VII}}$ - Cd2 - Cl3	90.0
Cl1$^{\mathrm{I}}$ - Cd1 - Cl1$^{\mathrm{V}}$	90.94 (3)	Cl3$^{\mathrm{VIII}}$ - Cd2 - Cl3	180.0
Cl1$^{\mathrm{II}}$ - Cd1 - Cl1$^{\mathrm{V}}$	89.06 (3)		

Symmetry codes: (i) −*x*+*y*, −*x*, *z*; (ii) −*x*, −*y*, −*z*; (iii) *x*−*y*, *x*, −*z*; (iv) −*y*, *x*−*y*, *z*; (v) *y*, −*x*+*y*, −*z*; (vi) −*y*+1, *x*−*y*, *z*; (vii) −*x*+*y*+1, −*x*+1, *z*; (viii) *y*+1/3, *x*−1/3, −*z*+1/6; (ix) −*x*+*y*, −*x*+1, *z*; (x) −*y*+1, *x*−*y*+1, *z*.

Table 3. Hydrogen-bond geometry (Å, º)

D - H···A	**D - H**	**H···A**	**D···A**	**D - H···A**
N1 - H1N···Cl4	0.88 (2)	2.19 (2)	3.069 (5)	180 (1)
N2 - H2A···Cl1	0.89	2.47	3.230 (3)	144
N2 - H2A···Cl1$^{\mathrm{i}}$	0.89	2.72	3.211 (3)	116
N2 - H2B···Cl2	0.89	2.99	3.542 (3)	122
N2 - H2B···Cl4$^{\mathrm{xi}}$	0.89	2.43	3.206 (3)	146
N2 - H2C···Cl3	0.89	2.39	3.281 (3)	176
C1 - H1B···Cl1	0.97	2.95	3.631 (3)	128
C1 - H1B···O2	0.97	2.62	3.246 (8)	122
C2 - H3A···Cl2$^{\mathrm{VII}}$	0.97	2.87	3.658 (4)	139
C2 - H3B···Cl2$^{\mathrm{IV}}$	0.97	2.93	3.816 (4)	153
O1 - H2···O2$^{\mathrm{XII}}$	1.24 (6)	1.30 (6)	2.459 (8)	151 (6)

Symmetry codes: (i)−*x*+*y*, −*x*, *z*; (iv) −*y*, *x*−*y*, *z*; (vii) −*x*+*y*+1, −*x*+1, *z*; (xi) *y*−2/3, *x*−1/3, −*z*+1/6; (xii) −*x*+1, −*y*+1, −*z*.

