

Search Overview

Search: search1
Date/Time done: Thu Jul 14 03:39:50 2011
Database(s): CSD version 5.32 (November 2010)
CSD version 5.32 updates (Nov 2010)
Restriction Info: No refcode restrictions applied
Filters: None
Percentage Completed: 100%
Number of Hits: 13

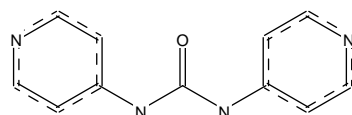
Summary of queries used. Search found structures that:

match

Query 2

Query 1

Query 1



Query 2

4M

Search: search1 (Thu Jul 14 03:39:50 2011): Hit 1

EKEJAF

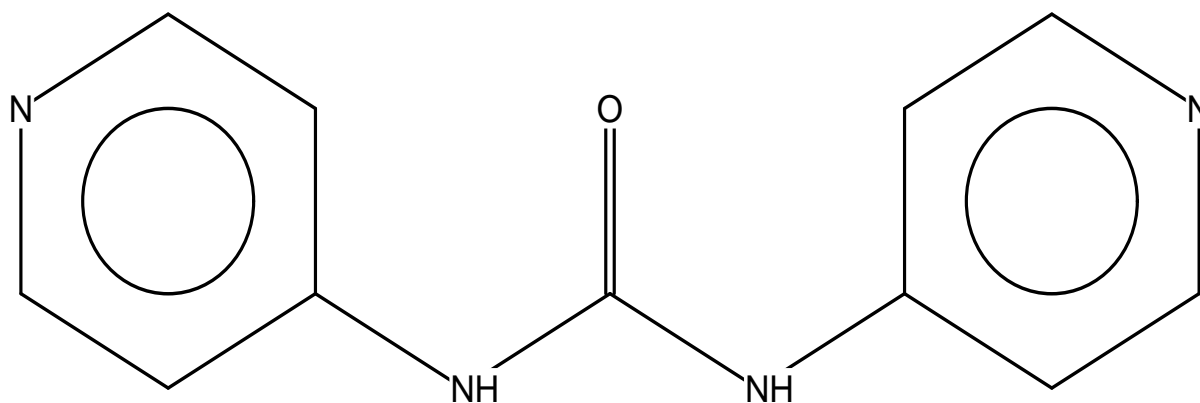
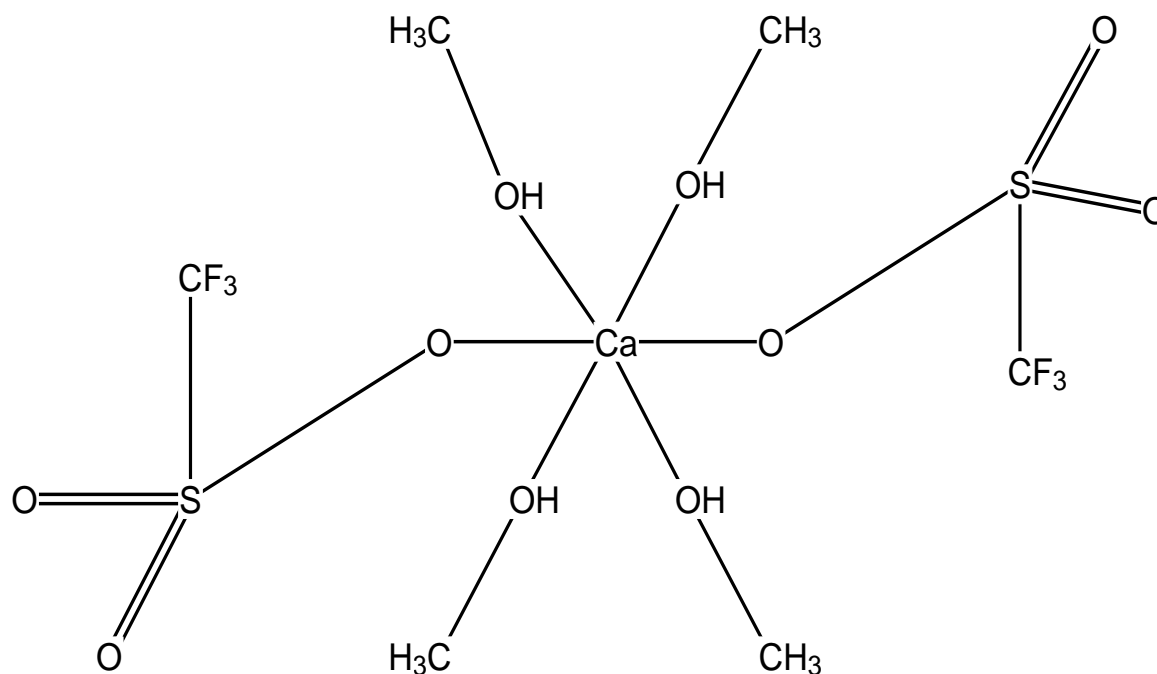
Reference: M.Barboiu, A.van der Lee (2003)
Acta Crystallogr., Sect. C: Cryst. Struct. Commun. ,59,m366

Formula: C₆ H₁₆ Ca₁ F₆ O₁₀ S₂, 2(C₁₁ H₁₀ N₄ O₁)

Compound Name: tetrakis(Methanol)-bis(trifluoromethanesulfonato)-calcium bis(1,3-di-4-pyridylurea)

Space Group: P-1 **Cell:** **a** 9.157(1) **b** 9.768(1) **c** 11.366(2)
Space Group No.: 2 **(Å, °)** **α** 98.95(1) **β** 97.14(1) **γ** 94.03(1)

R-Factor (%): 3.50 **Temperature(K):** 173 **Density(g/cm³):** 1.497



Search: search1 (Thu Jul 14 03:39:50 2011): Hit 2

KAZVAJ

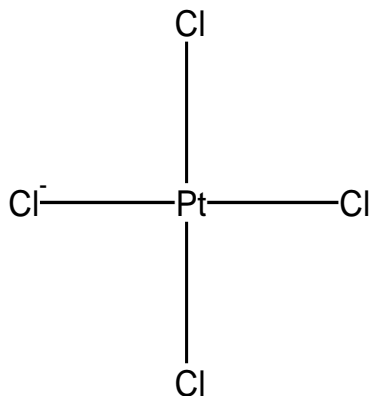
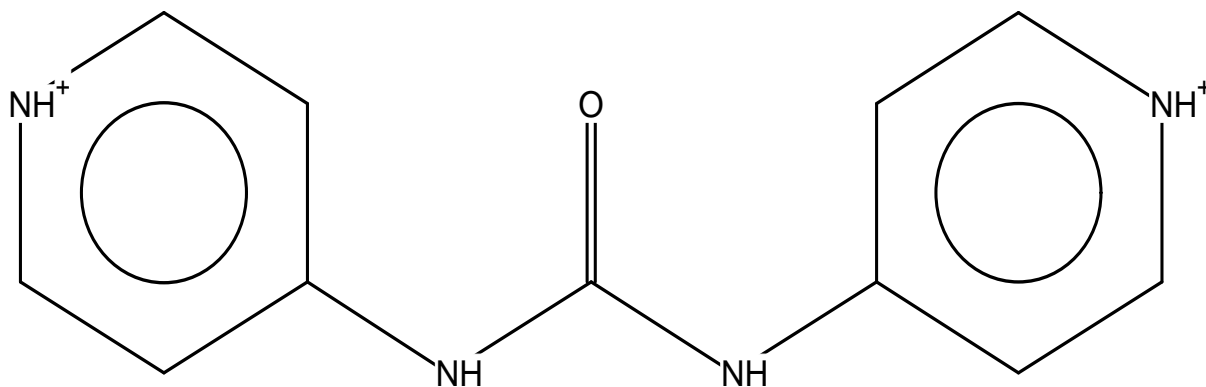
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *Cryst.Growth Des.* ,
6,216

Formula: C₁₁ H₁₂ N₄ O₁²⁺, Cl₄ Pt₁²⁻

Compound Name: N,N'-bis(4-Pyridinio)urea tetrachloro-platinum(ii)

Space Group: P21/c **Cell:** **a** 14.898(1) **b** 7.025(0) **c** 15.941(1)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 110.90(0) **γ** 90.00

R-Factor (%): 1.55 **Temperature(K):** 100 **Density(g/cm³):** 2.357



Search: search1 (Thu Jul 14 03:39:50 2011): Hit 3

KAZVEN

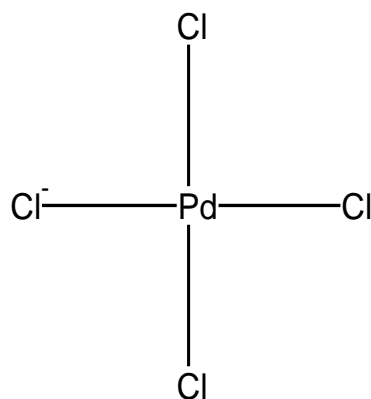
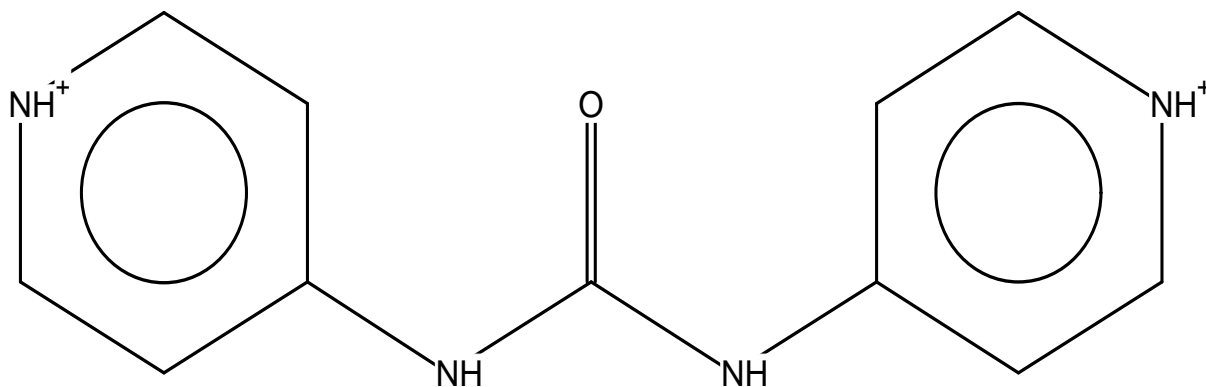
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *Cryst.Growth Des.* ,
6,216

Formula: C₁₁ H₁₂ N₄ O₁²⁺, Cl₄ Pd₁²⁻

Compound Name: N-(4-Pyridinio)isonicotinamidinium tetrachloro-palladium(ii)

Space Group: P21/c **Cell:** **a** 17.171(2) **b** 7.863(1) **c** 12.362(1)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 109.44(0) **γ** 90.00

R-Factor (%): 1.99 **Temperature(K):** 100 **Density(g/cm³):** 1.960



Search: search1 (Thu Jul 14 03:39:50 2011): Hit 4

LISDEX

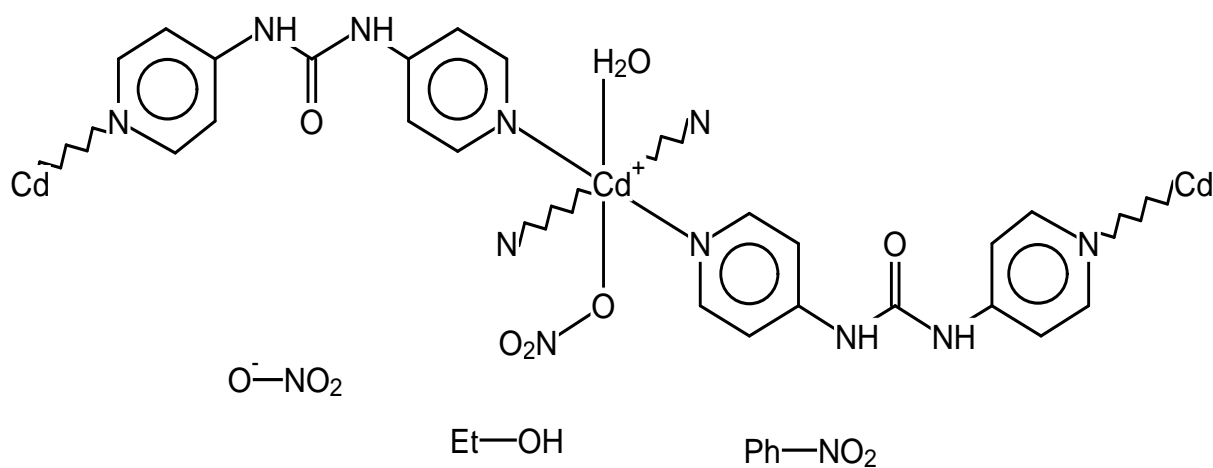
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *Cryst.Growth Des.* ,
7,2096

Formula: (C₂₂ H₂₂ Cd₁ N₉ O₆¹⁺)_n,n(N₁ O₃¹⁻),n(C₂ H₆ O₁),n(C₆ H₅ N₁ O₂)

Compound Name: catena-(bis(μ₂-N,N'-bis(4-Pyridyl)urea-N'',N''')-aqua-(nitrate-O)-cadmium nitrate ethanol nitrobenzene solvate)

Space Group: Fdd2 **Cell:** **a** 21.109(1) **b** 34.334(2) **c** 20.156(1)
Space Group No.: 43 **(Å, °)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 2.94 **Temperature(K):** 100 **Density(g/cm³):** 1.550



Search: search1 (Thu Jul 14 03:39:50 2011): Hit 5

LISDIB

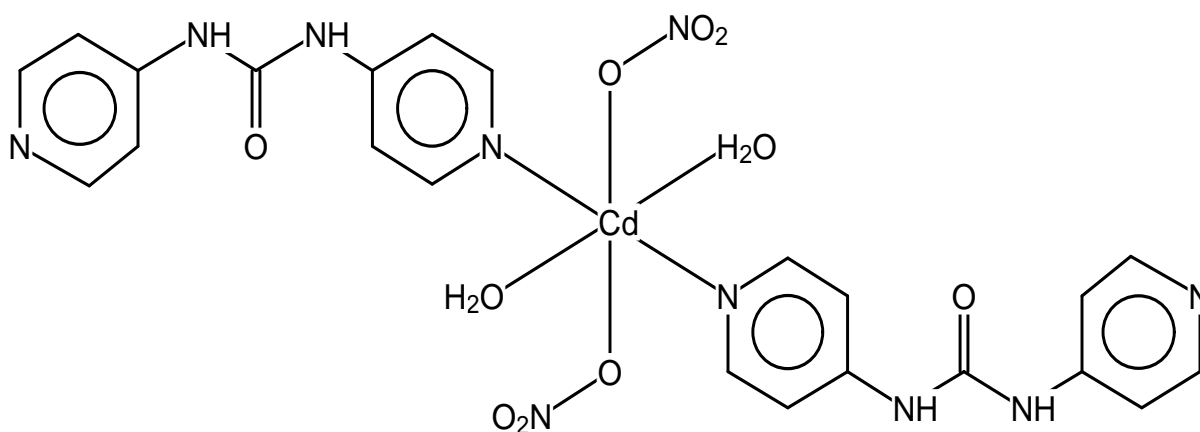
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *Cryst.Growth Des.* ,
7,2096

Formula: C₂₂ H₂₄ Cd₁ N₁₀ O₁₀

Compound Name: bis(N,N'-bis(4-Pyridyl)urea-N'')-diaqua-bis(nitrato-O)-cadmium

Space Group: P-1 **Cell:** **a** 6.182(1) **b** 10.254(3) **c** 10.921(3)
Space Group No.: 2 **(Å, °)** **α** 87.02(0) **β** 79.04(0) **γ** 77.89(0)

