SUPPLEMENTARY INFORMATION

THE CRYSTAL STRUCTURES OF TWO NOVEL CADMIUM-PICOLINIC ACID COMPLEXES IN RELATION TO THE SOLUTION SPECIES

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X-ray crystallography

Intensity data were collected on a Bruker SMART 1K CCD area detector diffractometer with graphite monochromated Mo K_α radiation (50kV, 30mA, λ = 71073 Å). The collection method involved ω-scans of width 0.5° and 512 × 512 bit data frames. Data reduction was carried out using the program *SAINT+,* version 6.02[9] and for complex **1** face empirical absorption corrections were made using the program SADABS. Both crystals were studied at -100 °C (173 K) by the aid of a CRYOSTREAM which is designed for operation over a wide temperature range. The crystal structures were solved by direct methods using *SHELX-97.*[10] Non-hydrogen atoms were first refined isotropically followed by anisotropic refinement by full matrix least-squares calculations based on F^2 using *SHELX-97.*[10] All hydrogen atoms were positioned geometrically and allowed to ride on their respective parent atoms, except those of O9 and O10 in complex **1** which were placed according to electron density and refined freely. Absorption corrections were made for complex **1**, but it was unnecessary to do so for complex **2** as no changes in the refinement were observed when applied. Diagrams and publication material were generated using *Win*GX,[11] *SHELX-97*,[10] *PLATON*,[12] *ORTEP-3* ,[13] and *Mercury*.[14]

See article for references.

Table S1 Crystal data and structure refinement for complexes **1** and **2**.

Complex	**1**	**2**
CCDC entry no.		
Empirical formula	$C_6H_9Cd\ N_3O_{10}$	$C_{18}H_{13.5}Cd\ N_4O_9$
Formula weight / g.mol^{-1}	395.56	1022.45
Temperature	173(2) K	173(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Triclinic	Trigonal
Space group	P -1	P-3
a	8.4374(8) Å	14.0290(5) Å
b	9.2353(7) Å	14.0290(5) Å
c	9.5588(8) Å	5.6564(2) Å
α	111.409(5)°	90°
β	116.156(5)°	90°
γ	94.582(6)°	120°
Volume	596.03(9) Å^3	964.10(6) Å^3
Z	2	2
Density (calculated)	2.204 Mg/m^3	1.761 Mg/m^3
Absorption coefficient	1.892 mm^{-1}	1.184 mm^{-1}
F(000)	388	508
Crystal size	0.46 x 0.36 x 0.28 mm^3	0.499 x 0.152 x 0.121 mm^3
Theta range for data collection	2.47 to 27.99°	1.68 to 27.97°
Index ranges	$-11 \le h \le 10, -12 \le k \le 12, -12 \le l \le 12$	$-9 \le h \le 18, -18 \le k \le 15, -7 \le l \le 7$
Reflections collected	11730	7838
Independent reflections	2863 [R(int) = 0.0223]	1556 [R(int) = 0.0453]
Completeness to theta	99.80%	99.90%
Absorption correction	Semi-empirical from equivalents	None
Max. and min. transmission	0.6194 and 0.3273	
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	2863 / 0 / 197	1556 / 1 / 91
Goodness-of-fit on F^2	1.184	1.104
Final R indices [I>2sigma(I)]	R_1 = 0.0166, wR_2 = 0.0440	R_1 = 0.0293, wR_2 = 0.0762
R indices (all data)	R_1 = 0.0171, wR_2 = 0.0442	R_1 = 0.0333, wR_2 = 0.0782
Largest diff. peak and hole	0.294 and -0.857 e.Å^{-3}	0.772 and -0.984 e.Å^{-3}

Table S2 Selected bond lengths (Å) and angles (°) for complexes **1** and **2**.