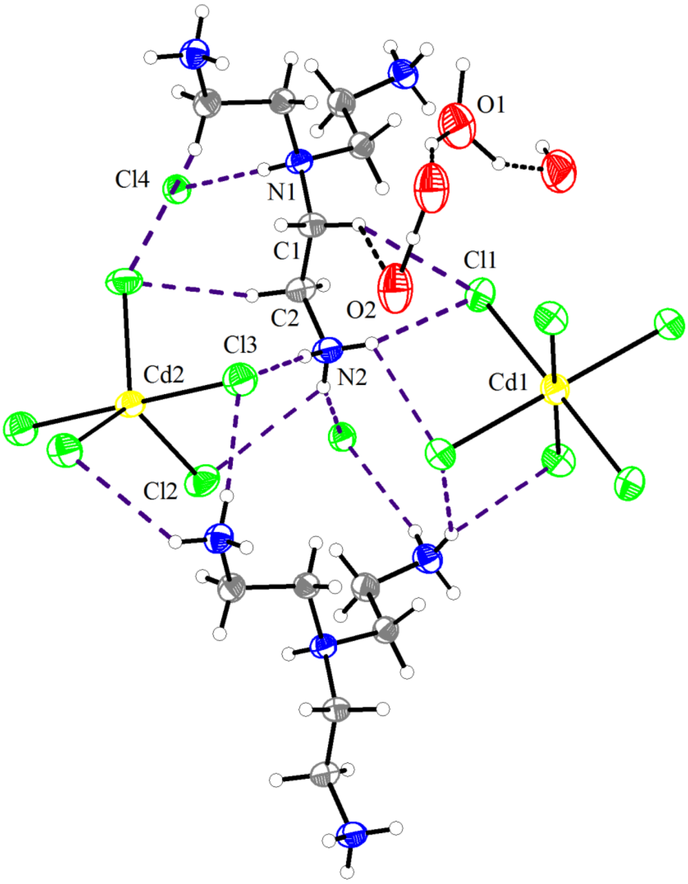

Figure. 1 ORTEP representation of the molecular configuration of the title compound, with atomic numbering sheme and thermal ellipsoids at 50 % of probability. Hydrogen bonds are shown as dashed lines.

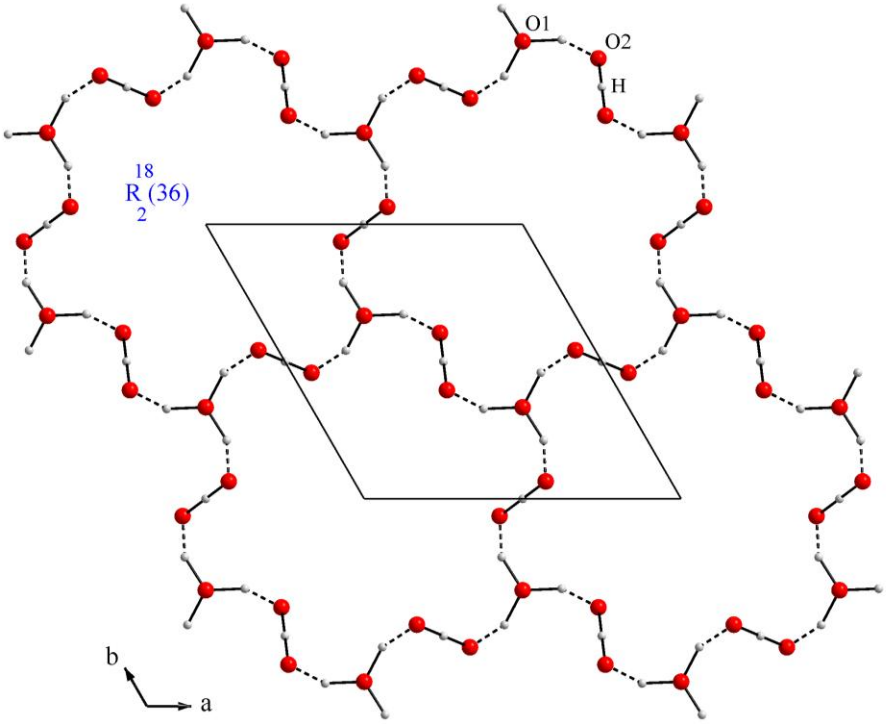

Figure. 2 Projection of a H_2O/H_3O^+ layer, viewed down the c direction, in the structure of the title compound. Hydrogen bonds are shown as dashed lines.