R-Factor (%): 3.93 **Temperature(K):** 298 **Density(g/cm³):** 1.751



Search: search1 (Thu Jul 14 03:39:50 2011): Hit 6

NAVWEN

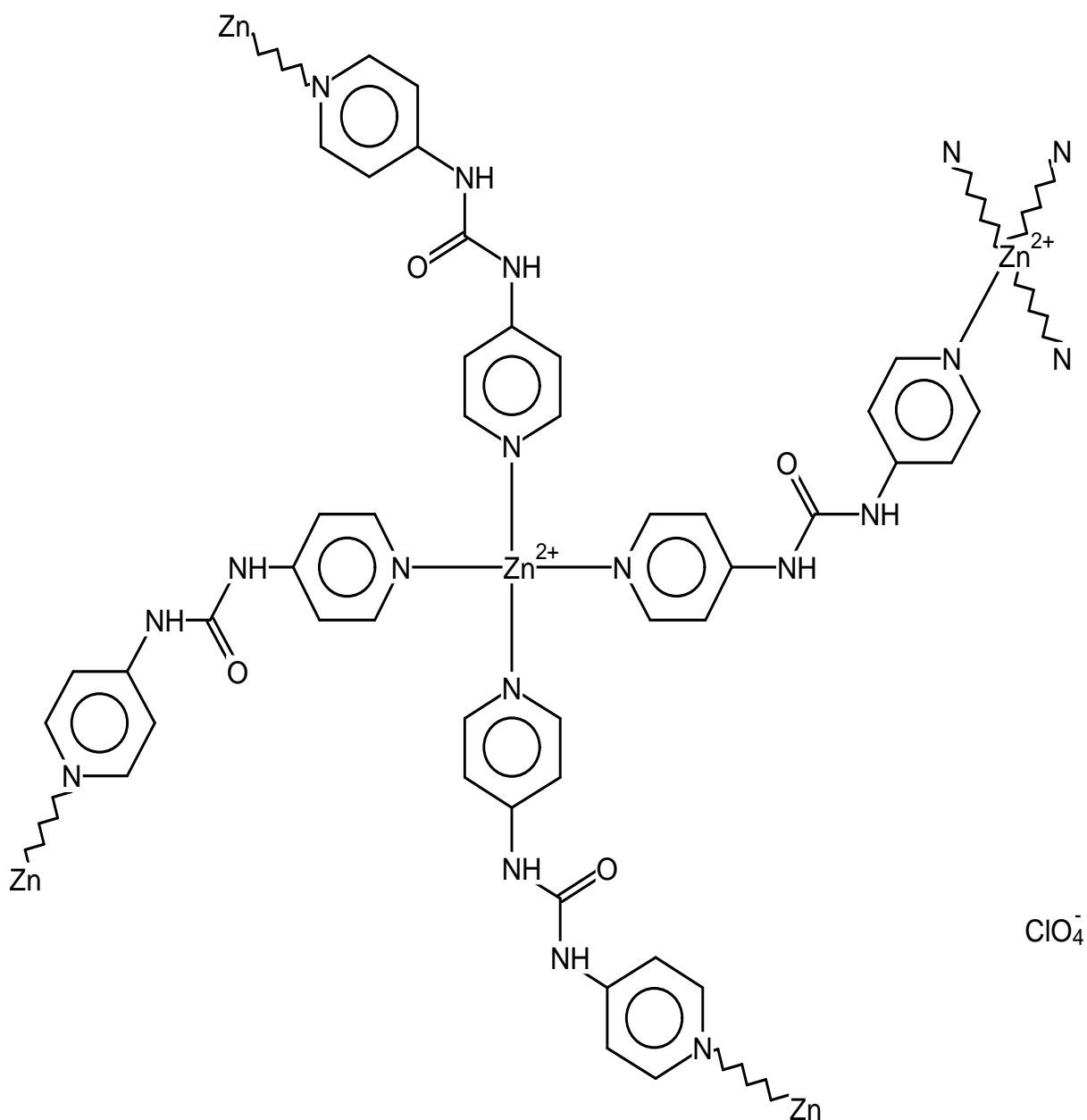
Reference: D.K.Kumar, D.A.Jose, A.Das, P.Dastidar (2005)
Inorg.Chem. ,**44**,6933

Formula: $(C_{44} H_{40} N_{16} O_4 Zn_2^{4+})n, 4n(Cl_1 O_4^{1-})$

Compound Name: catena-(tetrakis(μ_2 -N,N'-bis(4-Pyridyl)urea)-di-zinc(ii) tetraperchlorate)

Space Group: I-4 **Cell:** **a** 17.880(5) **b** 17.880(5) **c** 8.254(4)
Space Group No.: 82 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.43 **Temperature(K):** 100 **Density(g/cm³):** 1.744



Search: search1 (Thu Jul 14 03:39:50 2011): Hit 7

PAQLID

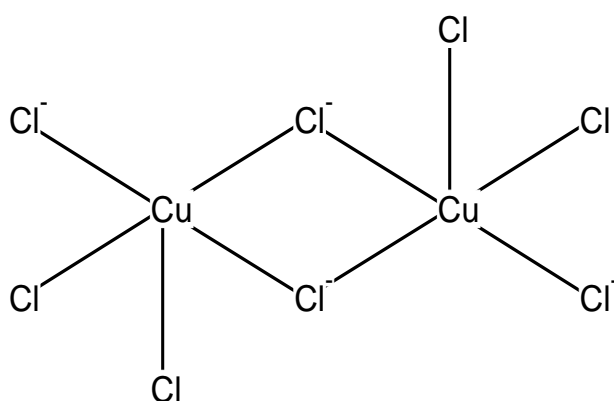
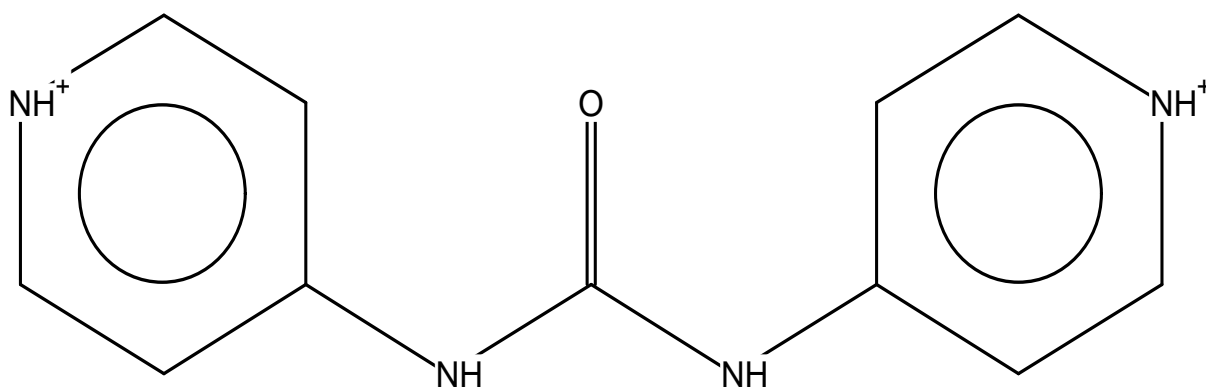
Reference: D.K.Kumar, A.Ballabh, D.A.Jose, P.Dastidar, A.Das
(2005) *Cryst.Growth Des.* ,5,651

Formula: $2(\text{C}_{11}\text{H}_{12}\text{N}_4\text{O}_1^{2+}), \text{Cl}_8\text{Cu}_2^{4-}$

Compound Name: bis(N,N'-bis(4-Pyridinio)urea) tetrachloro-copper

Space Group: P21/c **Cell:** **a** 7.734(5) **b** 17.448(5) **c** 11.609(3)
Space Group No.: 14 **(Å, °)** α 90.00 β 98.54(3) γ 90.00

R-Factor (%): 3.61 **Temperature(K):** 293 **Density(g/cm³):** 1.808



Search: search1 (Thu Jul 14 03:39:50 2011): Hit 8

SEQGEB

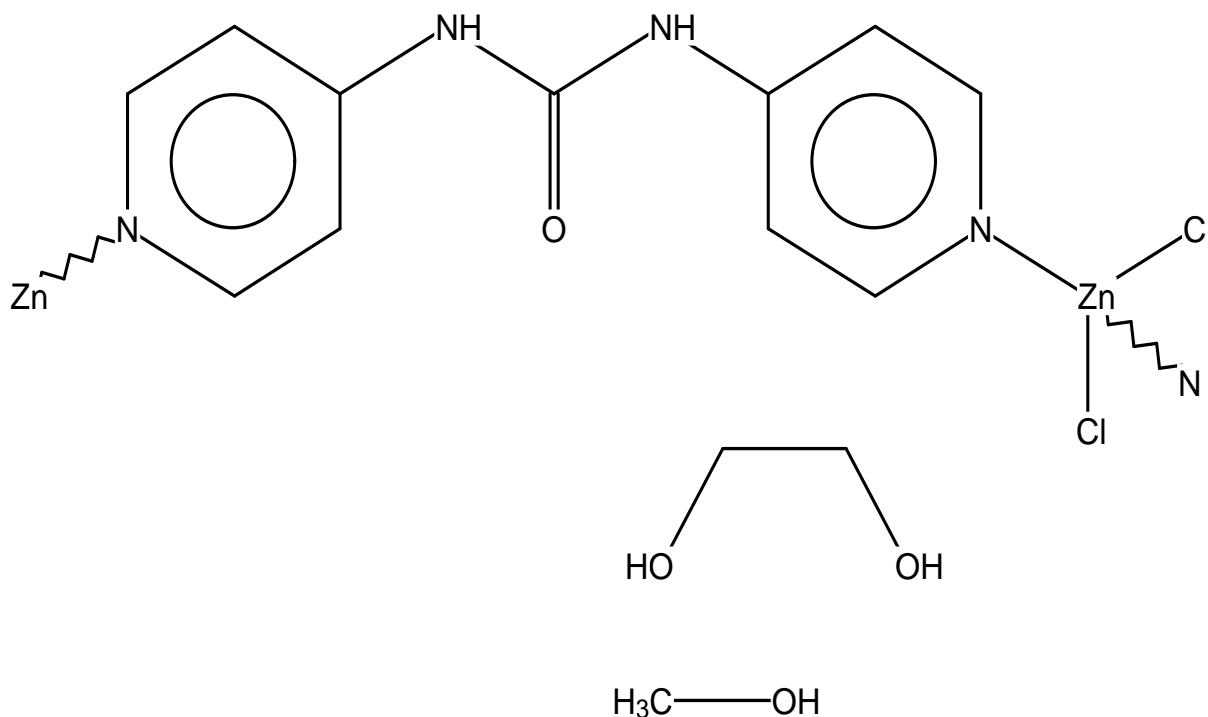
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *CrystEngComm*, **8**, 805

Formula: $(C_{11} H_{10} Cl_2 N_4 O_1 Zn_1)_n, n(C_2 H_6 O_2), n(C_1 H_4 O_1)$

Compound Name: catena-((μ_2 -N,N'-bis(4-Pyridyl)urea)-dichloro-zinc(ii) ethylene glycol methanol solvate)

Space Group: Pbcn **Cell:** **a** 19.193(1) **b** 7.198(0) **c** 24.428(1)
Space Group No.: 60 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.77 **Temperature(K):** 100 **Density(g/cm³):** 1.750



Search: search1 (Thu Jul 14 03:39:50 2011): Hit 9

SEQGIF

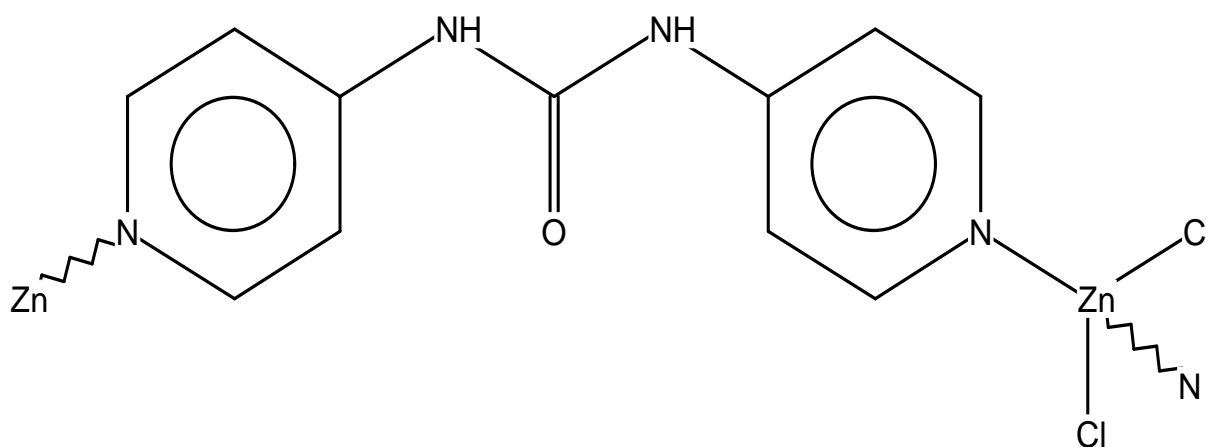
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *CrystEngComm*, **8**, 805

Formula: (C₁₁ H₁₀ Cl₂ N₄ O₁ Zn₁)_n, 2n(H₂ O₁)

Compound Name: catena-((μ₂-N,N'-bis(4-Pyridyl)urea)-dichloro-zinc(ii) dihydrate)

Space Group: Pbcn **Cell:** **a** 18.346(1) **b** 6.841(0) **c** 24.146(2)
Space Group No.: 60 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.48 **Temperature(K):** 100 **Density(g/cm³):** 1.695



Search: search1 (Thu Jul 14 03:39:50 2011): Hit 10

SEQGOL

Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *CrystEngComm*, **8**, 805

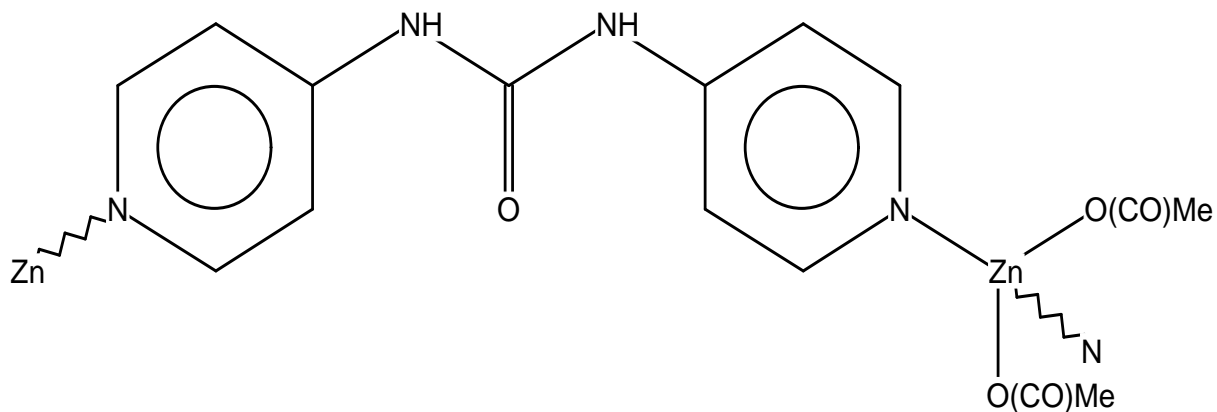
Formula: (C₁₅ H₁₆ N₄ O₅ Zn₁)_n,n(H₂ O₁)

Compound Name: catena-((μ₂-N,N'-bis(4-Pyridyl)urea)-diacetato-zinc(ii) monohydrate)

Space Group: C2/c **Cell:** **a** 10.758(0) **b** 16.552(1) **c** 19.285(1)