*Complex **1***			
O(1)-Cd(1)	2.3540(12)	O(10)-Cd(1)-O(4)	82.15(5)
O(2)-Cd(1)	2.5509(13)	O(6)-Cd(1)-O(4)	107.82(4)
O(3)-Cd(1)	2.5217(14)	O(1)-Cd(1)-O(4)	126.12(4)
O(4)-Cd(1)	2.4802(14)	O(9)-Cd(1)-O(3)	88.74(5)
O(6)-Cd(1)	2.3157(12)	O(10)-Cd(1)-O(3)	90.51(5)
O(9)-Cd(1)	2.2438(13)	O(6)-Cd(1)-O(3)	159.02(4)
		O(1)-Cd(1)-O(3)	74.90(4)
O(9)-Cd(1)-O(10)	167.51(5)	O(4)-Cd(1)-O(3)	51.22(4)
O(9)-Cd(1)-O(6)	91.38(5)	O(9)-Cd(1)-O(2)	93.34(5)
O(10)-Cd(1)-O(6)	84.88(5)	O(10)-Cd(1)-O(2)	96.85(4)
O(9)-Cd(1)-O(1)	92.27(5)	O(6)-Cd(1)-O(2)	72.32(4)
O(10)-Cd(1)-O(1)	99.57(4)	O(1)-Cd(1)-O(2)	53.72(4)
O(6)-Cd(1)-O(1)	126.04(4)	O(4)-Cd(1)-O(2)	178.96(4)
O(9)-Cd(1)-O(4)	87.68(5)	O(3)-Cd(1)-O(2)	128.62(4)
*Complex **2***			
O(1)-Cd(1)	2.3209(16)	N(1)#1-Cd(1)-O(1)#1	72.15(6)
N(1)-Cd(1)	2.2949(19)	N(1)-Cd(1)-O(1)#1	162.19(7)
		N(1)#2-Cd(1)-O(1)#1	91.75(7)
N(1)#1-Cd(1)-N(1)	105.68(5)	O(1)-Cd(1)-O(1)#1	90.15(6)
N(1)#1-Cd(1)-N(1)#2	105.68(5)	N(1)#1-Cd(1)-O(1)#2	162.19(7)
N(1)-Cd(1)-N(1)#2	105.68(5)	N(1)-Cd(1)-O(1)#2	91.75(7)
N(1)#1-Cd(1)-O(1)	91.75(7)	N(1)#2-Cd(1)-O(1)#2	72.15(6)
N(1)-Cd(1)-O(1)	72.15(6)	O(1)-Cd(1)-O(1)#2	90.15(6)
N(1)#2-Cd(1)-O(1)	162.19(7)	O(1)#1-Cd(1)-O(1)#2	90.15(6)

The Cambridge Crystallographic Data Centre deposition numbers are CCDC 821168 & 821169 for Complex **1** and **2** respectively.