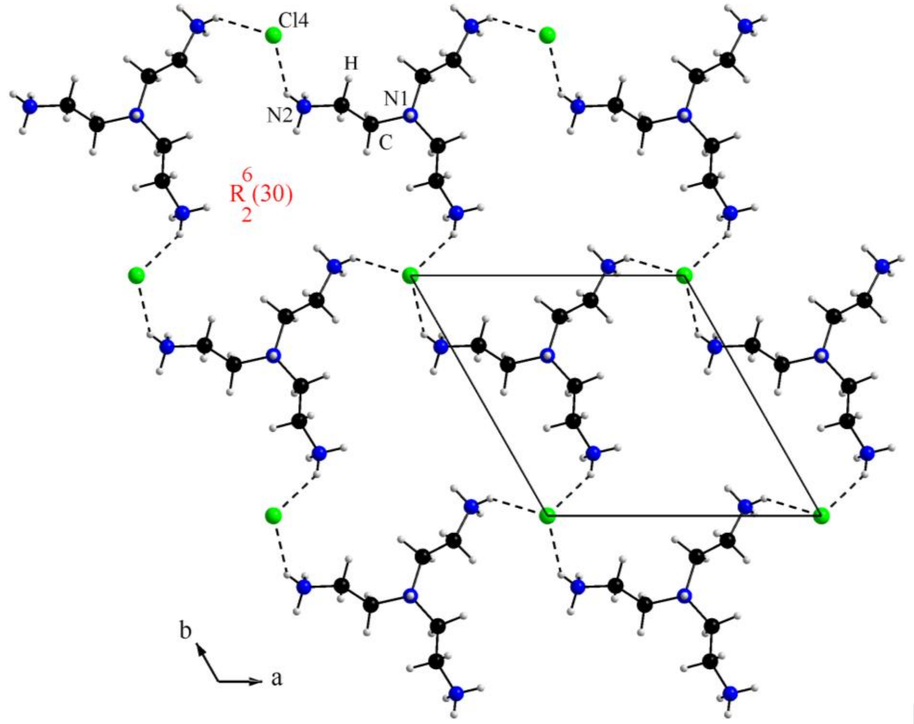

Figure. 3 Projection of a $[HN(C_6H_{21}N_3)]^{4+}/Cl^-$ layer, viewed down the c direction, in the structure of the title compound. Hydrogen bonds are shown as dashed lines.

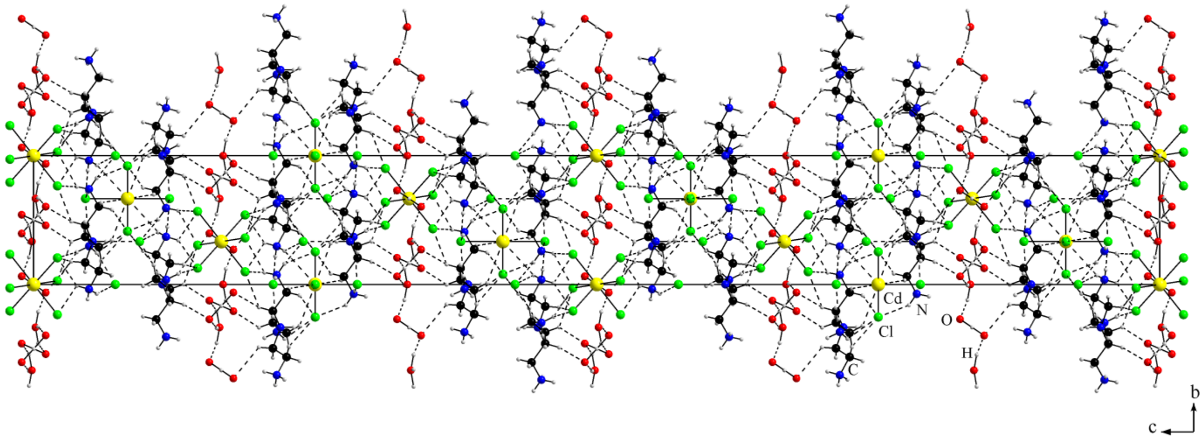

Figure. 4 Packing of the title compound, viewed down the c direction. Dotted lines show intermolecular hydrogen bonds.

The most salient feature of the crystal structure is $[Cl\cdots H_4]$ trigonal pyramidal configuration which is unknown until now (Figure. 5). This arise from the presence of isolated Cl^- anions together with $[HN(C_6H_{21}N_3)]^{4+}$ cations, rather than $[N(C_6H_{21}N_3)]^{3+}$, in the structure of the title compound.