Space Group No.: 15 **(Å, °)** **α** 90.00 **β** 96.31(0) **γ** 90.00

R-Factor (%): 2.83 **Temperature(K):** 100 **Density(g/cm³):** 1.618



H₂O

Search: search1 (Thu Jul 14 03:39:50 2011): Hit 11

SEQGUR

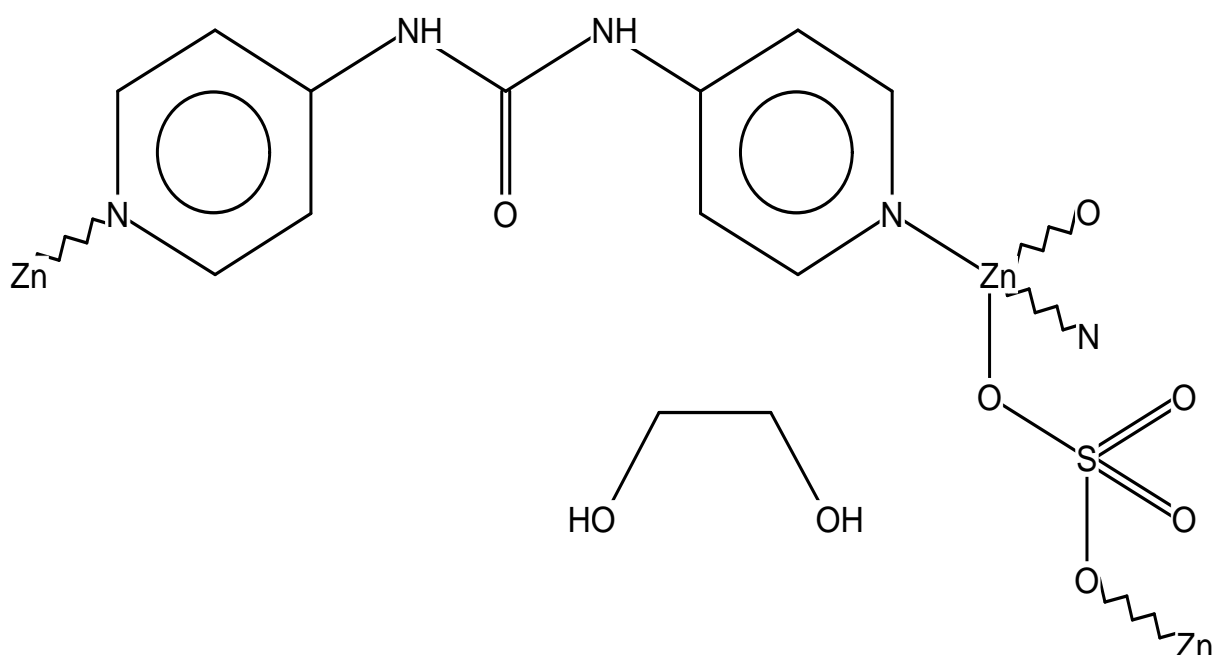
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *CrystEngComm* ,**8**, 805

Formula: (C₁₁ H₁₀ N₄ O₅ S₁ Zn₁)_n,2n(C₂ H₆ O₂)

Compound Name: catena-((μ₂-N,N'-bis(4-Pyridyl)urea)-(μ₂-sulfato)-zinc(ii) ethylene glycol solvate)

Space Group: P21/c **Cell:** **a** 4.853(0) **b** 16.207(1) **c** 24.048(2)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 100.39(0) **γ** 90.00

R-Factor (%): 4.09 **Temperature(K):** 100 **Density(g/cm³):** 1.785



Search: search1 (Thu Jul 14 03:39:50 2011): Hit 12

VIMZAT

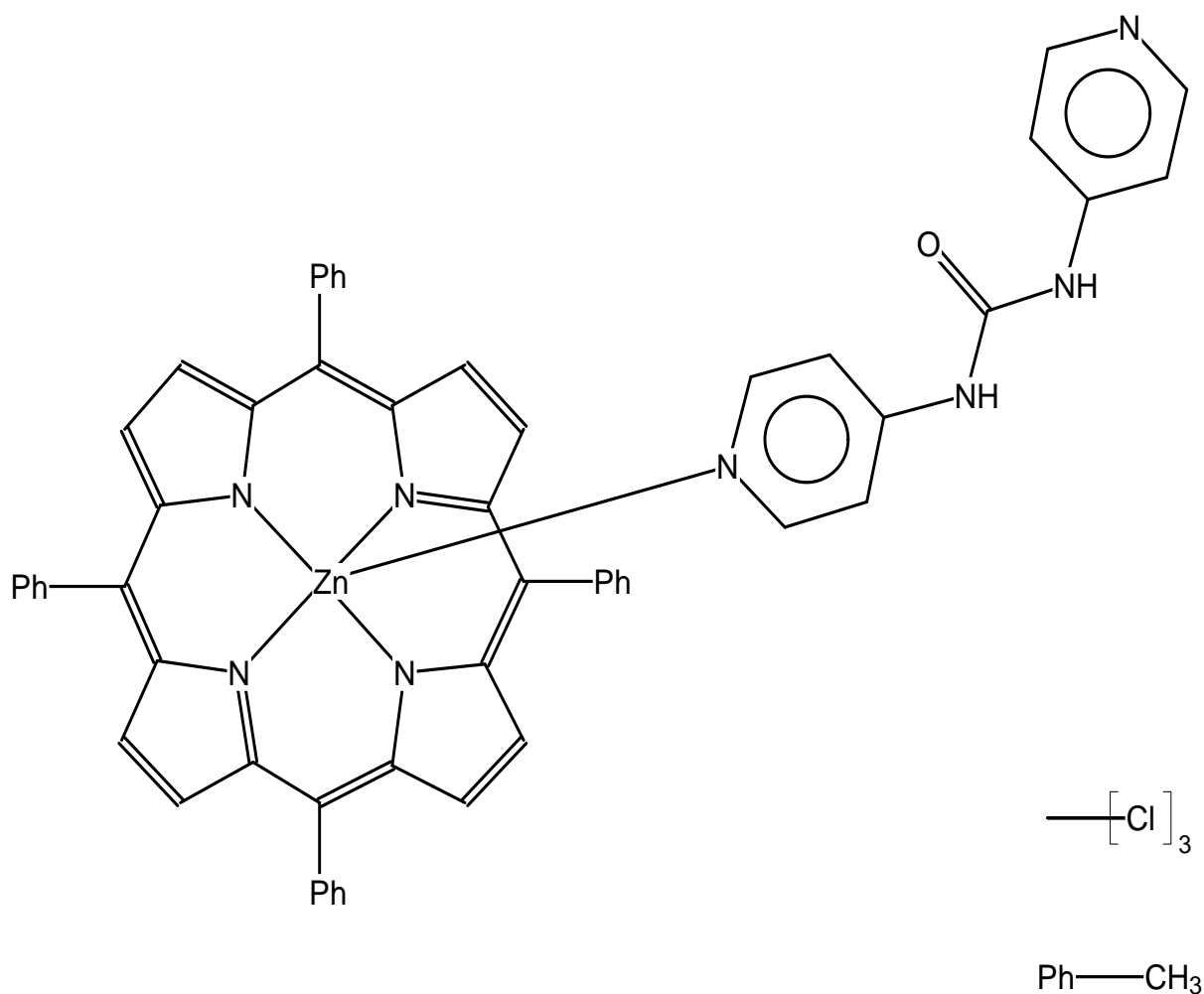
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *Inorg.Chem.* ,**46**, 7351

Formula: C₅₅ H₃₈ N₈ O₁ Zn₁.0.33(C₁ H₁ Cl₃),1.44(C₇ H₈)

Compound Name: (N,N'-bis(4-Pyridyl)urea)-(5,10,15,20-tetraphenylporphyrinato)-zinc(ii) toluene chloroform clathrate toluene solvate

Space Group: R-3 **Cell:** **a** 39.647(1) **b** 39.647(1) **c** 17.055(1)
Space Group No.: 148 **(Å, °)** α 90.00 β 90.00 γ 120.00

R-Factor (%): 6.92 **Temperature(K):** 100 **Density(g/cm³):** 1.370



Search: search1 (Thu Jul 14 03:39:50 2011): Hit 13

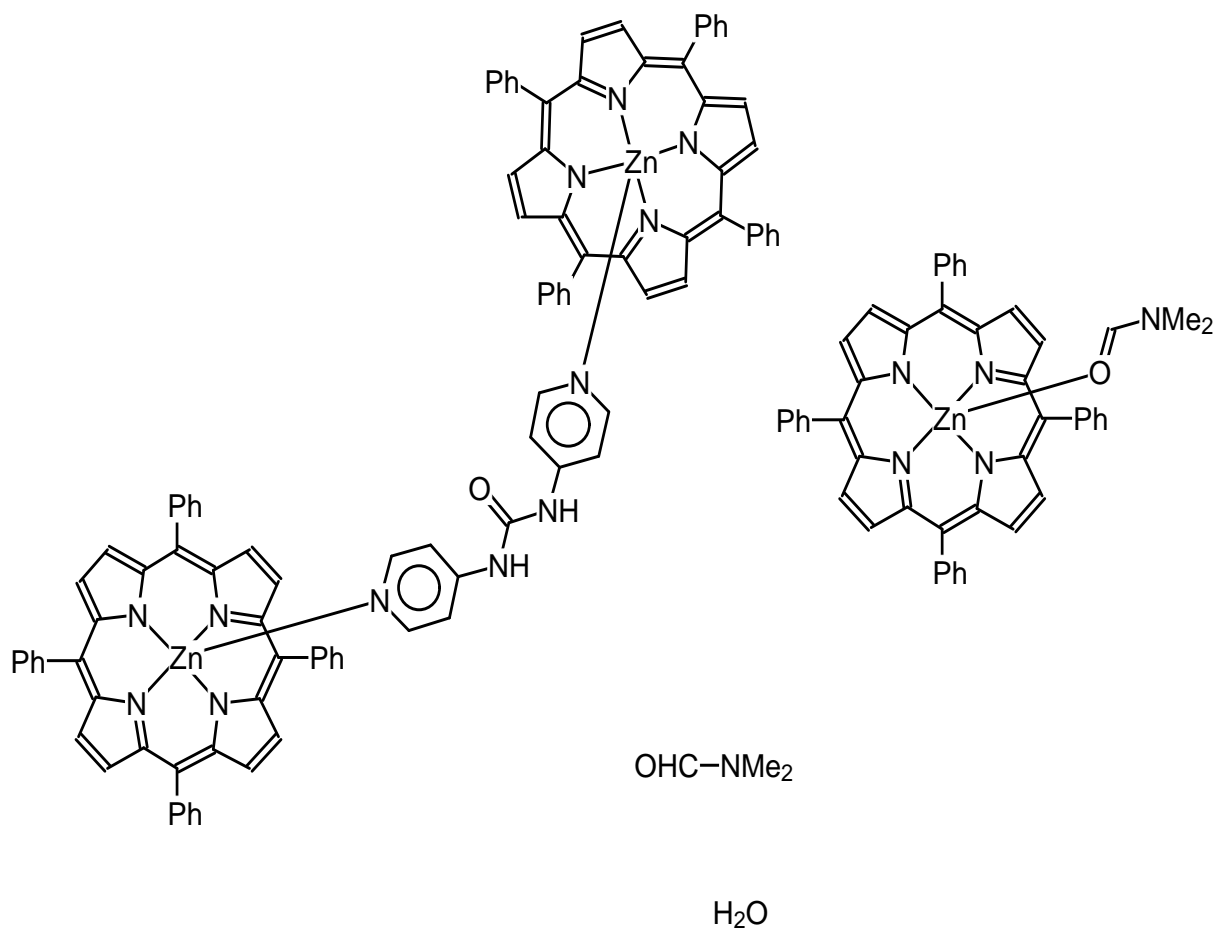
VINBOK

Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *Inorg.Chem.* ,**46**, 7351

Formula: C₉₉ H₆₆ N₁₂ O₁ Zn₂, C₄₇ H₃₅ N₅ O₁ Zn₁, 6(C₃ H₇ N₁ O₁), 2(H₂ O₁)

Compound Name: (μ₂-N,N'-bis(4-Pyridyl)urea)-bis(5,10,15,20-tetraphenylporphyrinato)-di-zinc(ii) (5,10,15,20-tetraphenylporphyrinato)-zinc(ii) tris(dimethylformamide) clathrate dimethylformamide solvate dihydrate

Space Group:	P-1	Cell:	a 13.365(0)	b 17.511(1)	c 28.996(1)
Space Group No.:	2	(Å, °)	α 92.68(0)	β 91.20(0)	γ 93.49(0)
R-Factor (%):	6.55	Temperature(K):	298	Density(g/cm³):	1.373



Search Overview

Search: search2
Date/Time done: Sun Nov 20 19:30:17 2011
Database(s): CSD version 5.32 (November 2010)
CSD version 5.32 updates (Nov 2010)
Restriction Info: No refcode restrictions applied
Filters: None
Percentage Completed: 100%
Number of Hits: 38

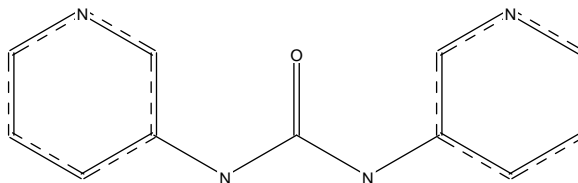
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

4M

Search: search2 (Sun Nov 20 19:30:17 2011): Hit 1

DEPCIL

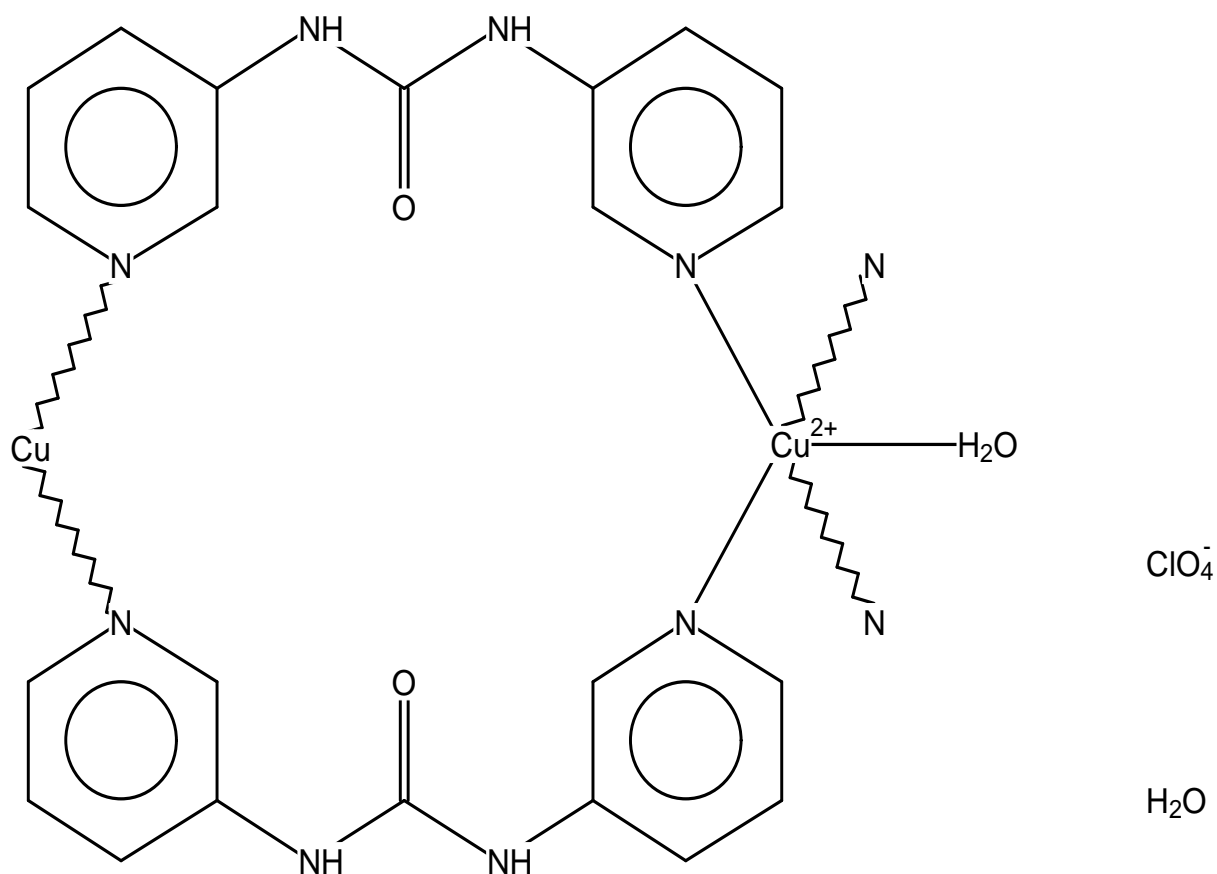
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *New J.Chem.* ,**30**, 1267

Formula: $(C_{22} H_{22} Cu_1 N_8 O_3^{2+})_n, 2n(Cl_1 O_4^{1-}), n(H_2 O_1)$

Compound Name: catena-(bis(μ_3 -N,N'-bis(3-pyridyl)urea)-aqua-copper(ii) diperchlorate monohydrate)

Space Group: P21/c **Cell:** **a** 8.797(0) **b** 17.983(1) **c** 17.520(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 90.36(0) γ 90.00