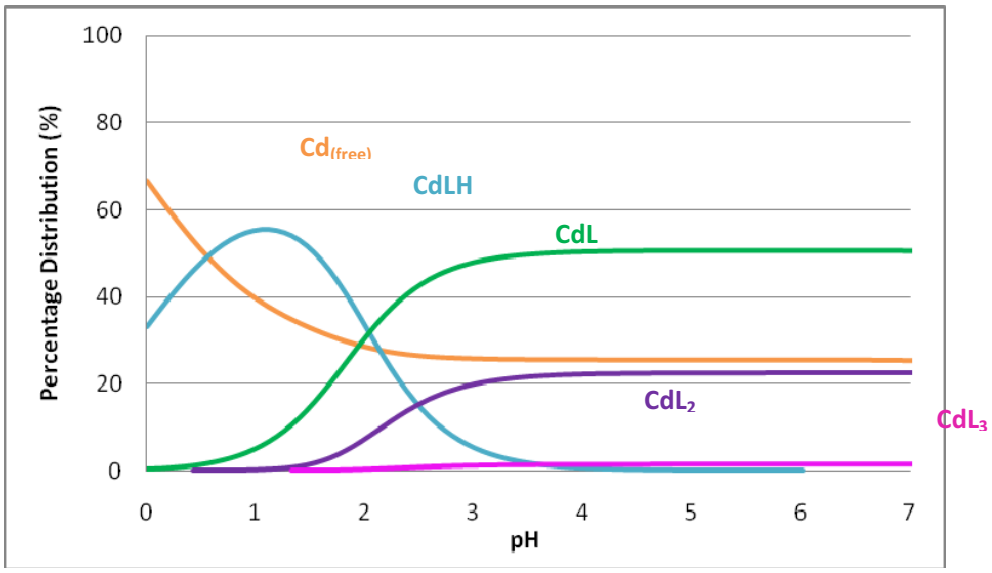


Figure S1 Species distribution diagram for the cadmium-picolinic acid system using formation constant values as follows: log β(CdLH) = 6.27 ± 0.07, log β(CdL) = 4.23 ± 0.01, log β(CdL_2) = 7.81 ± 0.09 and log β(CdL_3) = 10.53 ± 0.08 at 25 °C and 0.25 – 0.5 M H/$NaNO_3$ ionic strength.[2] $[Cd^{2+}]$ = [L]= 0.5 M.