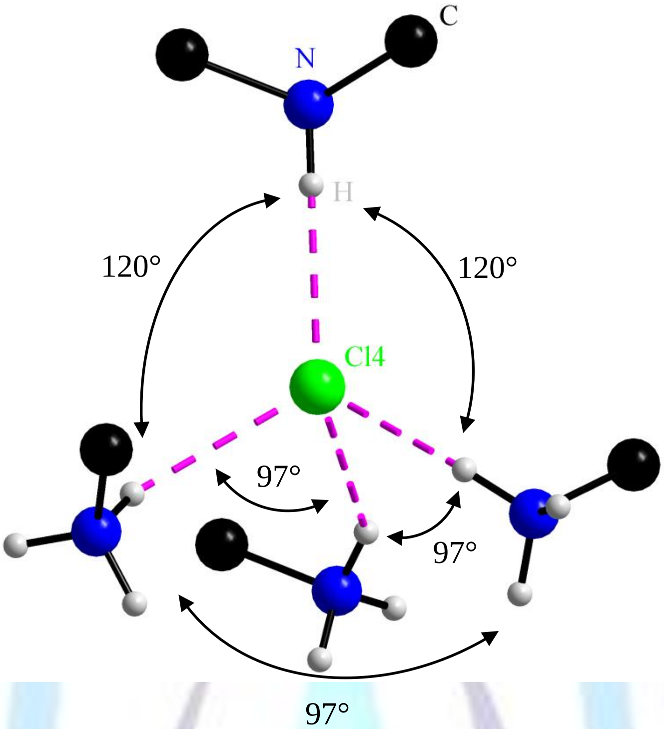

Figure. 5 Trigonal pyramidal configuration of the chloride ion in the title compound.

Regarding the hydronium ion-3H_2O hydrogen bonded complex, $H_9O_4^+$, structural features (Figure. 6) shows that the configuration of this cation is a little bit different from the counterparts in previous papers [21], which is due to the fact that the oxygen atoms O(1) and O(2) have a half occupancy (Table 4). This arises from the symmetry restriction. Both O(1) and H(1) are located at a special position. The O(1)-H(2) bond distance of 1.179(8) Å is much longer than the expected value of about 0.82 Å from X-ray diffraction in free hydroxyl group [22]. Indeed, the presence of the H(1) hydrogen atom on a special position at -1 leads to the abnormally long distance of O-H bond close to 1.2 Å. Hydrogen atom situated at an inversion center is commonly reported [22]. The hydronium ion is confined by a trigonal axis. The most interesting feature of the $H_9O_4^+$ entity is the presence of a very strong hydrogen bond [d(O…O) < 2.5 Å], where the distance O(1)…O(2)^{xii} is 2.459(8) Å (Table 3).

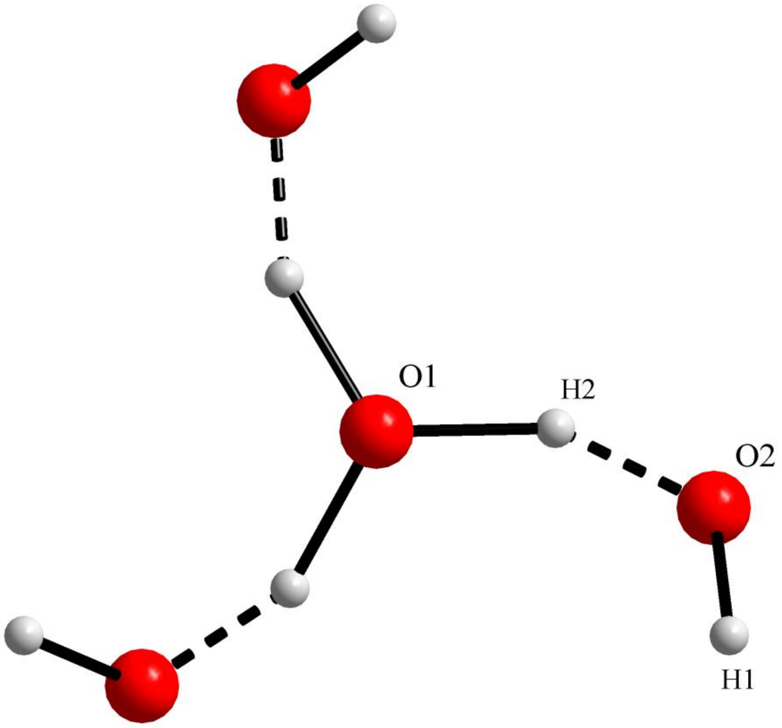

Figure. 6 Hydronium ion-3H_2O hydrogen bonded complex in the title complex. O(1) and O(2) are a half occupancy. O(1) and H(1) lie on a special position. H(1) is situated at an inversion center.