R-Factor (%): 4.06 **Temperature(K):** 100 **Density(g/cm³):** 1.742



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 2

DEPCOR

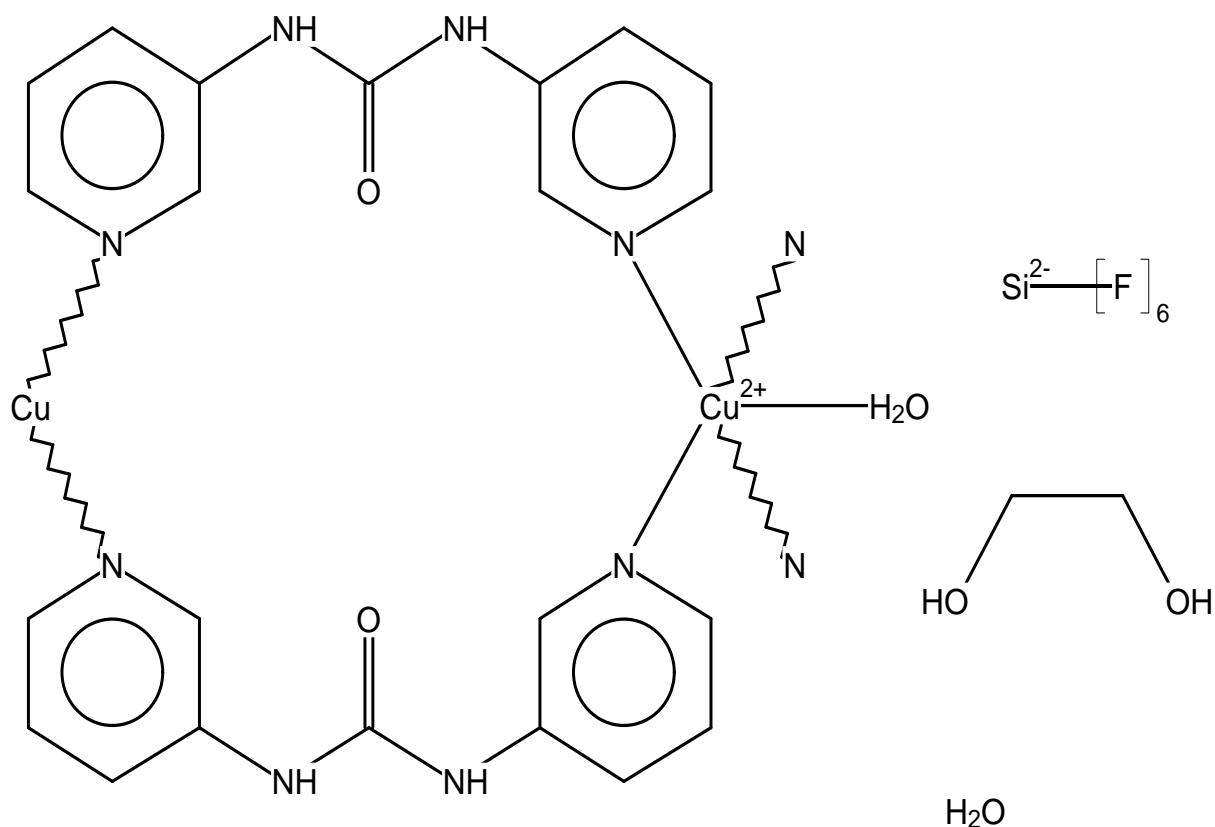
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *New J.Chem.* ,**30**, 1267

Formula: $(C_{22} H_{22} Cu_1 N_8 O_3^{2+})_n, n(F_6 Si_1^{2-}), 2n(C_2 H_6 O_2), n(H_2 O_1)$

Compound Name: catena-(bis(μ_2 -N,N'-bis(3-Pyridyl)urea)-aqua-copper(ii) hexafluorosilicate ethylene glycol solvate monohydrate)

Space Group: C2/c **Cell:** **a** 21.398(2) **b** 17.904(1) **c** 17.439(1)
Space Group No.: 15 **(Å, °)** α 90.00 β 105.30(0) γ 90.00

R-Factor (%): 7.26 **Temperature(K):** 100 **Density(g/cm³):** 1.637



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 3

DEPCUX

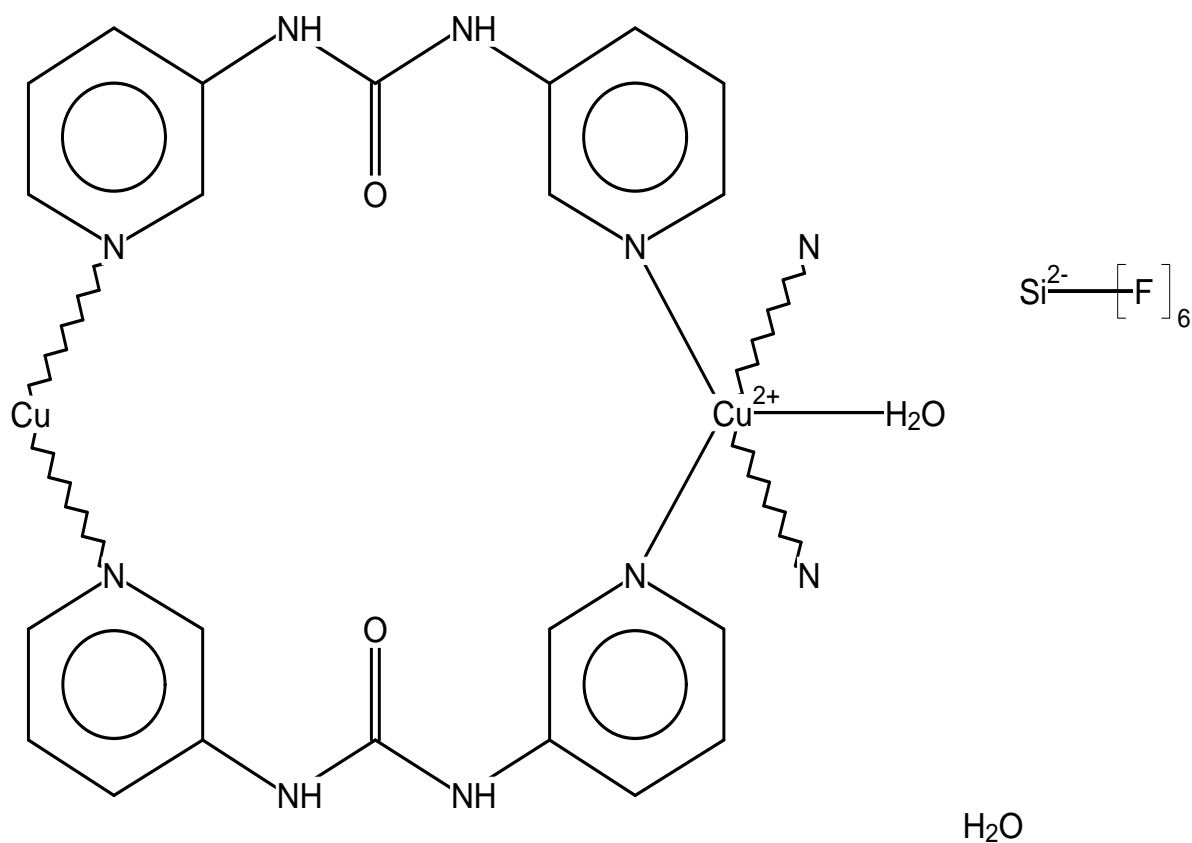
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *New J.Chem.* ,**30**, 1267

Formula: $(C_{22} H_{22} Cu_1 N_8 O_3^{2+})_n, n(F_6 Si_1^{2-}), 5n(H_2 O_1)$

Compound Name: catena-(bis(μ_2 -N,N'-bis(3-Pyridyl)urea)-aqua-copper(ii) hexafluorosilicate pentahydrate)

Space Group: C2/c **Cell:** **a** 21.211(1) **b** 17.934(1) **c** 17.546(1)
Space Group No.: 15 (**Å, °**) α 90.00 β 104.88(0) γ 90.00

R-Factor (%): 4.03 **Temperature(K):** 100 **Density(g/cm³):** 1.528



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 4

DEPDAE

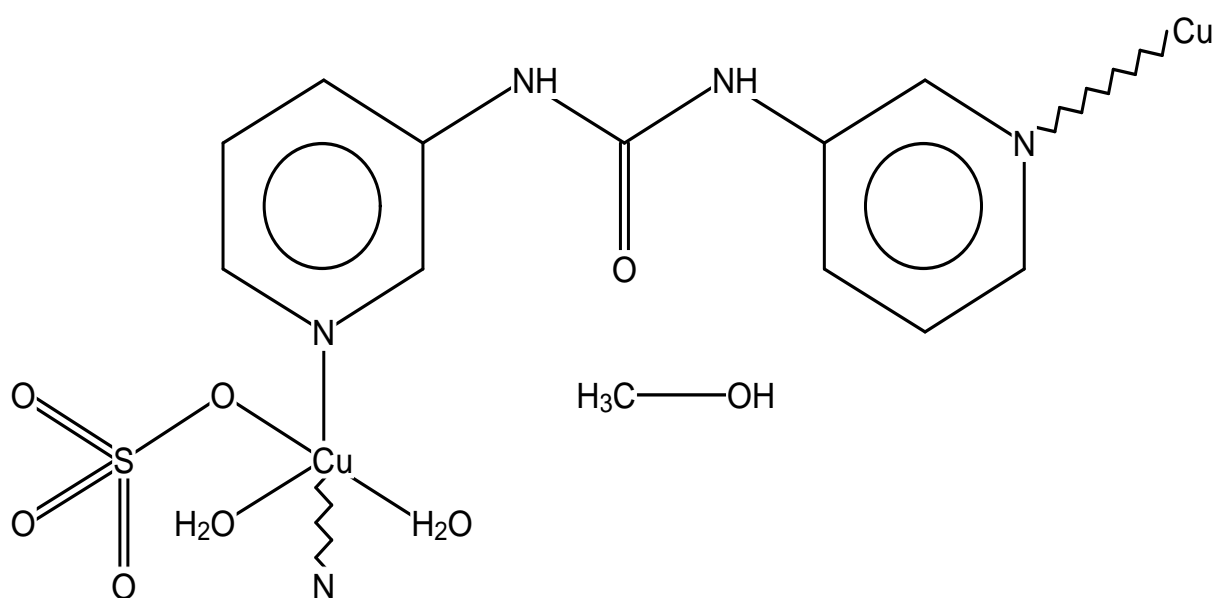
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *New J.Chem.* ,**30**, 1267

Formula: (C₁₁ H₁₄ Cu₁ N₄ O₇ S₁)_n,n(C₁ H₄ O₁)

Compound Name: catena-((μ_2 -N,N'-bis(3-Pyridyl)urea)-diaqua-(sulfato-O)-copper(ii) methanol solvate)

Space Group: P21/c **Cell:** **a** 7.704(4) **b** 21.708(11) **c** 12.165(5)
Space Group No.: 14 **(Å, °)** α 90.00 β 122.77(2) γ 90.00

R-Factor (%): 4.72 **Temperature(K):** 298 **Density(g/cm³):** 1.716



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 5

DEPDEI

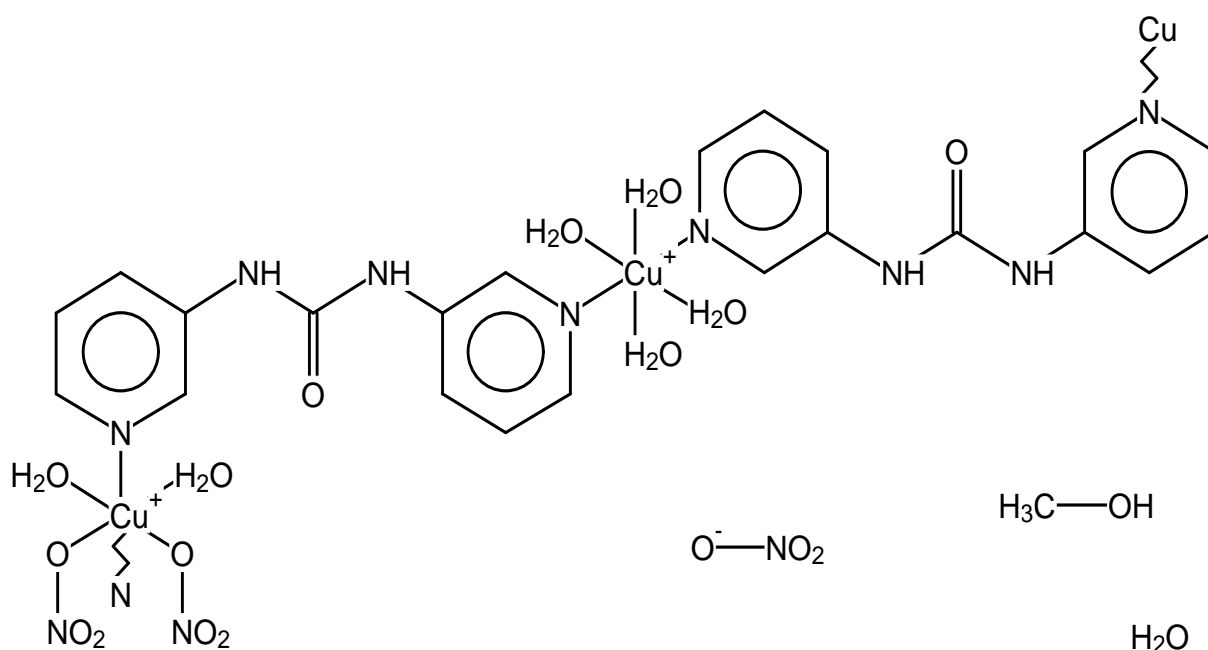
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *New J.Chem.* ,**30**, 1267

Formula: $(C_{22} H_{32} Cu_2 N_{10} O_{14}^{2+})_n, 2n(N_1 O_3^{1-}), n(C_1 H_4 O_1), n(H_2 O_1)$

Compound Name: catena-(μ_2 -bis(N,N'-bis(3-pyridyl)urea)-hexa-aqua-bis(nitrato)-di-copper(ii) dintrate methanol solvate monohydrate)

Space Group: P-1 **Cell:** **a** 8.329(0) **b** 9.799(0) **c** 13.155(1)
Space Group No.: 2 **(Å, °)** α 80.12(0) β 74.89(0) γ 88.20(0)

R-Factor (%): 4.28 **Temperature(K):** 100 **Density(g/cm³):** 1.564



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 6

JEXNEG

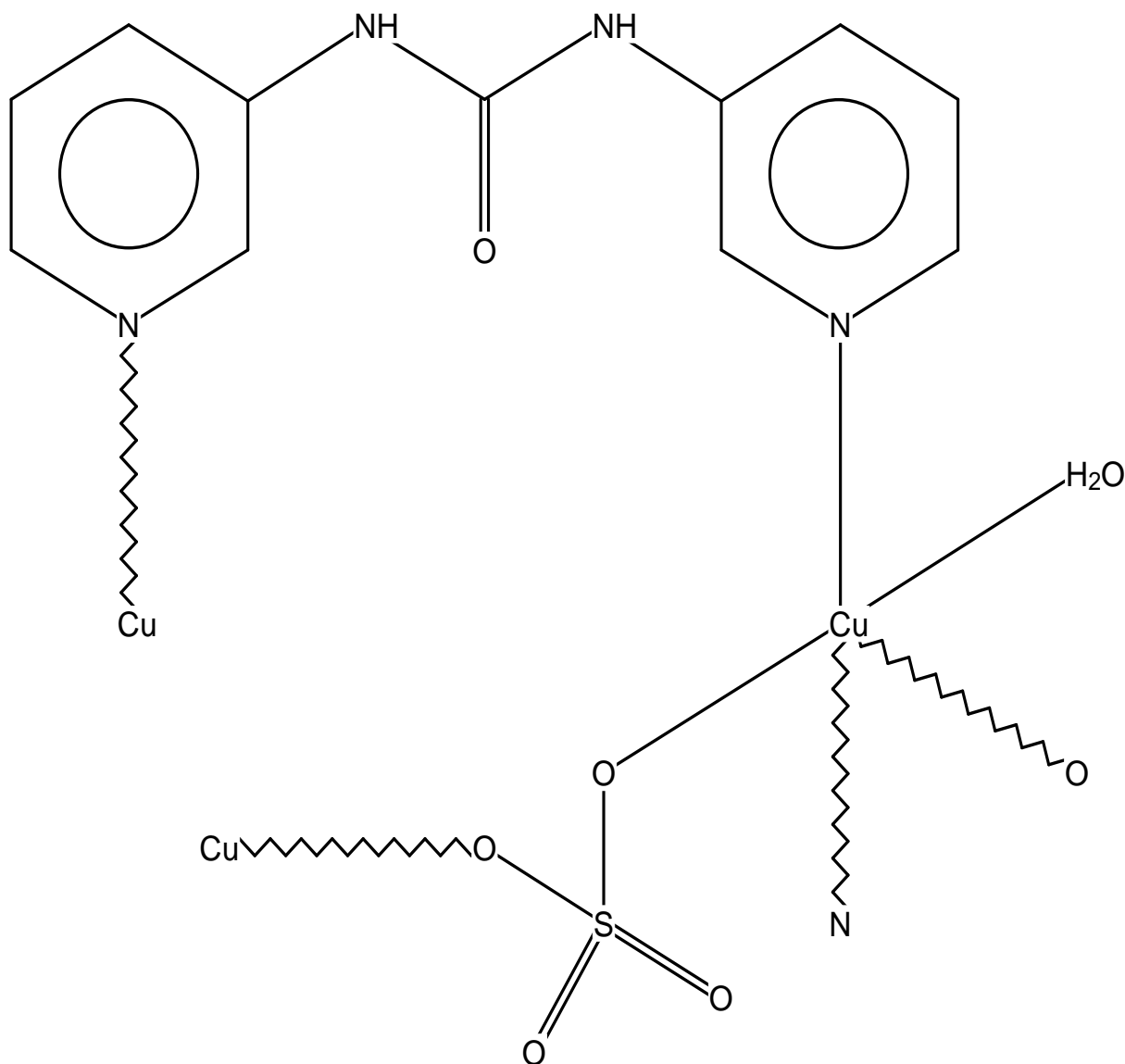
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *Cryst.Growth Des.* ,
7,205