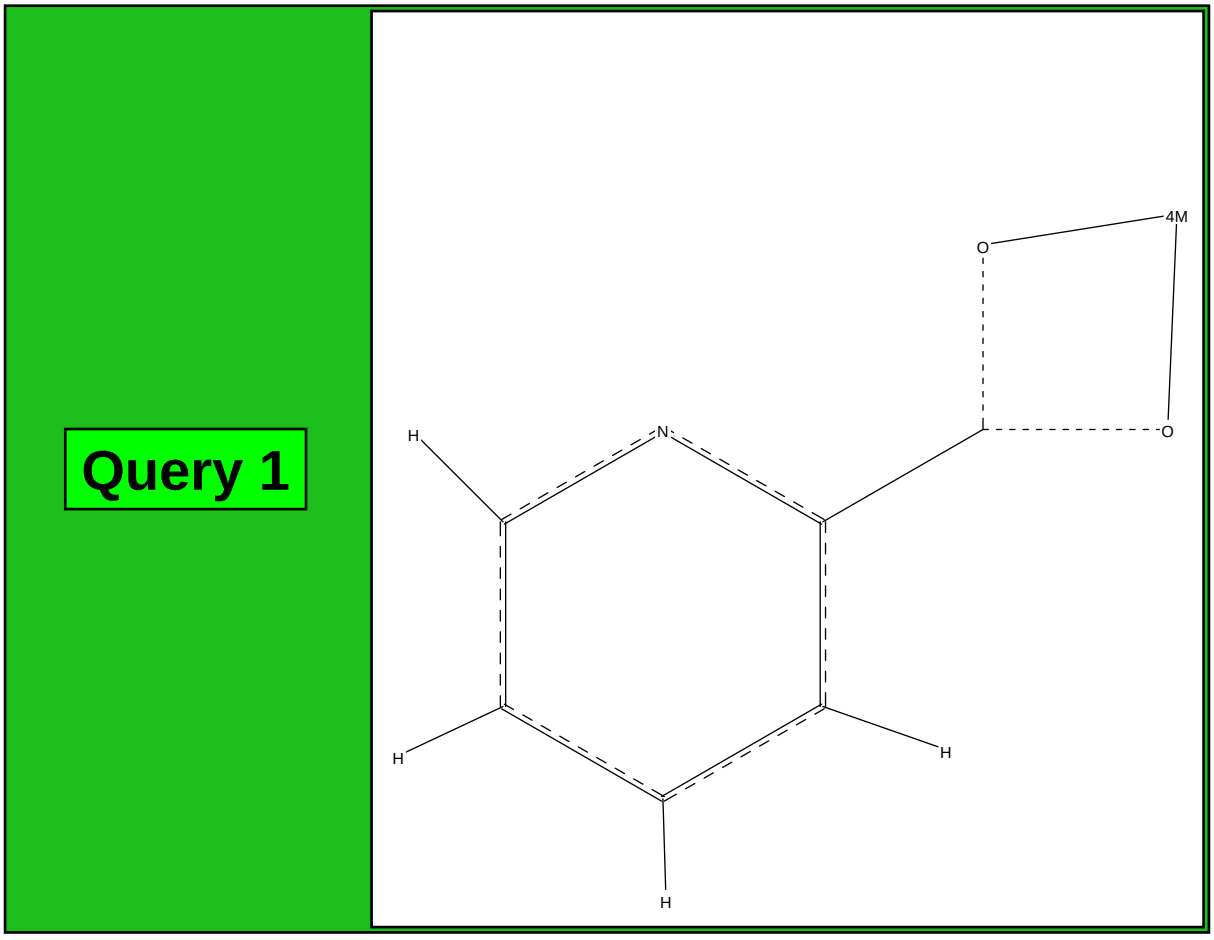
Search Overview

Search:	search2
Date/Time done:	Tue Dec 7 15:35:25 2010
Database(s):	CSD version 5.31 (November 2009) CSD version 5.31 updates (Nov 2009) CSD version 5.31 updates (Feb 2010) CSD version 5.31 updates (May 2010) CSD version 5.31 updates (Aug 2010)
Restriction Info:	No refcode restrictions applied
Filters:	None
Percentage Completed:	100%
Number of Hits:	42

Single query used. Search found structures that:

match

Query 1



Search: search2 (Tue Dec 7 15:35:25 2010): Hits 1-2

TEQTAK

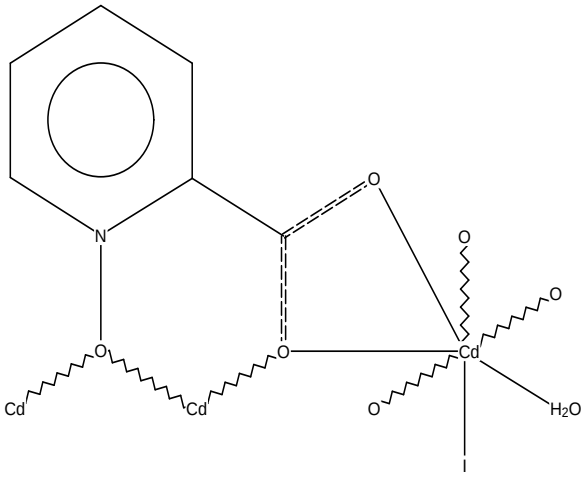
Reference: E.Bermejo, A.Castineiras, R.Dominguez, J.Strahle, C.Maichle-Mossmer (1996) *Polyhedron* ,**15,**1923

Formula: $(C_6 H_6 Cd_1 I_1 N_1 O_4)n$

Compound Name: catena-($(\mu_2$-Pyridine-1-oxide-2-carboxylato)-aqua-iodo-cadmium(ii))

Space Group:	P21/c	***Cell:***	***a***	10.848(4)	***b***	8.488(1)	***c***	10.604(4)
Space Group No.:	14	***(Å,°)***	α	90.00	β	90.77(2)	γ	90.00

R-Factor (%): 4.60 ***Temperature(K):*** 295 ***Density(g/cm^3):*** 2.690



YILBIF

Reference: C.Papatriantafyllopoulou, C.P.Raptopoulou, A.Terzis, J.F.Janssens, E.Manessi-Zoupa, S.P.Perlepes, J.C.Plakatouras (2007) *Polyhedron* ,**26,**4053

Formula: $(C_{12} H_{14} Cd_2 N_2 O_{11} S_1)n,n(H_2 O_1)$

Compound Name: catena-($(\mu_2$-Picolinato-N,O,O)-(μ_2-picolinato-N,O,O,O')-(μ_2-aqua)-(μ_2-sulfato-O,O')-diaqua-di-cadmium(ii) monohydrate)

Space Group:	P21/c	***Cell:***	***a***	11.200(5)	***b***	13.231(6)	***c***	13.650(6)
Space Group No.:	14	***(Å,°)***	α	90.00	β	110.36(1)	γ	90.00

R-Factor (%): 5.93 ***Temperature(K):*** 298 ***Density(g/cm^3):*** 2.232