Table 4. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	X	*Y*	*Z*	U_{iso}*/U_{eq}	*Occ. (<1)*
Cd1	0.0000	0.0000	0.0000	0.0339 (2)	
Cd2	0.6667	0.3333	0.0833	0.03012 (19)	
Cl1	0.02799 (11)	0.23444 (11)	0.02109 (2)	0.0386 (2)	
Cl2	0.41303 (13)	0.07970 (13)	0.0833	0.0427 (3)	
Cl3	0.6667	0.3333	0.04597 (2)	0.0441 (4)	
Cl4	0.3333	0.6667	0.09410 (2)	0.0303 (3)	
N1	0.3333	0.6667	0.05239 (7)	0.0248 (9)	
H1N	0.3333	0.6667	0.0643 (3)	0.04 (2)*	
N2	0.2968 (4)	0.2596 (3)	0.04916 (4)	0.0318 (6)	
H2A	0.2510	0.2408	0.0383	0.048*	
H2B	0.2448	0.1727	0.0561	0.048*	
H2C	0.3983	0.2839	0.0480	0.048*	
C1	0.3704 (4)	0.5406 (4)	0.04575 (4)	0.0260 (6)	
H1A	0.4852	0.5836	0.0458	0.031*	
H1B	0.3322	0.5108	0.0334	0.031*	
C2	0.2910 (4)	0.3942 (4)	0.05787 (5)	0.0297 (7)	
H3A	0.3455	0.4180	0.0695	0.036*	
H3B	0.1806	0.3651	0.0600	0.036*	
O1	0.3333	0.6667	−0.00158 (15)	0.065 (4)	0.5
O2	0.4589 (9)	0.3957 (10)	0.01069 (9)	0.066 (2)	0.5
H1	0.5000	0.5000	0.0000	0.079*	
H2	0.461 (7)	0.669 (8)	−0.0044 (8)	0.079*	

With regard to the hexachloridocadmate anion geometrical features (Table 2), the values of the Cd-Cl bond lengths equal to 2.6441 (9) Å and the Cl-Cd(1)-Cl bond angles average exactly 90.0°, range between 89.06 (3) and 90.94 (3)°. These geometrical parameters, which agree with those found in other compounds [23, 24], confirm the close to symmetric octahedral nature of the Cd(1)Cl_6 building units [25]. Moreover, for the pentachloridocadmate(II) anion, the structural index τ, namely the Addison parameter $\tau = (\beta - \alpha)/60$ with α and β being the two largest angles, is zero for an ideal square pyramidal and becomes equal to one for an ideal trigonal bipyramid [26]. The calculated τ values of the title compound are τ (Cd2) = 1.00 (where α = 180° and β = 120°) indicating that the geometry around the Cd(2) cation has a perfectly regular trigonal bipyramidal structure. Both Cd(1) and Cd(2) cadmium atoms are located on special positions. The bond valence sums (BVS) calculations on the cadmium sites give the values at 1.960 and 2.153 *uv* (unit valence) for Cd(1) and Cd(2) respectively, indicating both Cd atoms in the oxidation state of +2 [27].

3.2 IR absorption spectroscopy

The IR spectrum of the crystalline title compound is shown in Figure. 7. The characteristic vibrational modes can be compared to those of similar materials containing alkylammonium cation [28]. In the high-frequency region, the bands between 3600 and 2700 cm^{-1} correspond to the stretching of the organic and hydroxyl groups (νN-H, νC-H and νO-H). Bands of weak intensities observed in the 2650-2370 cm^{-1} spectral region are assigned to combination and overtone bands involving probably the NH deformation modes and the C-NH_3 torsion modes around the C-N bond [30]. The bands observed at 1598, 1566 and 1494 cm^{-1} are assigned to the δ(OH) bending mode, the asymmetric $\delta_{as}(NH_3)$ and the symmetric $\delta_s(NH_3)$ bending modes, respectively. The adjacent carbon atoms attached to the CH_2 groups were also involved in the wagging, twisting and rocking modes of these groups. This has induced a coupling between the adjacent CH_2 groups. Thus, the bands observed at 1426 and 1140 cm^{-1} are assigned to the waging modes, those observed at 1289 and 1013 cm^{-1} to the twisting modes and, finally, those observed between 1013 and 782 cm^{-1} to the rocking modes.