Formula: (C₁₁ H₁₂ Cu₁ N₄ O₆ S₁)_n

Compound Name: catena-((μ₂-syn,syn-N,N'-bis(3-Pyridyl)urea)-(μ₂-sulfato)-aqua-
copper(ii))

Space Group: P21/c **Cell:** **a** 4.962(1) **b** 16.979(5) **c** 18.354(5)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 91.97(0) **γ** 90.00

R-Factor (%): 6.43 **Temperature(K):** 298 **Density(g/cm³):** 1.684



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 7

JEYZET

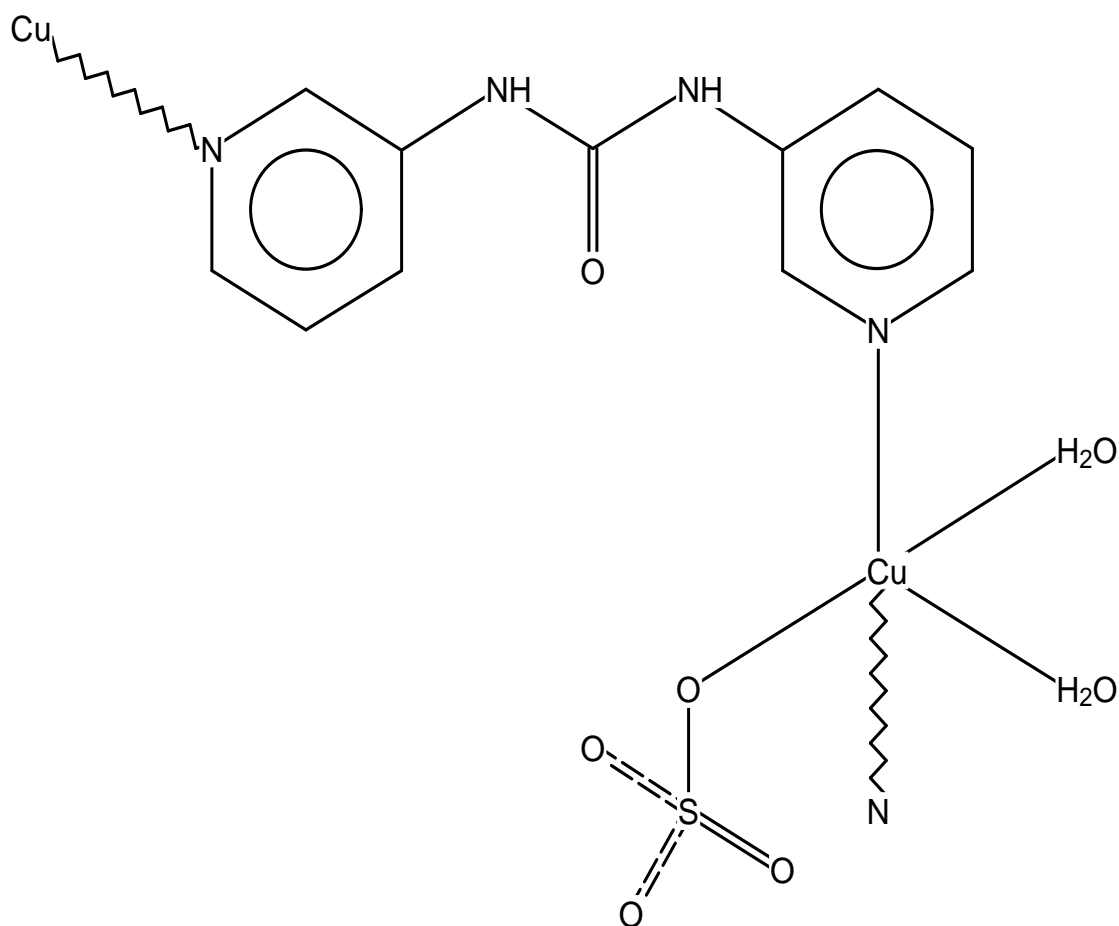
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *Cryst.Growth Des.* ,
7,205

Formula: $(C_{11}H_{14}Cu_1N_4O_7S_1)_n \cdot 2n(H_2O)_1$

Compound Name: catena-((μ_2 -syn,anti-N,N'-bis(3-Pyridyl)urea)-diaqua-(sulfato-O)-
copper(ii) dihydrate)

Space Group: P21/c **Cell:** **a** 7.517(0) **b** 21.771(2) **c** 12.105(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 122.87(0) γ 90.00

R-Factor (%): 4.78 **Temperature(K):** 100 **Density(g/cm³):** 1.780



H₂O

Search: search2 (Sun Nov 20 19:30:17 2011): Hit 8

KAZWAK

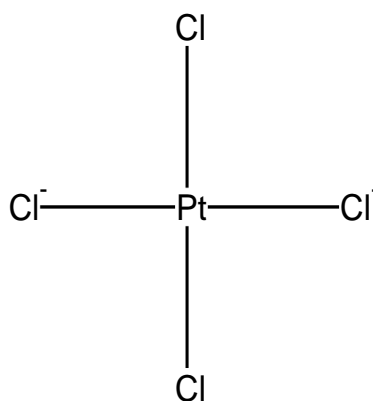
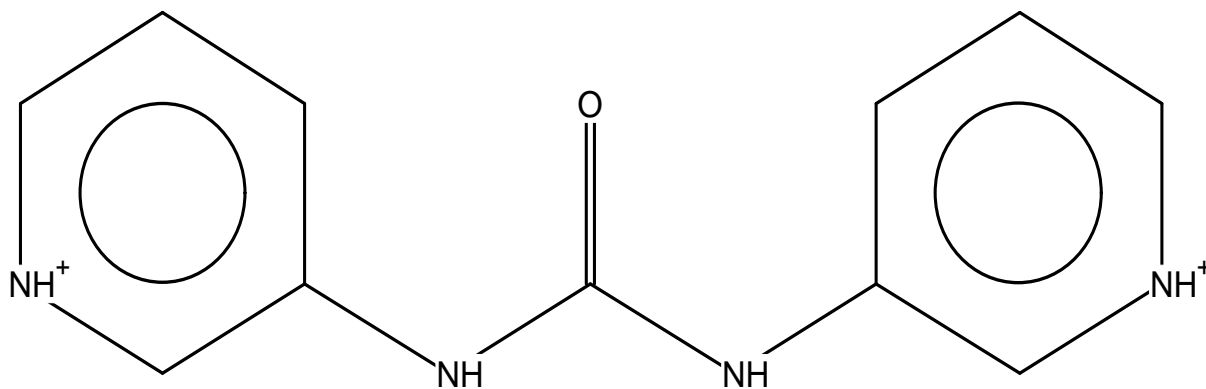
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *Cryst.Growth Des.* ,
6,216

Formula: C₁₁ H₁₂ N₄ O₁²⁺, Cl₄ Pt₁²⁻, H₂ O₁

Compound Name: N,N'-bis(3-Pyridinio)urea tetrachloro-platinum monohydrate

Space Group: P-1 **Cell:** **a** 6.743(0) **b** 8.114(1) **c** 16.254(2)
Space Group No.: 2 **(Å, °)** α 102.91(0) β 90.13(0) γ 106.97(0)

R-Factor (%): 2.39 **Temperature(K):** 278 **Density(g/cm³):** 2.294



H₂O

Search: search2 (Sun Nov 20 19:30:17 2011): Hit 9

LISCAS

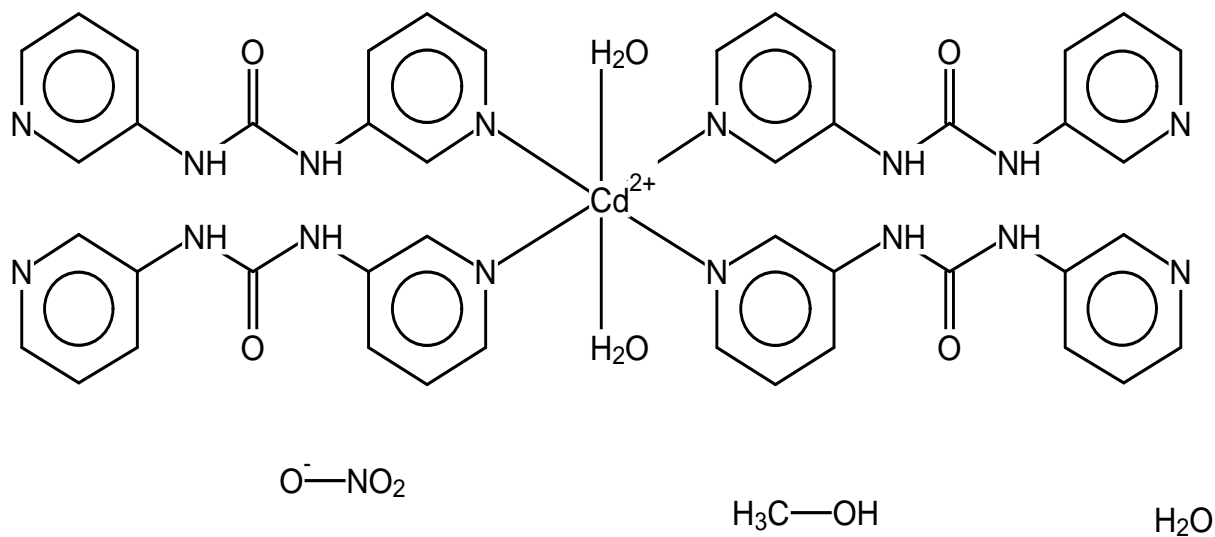
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *Cryst.Growth Des.* ,
7,2096

Formula: $C_{44} H_{44} Cd_1 N_{16} O_6^{2+}, 2(N_1 O_3^{1-}), 2(C_1 H_4 O_1), 6(H_2 O_1)$

Compound Name: Diaqua-tetrakis(N,N'-bis(3-pyridyl)urea-N'')-cadmium(ii) dinitrate
methanol solvate hexahydrate

Space Group: P-1 **Cell:** **a** 9.864(0) **b** 11.262(0) **c** 14.312(1)
Space Group No.: 2 **(Å, °)** α 69.65(0) β 78.81(0) γ 81.99(0)

R-Factor (%): 4.10 **Temperature(K):** 100 **Density(g/cm³):** 1.482



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 10

LISCEW

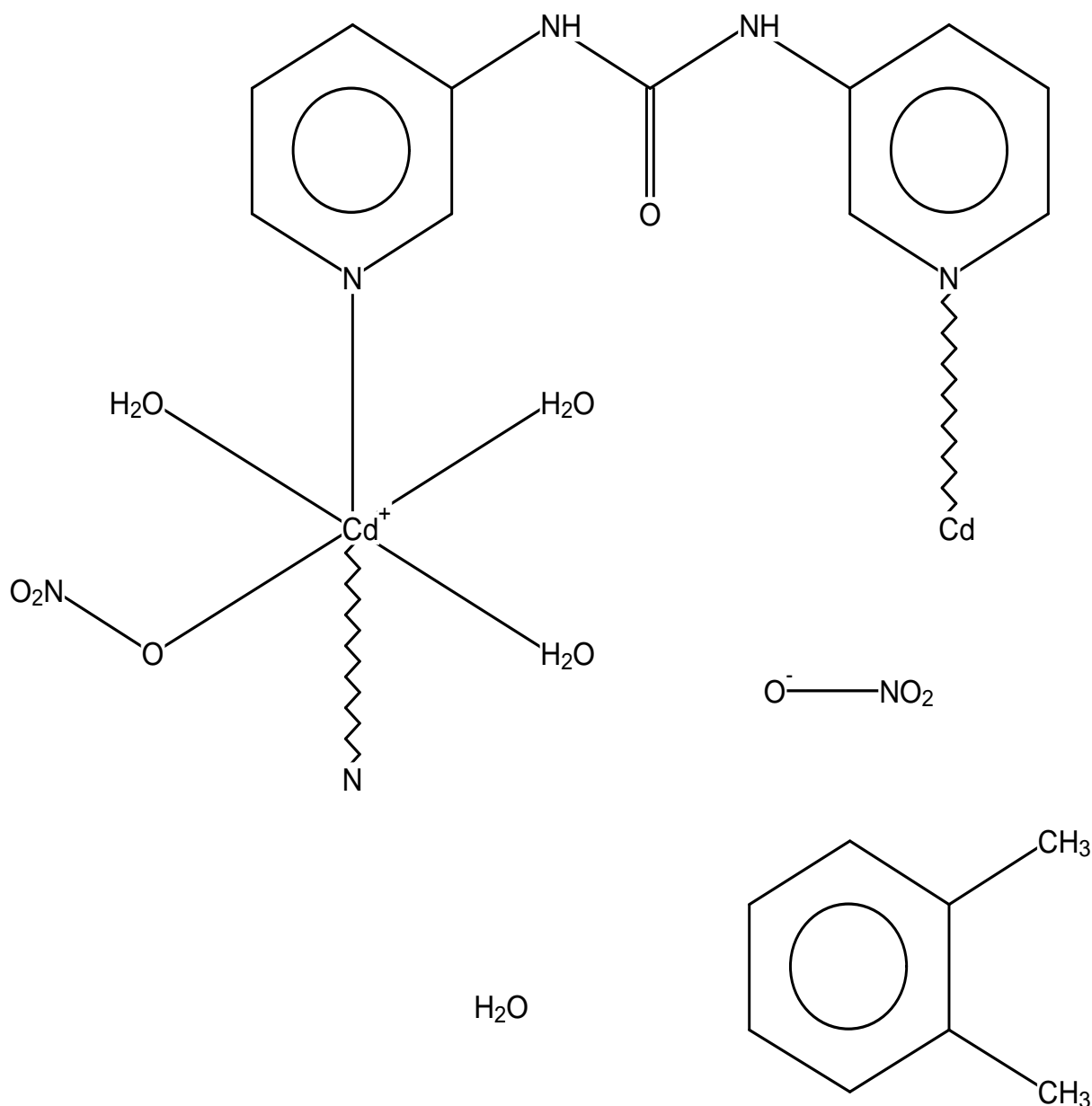
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *Cryst.Growth Des.* ,
7,2096

Formula: $(C_{11}H_{16}Cd_1N_5O_7^{1+})_n, n(N_1O_3^{1-}), 0.5n(C_8H_{10}), n(H_2O_1)$

Compound Name: catena-((μ_2 -N,N'-bis(3-Pyridyl)urea-N'',N''')-triaqua-(nitrate-O)-cadmium nitrate o-xylene solvate monohydrate)

Space Group: P21/n **Cell:** **a** 7.591(0) **b** 17.512(1) **c** 16.596(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 99.38(0) γ 90.00