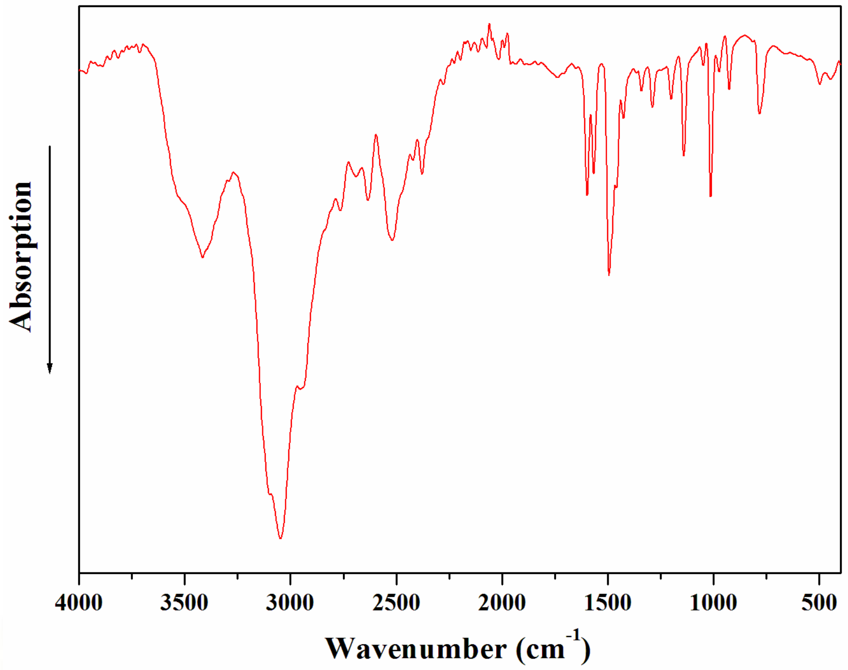

Figure. 7 IR absorption spectrum of the title compound.

3.3 DFT calculations

The DFT calculations show that the inorganic entities lead to vibrations below 500 cm^{-1} which are not observed experimentally in our conditions. So we focused only on the vibration of the organic cation. However the X-ray diffraction data give C-H or N-H distances which are too small compared to what is usually observed (typically below 0.1 nm) due to the fact that this method is not sensitive to the nuclei but to the electrons and so gives values corresponding to distances between the bary centers of electronic charges. As a consequence the positions of protons were first optimized, the C and N atoms being located at the positions given by the X-ray study. The resulting C-H and N-H distances correspond to what is usually obtained (typically 0.109 nm for C-H and 0.104 nm for N-H, see supplementary material) and the frequencies calculation was made on the semi-optimized geometry. The resulting IR spectrum between 500 and 1800 cm^{-1} is shown on Figure. 8 and is very similar to the experimental spectrum allowing a good correlation between the experimental and theoretical data as shown on Figure. 9. The scale factor is smaller than the values obtained for the B3LYP/6-311++G** method (ca. 0.97) and this is probably related to the fact that the frequencies were calculated for an isolated cation without taking into account the surrounding and the presence of numerous hydrogen bonds. However the precision is sufficient to assign the experimental frequencies and to confirm the attributions proposed above. The list of all calculated frequencies with the corresponding vibrations is listen in the supplementary material.