R-Factor (%): 4.37 **Temperature(K):** 100 **Density(g/cm³):** 1.757



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 11

LISCIA

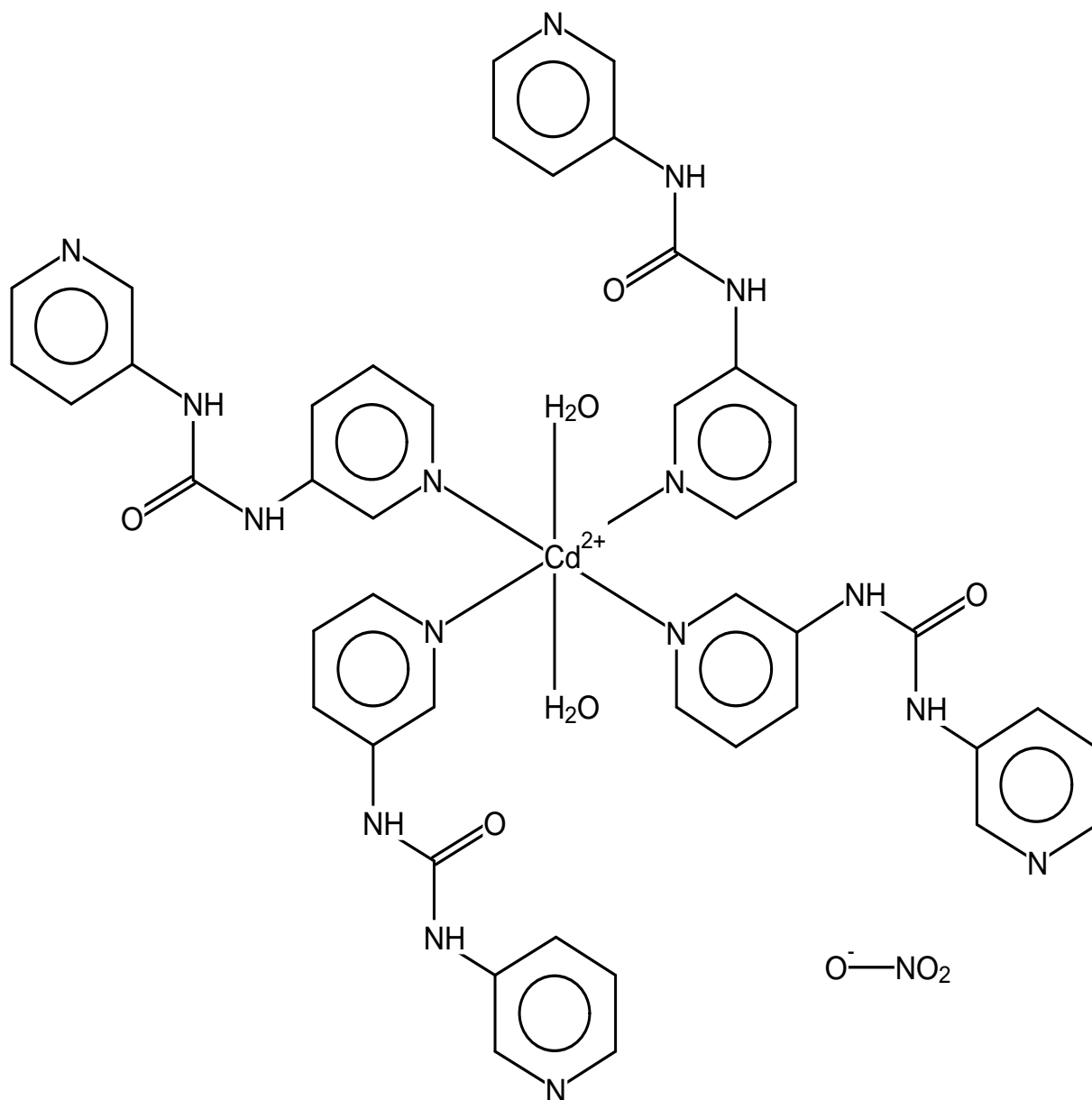
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *Cryst.Growth Des.* ,
7,2096

Formula: $C_{44} H_{44} Cd_1 N_{16} O_6^{2+}, 2(N_1 O_3^{1-})$

Compound Name: Diaqua-tetrakis(N,N'-bis(3-pyridyl)urea-N'')-cadmium(ii) dinitrate

Space Group: C2/c **Cell:** **a** 24.516(3) **b** 15.330(1) **c** 14.531(1)
Space Group No.: 15 **(Å, °)** α 90.00 β 120.43(0) γ 90.00

R-Factor (%): 3.51 **Temperature(K):** 100 **Density(g/cm³):** 1.593



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 12

LISCOG

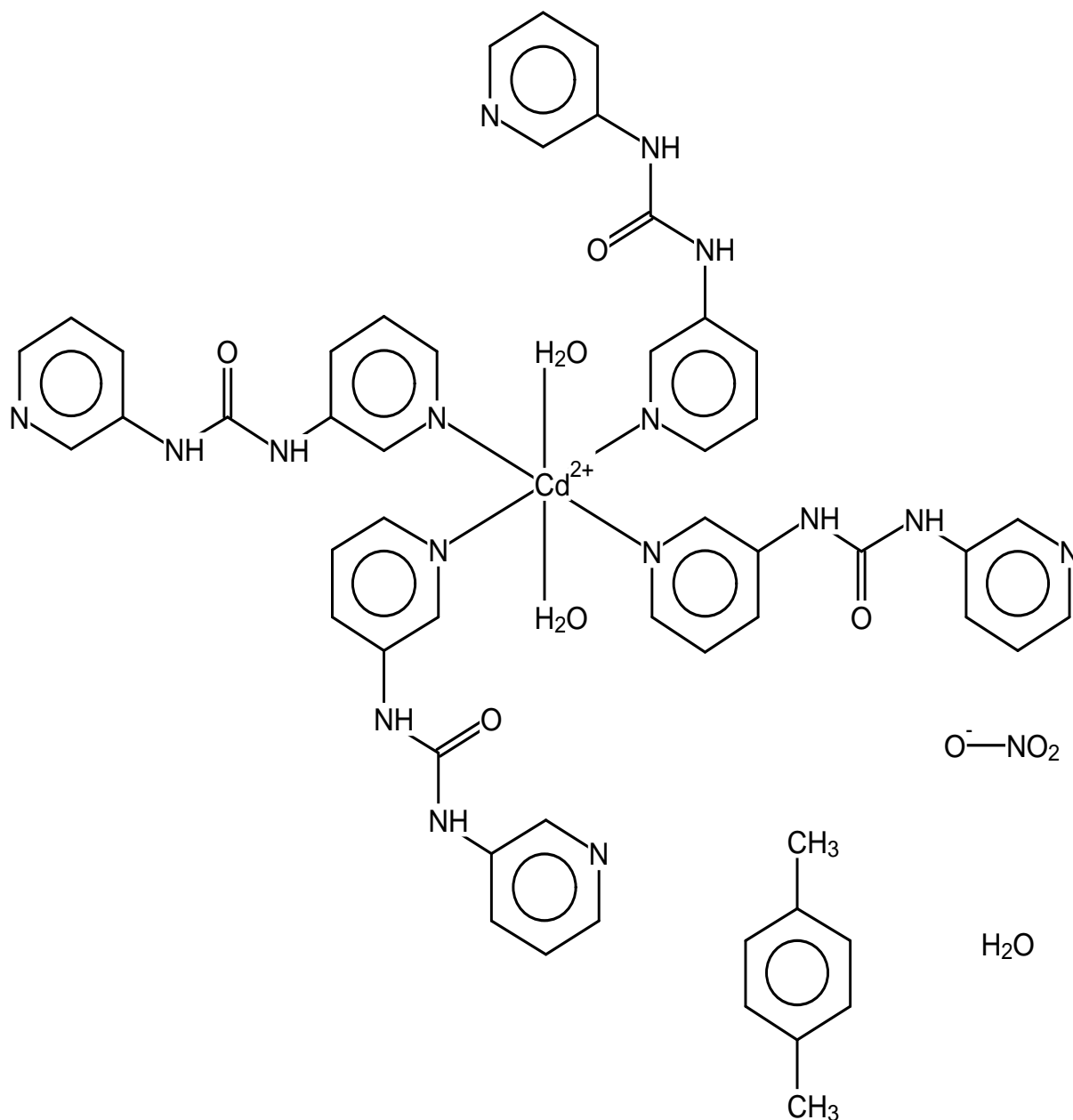
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *Cryst.Growth Des.* ,
7,2096

Formula: $C_{44} H_{44} Cd_1 N_{16} O_6^{2+}, 2(N_1 O_3^{1-}), C_8 H_{10}, 2(H_2 O_1)$

Compound Name: Diaqua-tetrakis(N,N'-bis(3-pyridyl)urea-N'')-cadmium(ii) dinitrate p-xylene solvate dihydrate

Space Group: P-1 **Cell:** **a** 7.435(2) **b** 13.696(4) **c** 14.030(4)
Space Group No.: 2 **(Å, °)** α 102.14(0) β 92.28(0) γ 92.16(0)

R-Factor (%): 4.89 **Temperature(K):** 150 **Density(g/cm³):** 1.515



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 13

LISCUM

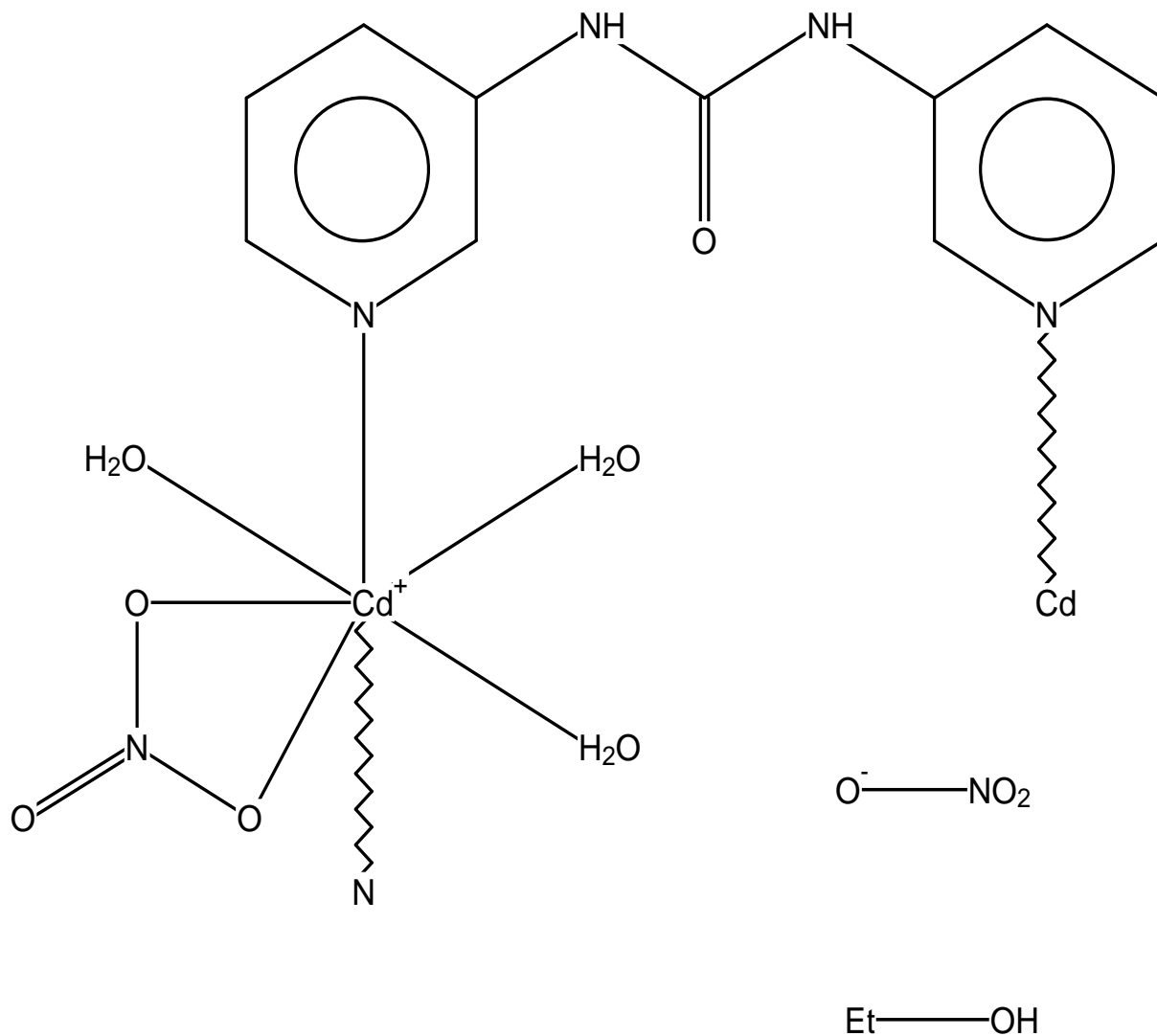
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *Cryst.Growth Des.* ,
7,2096

Formula: (C₁₁ H₁₆ Cd₁ N₅ O₇¹⁺)_n,n(N₁ O₃¹⁻),n(C₂ H₆ O₁)

Compound Name: catena-((μ₂-N,N'-bis(3-Pyridyl)urea-N'',N''')-triaqua-(nitrate-O,O')-
cadmium nitrate ethanol solvate)

Space Group: Pbcn **Cell:** **a** 16.212(4) **b** 18.776(5) **c** 13.907(4)
Space Group No.: 60 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 7.48 **Temperature(K):** 100 **Density(g/cm³):** 1.728



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 14

LISDAT

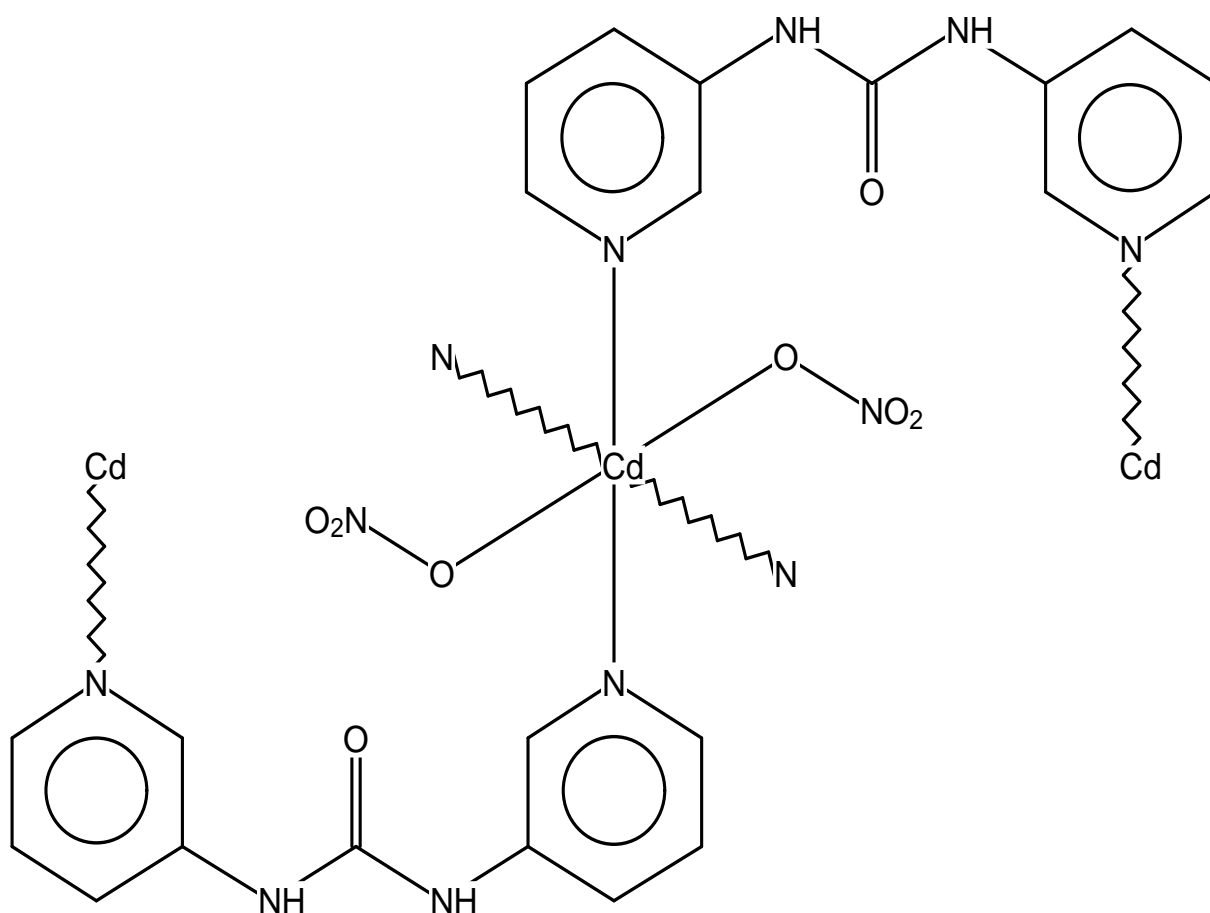
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *Cryst.Growth Des.* ,
7,2096