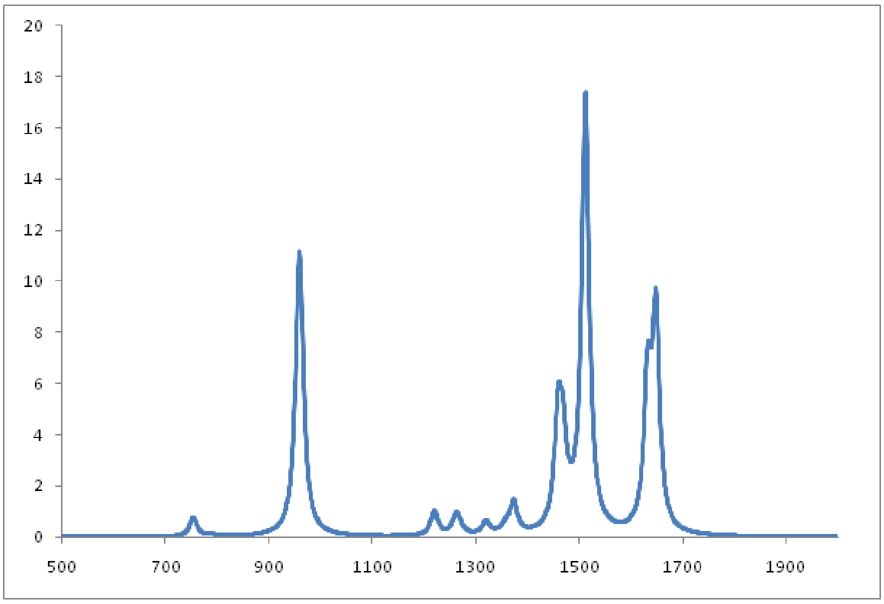

Figure. 8 Calculated IR absorption spectrum in the 500 - 2000 cm^{-1} range.

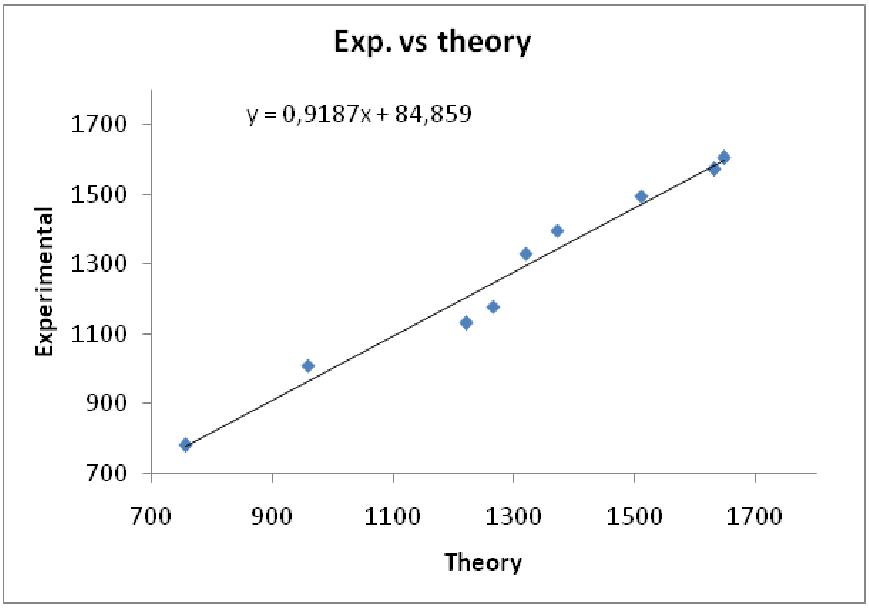

Figure. 9 Comparison between experimental and calculated IR frequencies.

4. Conclusions

A new, $(C_6H_{22}N_4)_2H_9O_4CdCl_6CdCl_5Cl_2$, was synthesized at room temperature and characterized by X-ray diffraction and IR spectroscopy. On the structural level, the atomic arrangement is characterized by the presence the hydronium ion-3H_2O hydrogen bonded complexes interconnected via O-H…O hydrogen bonds, leading to the formation of layers arranged parallel to (a, b) planes. The presence of the H(1) hydrogen atom on a special position at -1 leads to the abnormally long distance of O-H bond in the compound, the Cd(1) and Cd(2) cadmium atoms are six and five-coordinated with the chloride ions, respectively. All the components of the title material are held together through a set of hydrogen bonds, three of which are three-center interactions. The vibrational properties of this structure were studied by infrared spectroscopy.

Supplementary data

Crystallographic data for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre, CCDC No 1001353. These data can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html, or from the CCDC, 12 Union Road, Cambridge, CB2 1EZ, UK: fax: (+44) 01223-336-033; e-mail: deposit@ccdc.cam.ac.

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