Formula: (C₂₂ H₂₀ Cd₁ N₁₀ O₈)_n

Compound Name: catena-(bis(μ₂-N,N'-bis(3-Pyridyl)urea-N'',N''')-bis(nitrato-O)-cadmium)

Space Group: P21/n **Cell:** **a** 9.622(1) **b** 10.242(1) **c** 12.840(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 95.36(0) γ 90.00

R-Factor (%): 3.31 **Temperature(K):** 100 **Density(g/cm³):** 1.753



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 15

NAVWIR

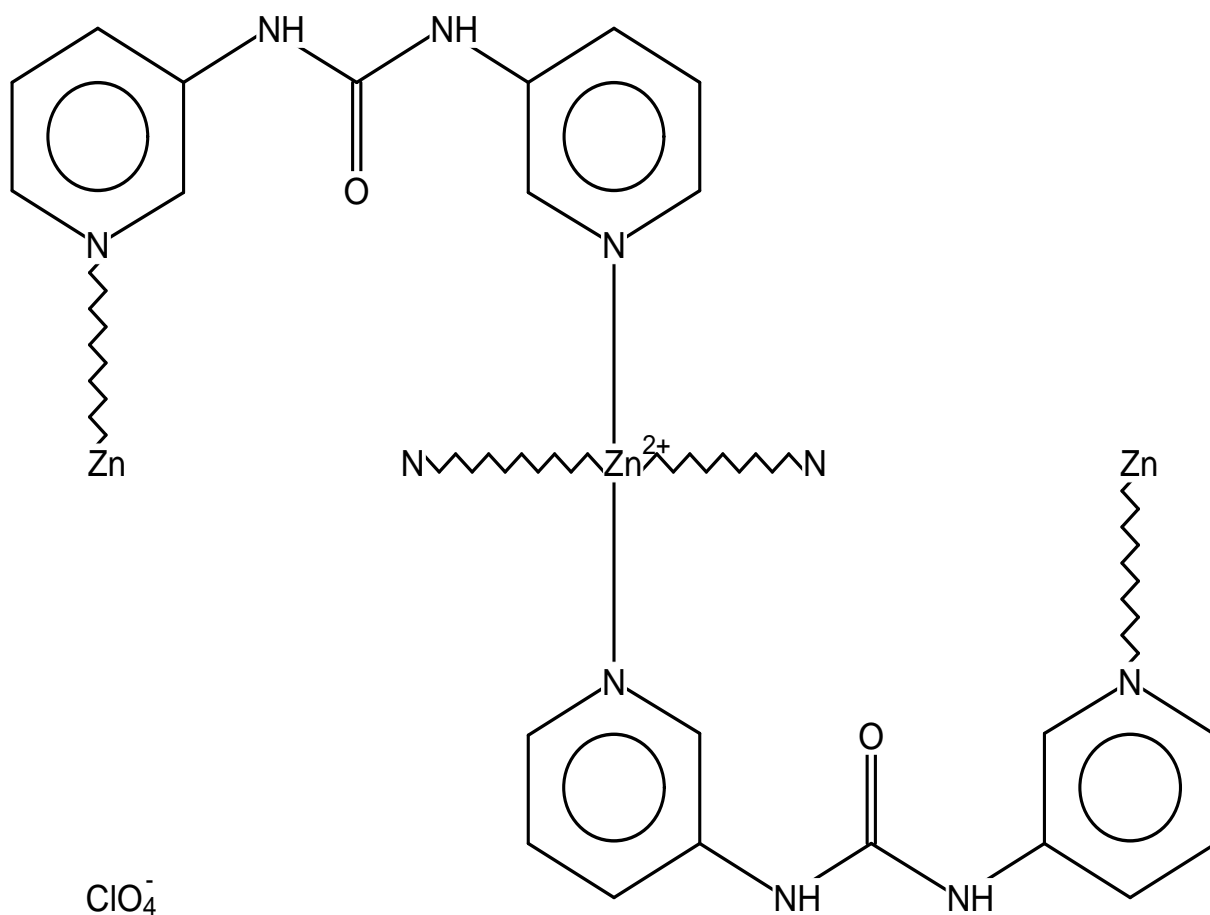
Reference: D.K.Kumar, D.A.Jose, A.Das, P.Dastidar (2005)
Inorg.Chem. ,**44**,6933

Formula: (C₂₂ H₂₀ N₈ O₂ Zn₁ ²⁺)_n,2n(Cl₁ O₄ ¹⁻)

Compound Name: catena-(μ₂-bis(N,N'-bis(3-Pyridyl)urea)-zinc(ii) diperchlorate)

Space Group: P42/n **Cell:** **a** 12.054(1) **b** 12.054(1) **c** 9.280(1)
Space Group No.: 86 **(Å, °)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 5.80 **Temperature(K):** 298 **Density(g/cm³):** 1.706



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 16

NAVWIR01

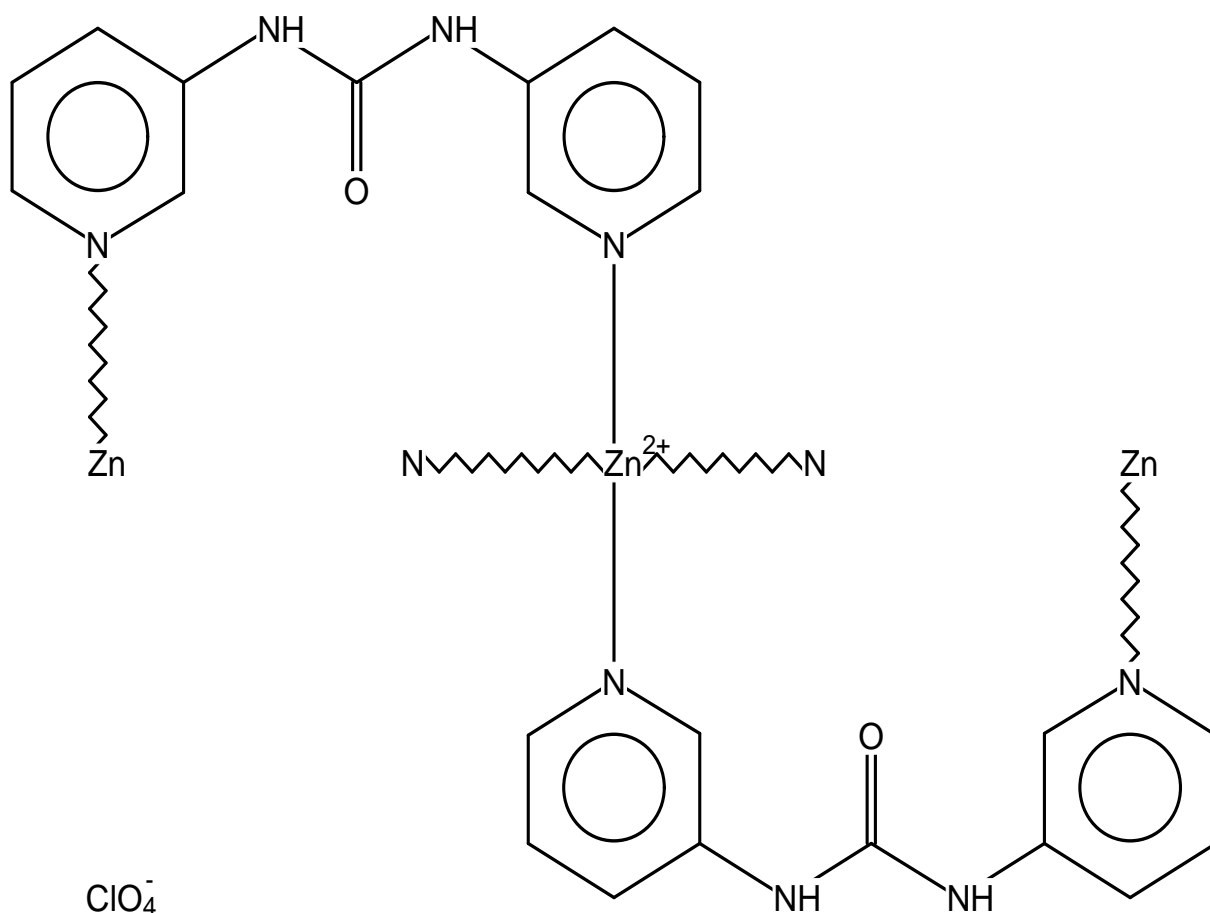
Reference: D.K.Kumar, D.A.Jose, A.Das, P.Dastidar (2005)
Inorg.Chem. ,**44**,6933

Formula: (C₂₂ H₂₀ N₈ O₂ Zn₁²⁺)_n,2n(Cl₁ O₄¹⁻)

Compound Name: catena-(bis(μ₂-N,N'-bis(3-Pyridyl)urea)-zinc(ii) diperchlorate)

Space Group: I41/a **Cell:** **a** 16.899(0) **b** 16.899(0) **c** 18.460(1)
Space Group No.: 88 **(Å, °)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 2.51 **Temperature(K):** 100 **Density(g/cm³):** 1.746



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 17

NAVWIR02

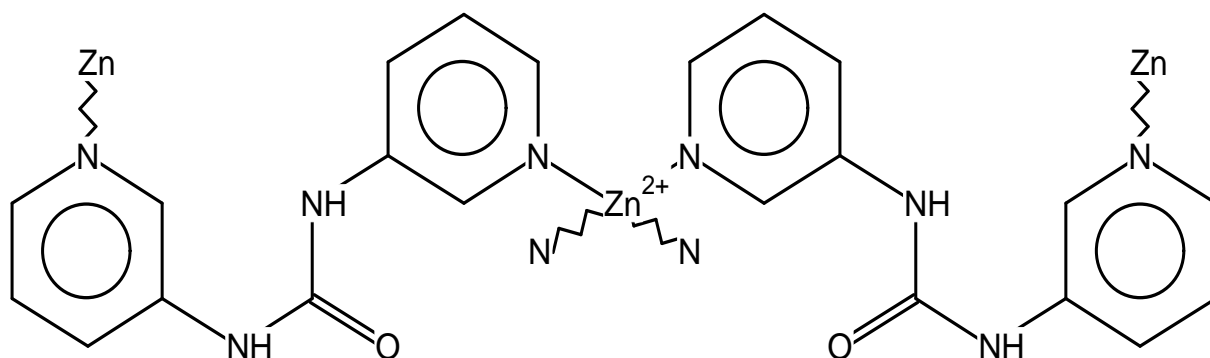
Reference: R.Custelcean, B.A.Moyer, V.S.Bryantsev, B.P.Hay (2006)
Cryst.Growth Des. ,6,555

Formula: (C₂₂ H₂₀ N₈ O₂ Zn₁ ²⁺)_n,2n(Cl₁ O₄ ¹⁻)

Compound Name: catena-(bis(μ₂-N,N'-bis(3-Pyridyl)urea-N,N')-zinc diperchlorate)

Space Group: I41/a **Cell:** **a** 16.946(1) **b** 16.946(1) **c** 18.477(3)
Space Group No.: 88 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 6.32 **Temperature(K):** 173 **Density(g/cm³):** 1.734



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 18

NEMJOF

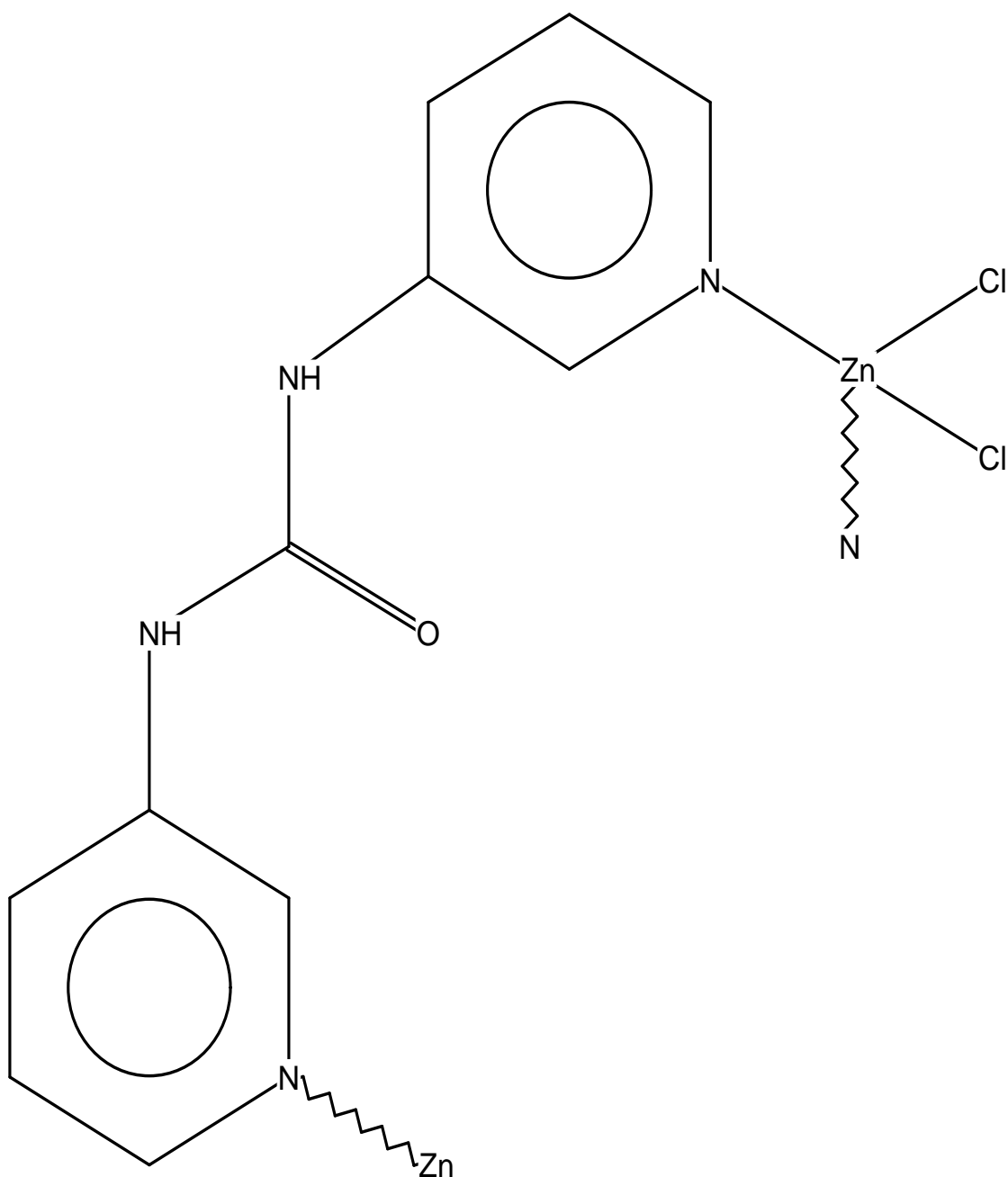
Reference: R.Custelcean, T.H.Haverlock, B.A.Moyer (2006)
Inorg.Chem. ,**45**,6446

Formula: (C₁₁ H₁₀ Cl₂ N₄ O₁ Zn₁)_n

Compound Name: catena-((μ₂-N,N'-bis(3-pyridyl)urea)-dichloro-zinc)

Space Group: Fdd2 **Cell:** **a** 18.230(2) **b** 9.829(1) **c** 15.879(1)
Space Group No.: 43 **(Å, °)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 1.52 **Temperature(K):** 173 **Density(g/cm³):** 1.636



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 19

NEMJOF01

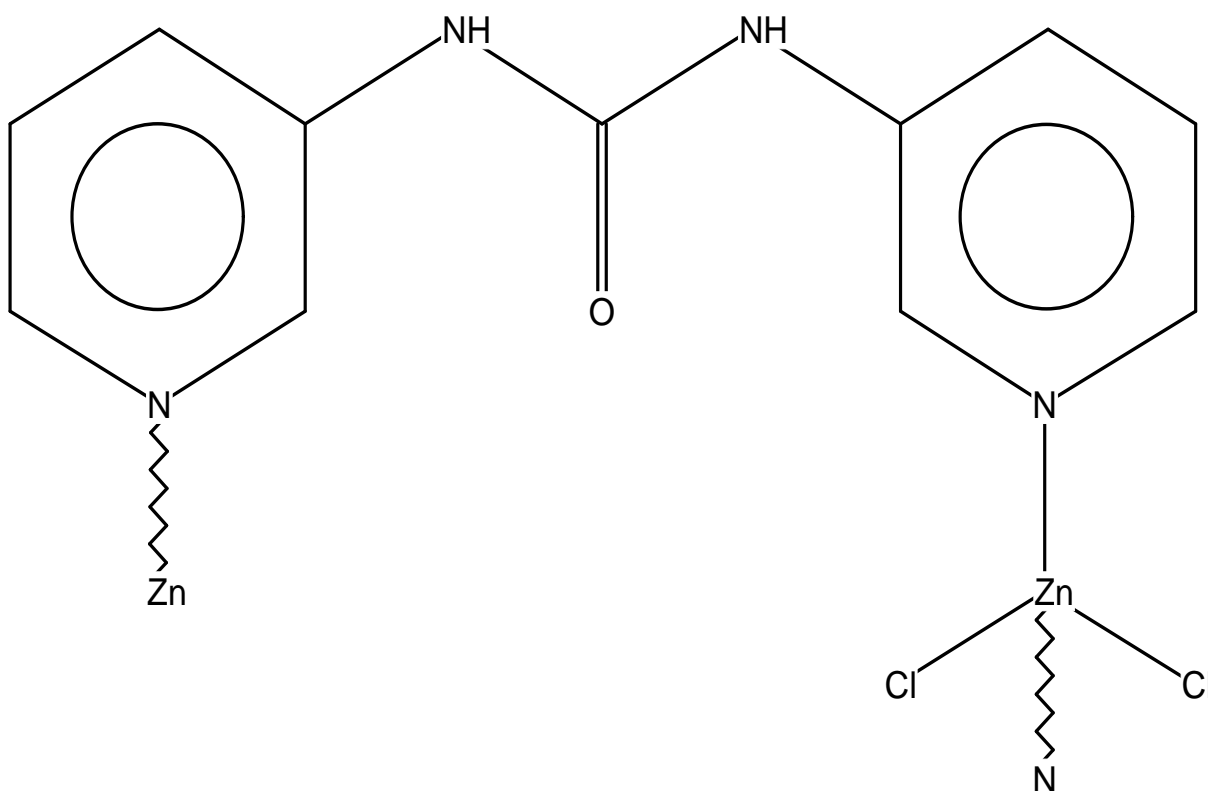
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *CrystEngComm*, **8**, 805

Formula: (C₁₁ H₁₀ Cl₂ N₄ O₁ Zn₁)_n

Compound Name: catena-((μ₂-N,N'-bis(3-Pyridyl)urea)-dichloro-zinc(ii))

Space Group: Fdd2 **Cell:** **a** 18.371(3) **b** 9.867(1) **c** 15.866(3)
Space Group No.: 43 (**Å, °**) **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 3.01 **Temperature(K):** 100 **Density(g/cm³):** 1.619



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 20

NEMJUL

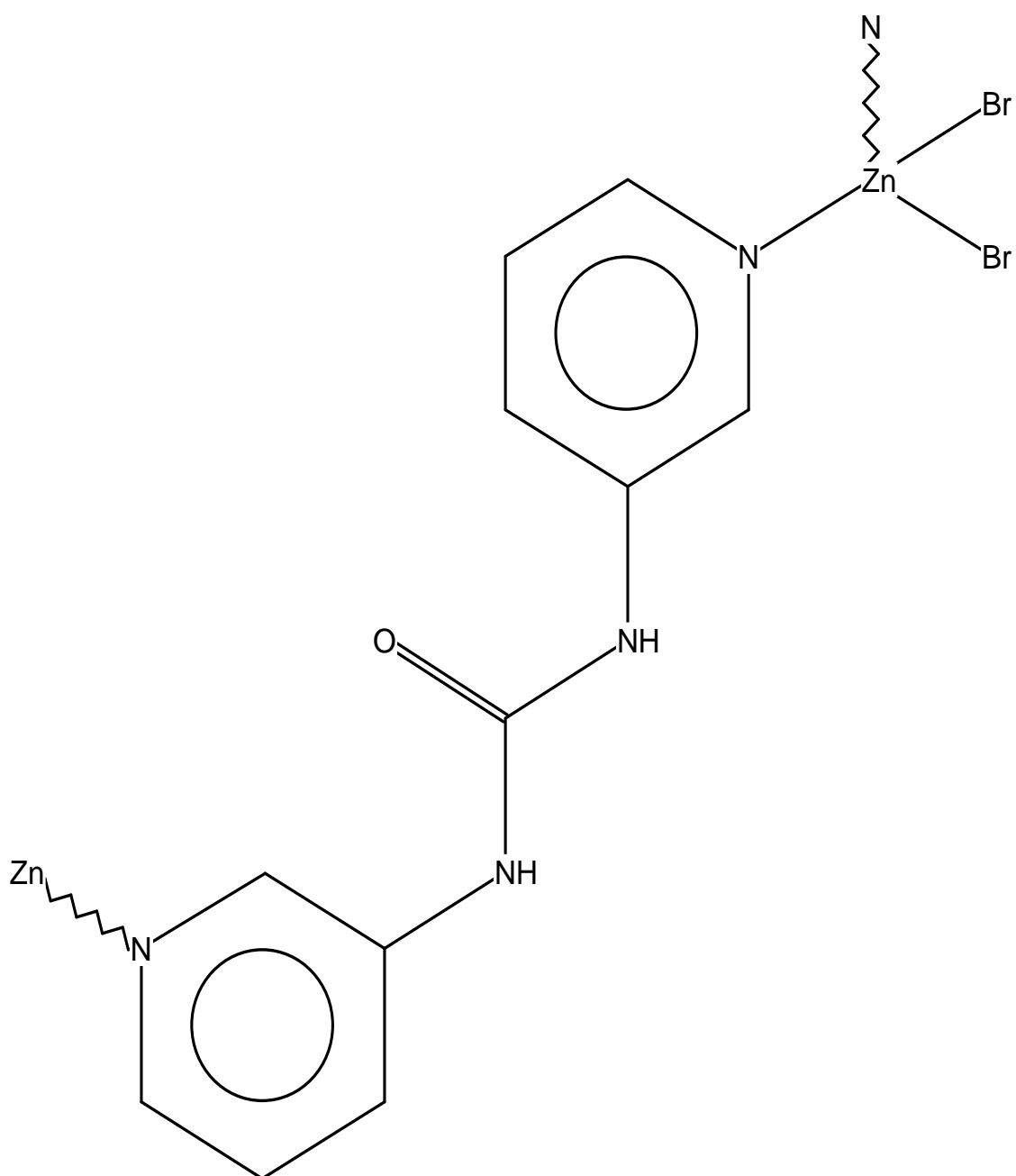
Reference: R.Custelcean, T.H.Haverlock, B.A.Moyer (2006)
Inorg.Chem. ,**45**,6446

Formula: (C₁₁ H₁₀ Br₂ N₄ O₁ Zn₁)_n

Compound Name: catena-((μ₂-N,N'-bis(3-pyridyl)urea)-dibromo-zinc)

Space Group: P21/c **Cell:** **a** 10.060(1) **b** 16.763(1) **c** 8.420(0)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 104.00(0) **γ** 90.00

R-Factor (%): 1.90 **Temperature(K):** 273 **Density(g/cm³):** 2.119



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 21

NEMKAS

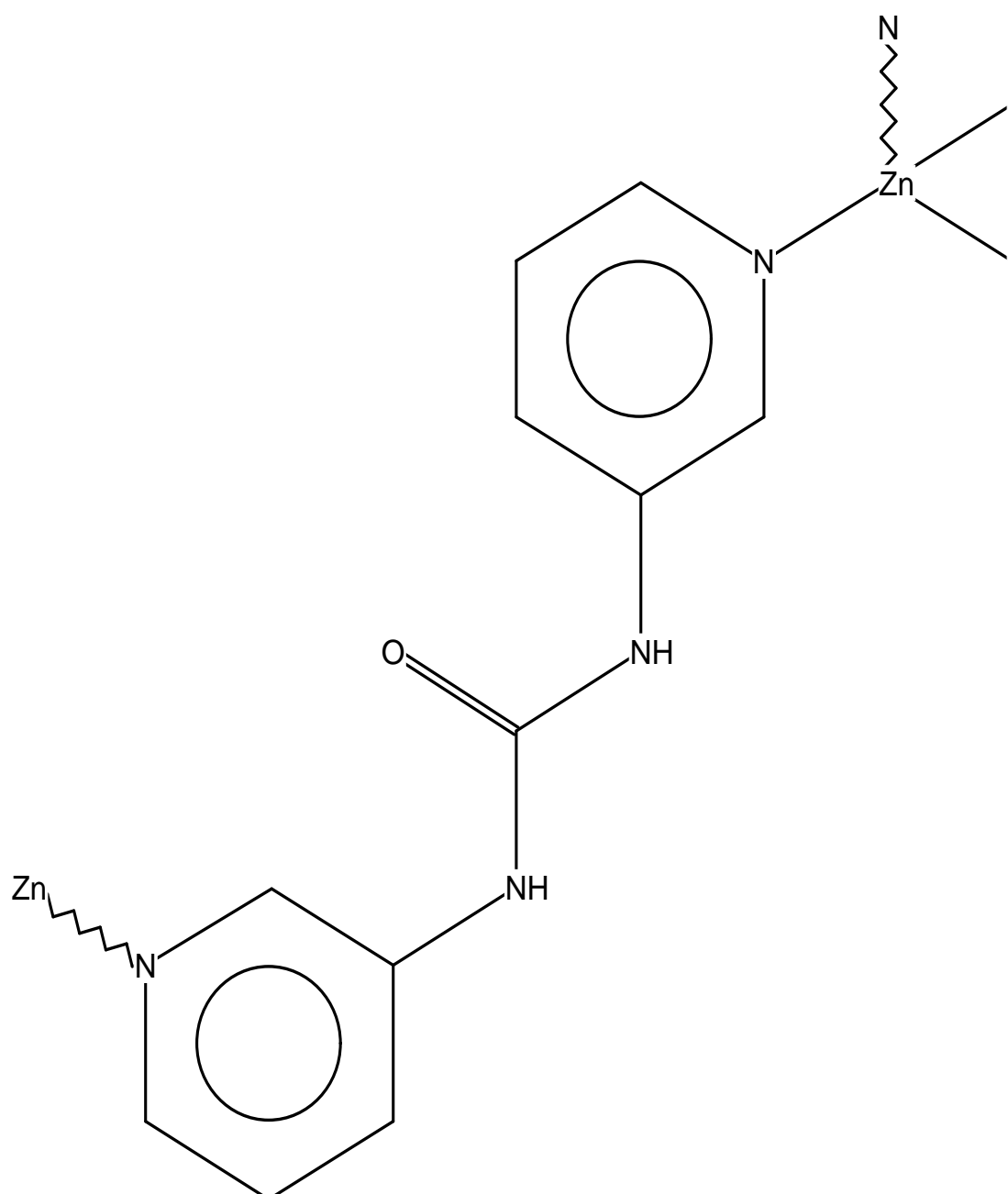
Reference: R.Custelcean, T.H.Haverlock, B.A.Moyer (2006)
Inorg.Chem. ,**45**,6446

Formula: (C₁₁ H₁₀ I₂ N₄ O₁ Zn₁)_n

Compound Name: catena-((μ₂-N,N'-bis(3-pyridyl)urea)-diiodo-zinc)

Space Group: P21/c **Cell:** **a** 10.150(1) **b** 17.116(1) **c** 8.758(1)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 104.88(0) **γ** 90.00

R-Factor (%): 1.95 **Temperature(K):** 173 **Density(g/cm³):** 2.410



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 22

NEMKEW

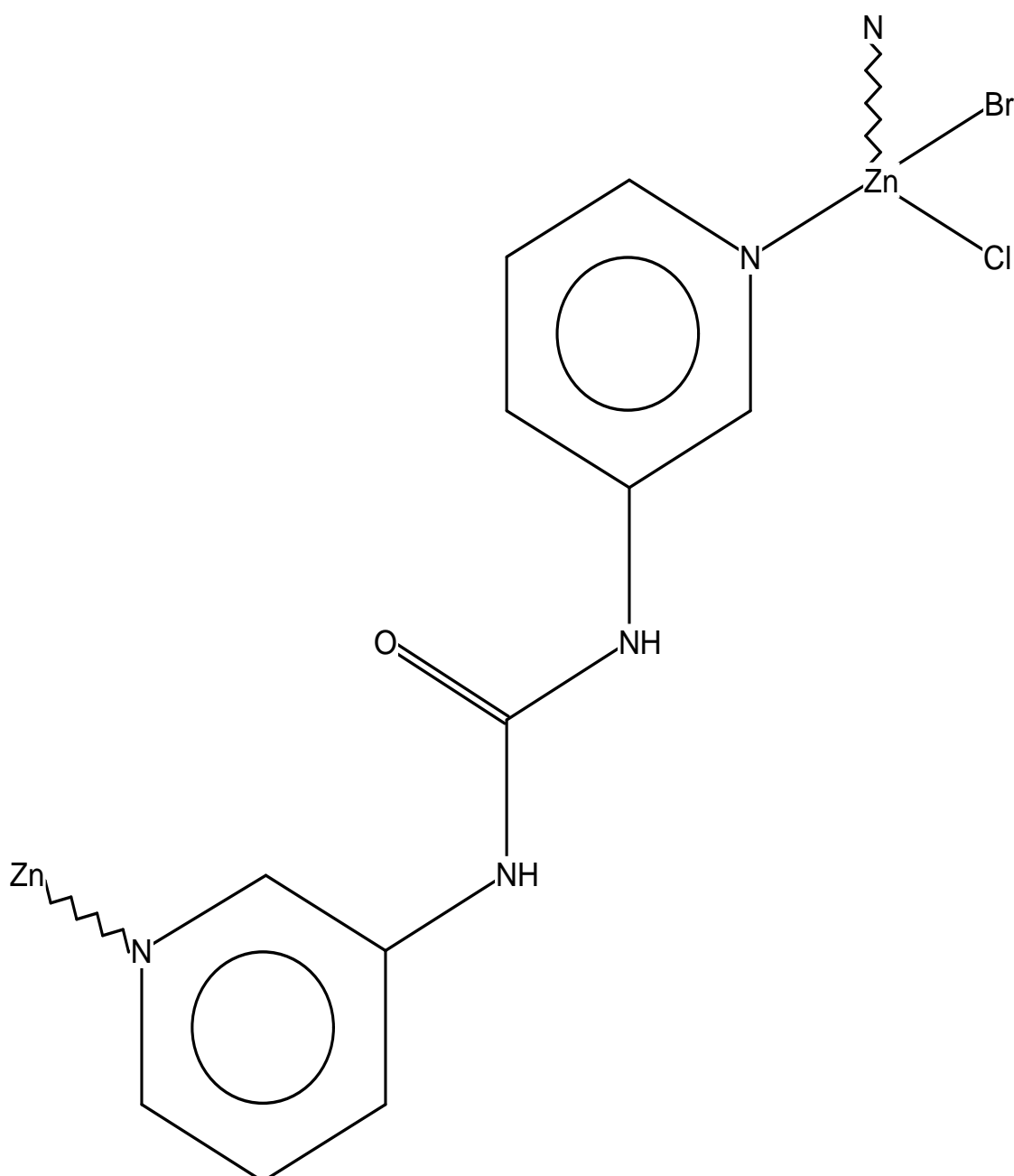
Reference: R.Custelcean, T.H.Haverlock, B.A.Moyer (2006)
Inorg.Chem. ,**45**,6446

Formula: (C₁₁ H₁₀ Br₁ Cl₁ N₄ O₁ Zn₁)_n

Compound Name: catena-((μ₂-N,N'-bis(3-pyridyl)urea)-bromo-chloro-zinc)

Space Group: P21/c **Cell:** **a** 10.030(1) **b** 16.765(1) **c** 8.359(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 105.10(1) γ 90.00

R-Factor (%): 2.66 **Temperature(K):** 173 **Density(g/cm³):** 1.933



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 23

NEMKIA

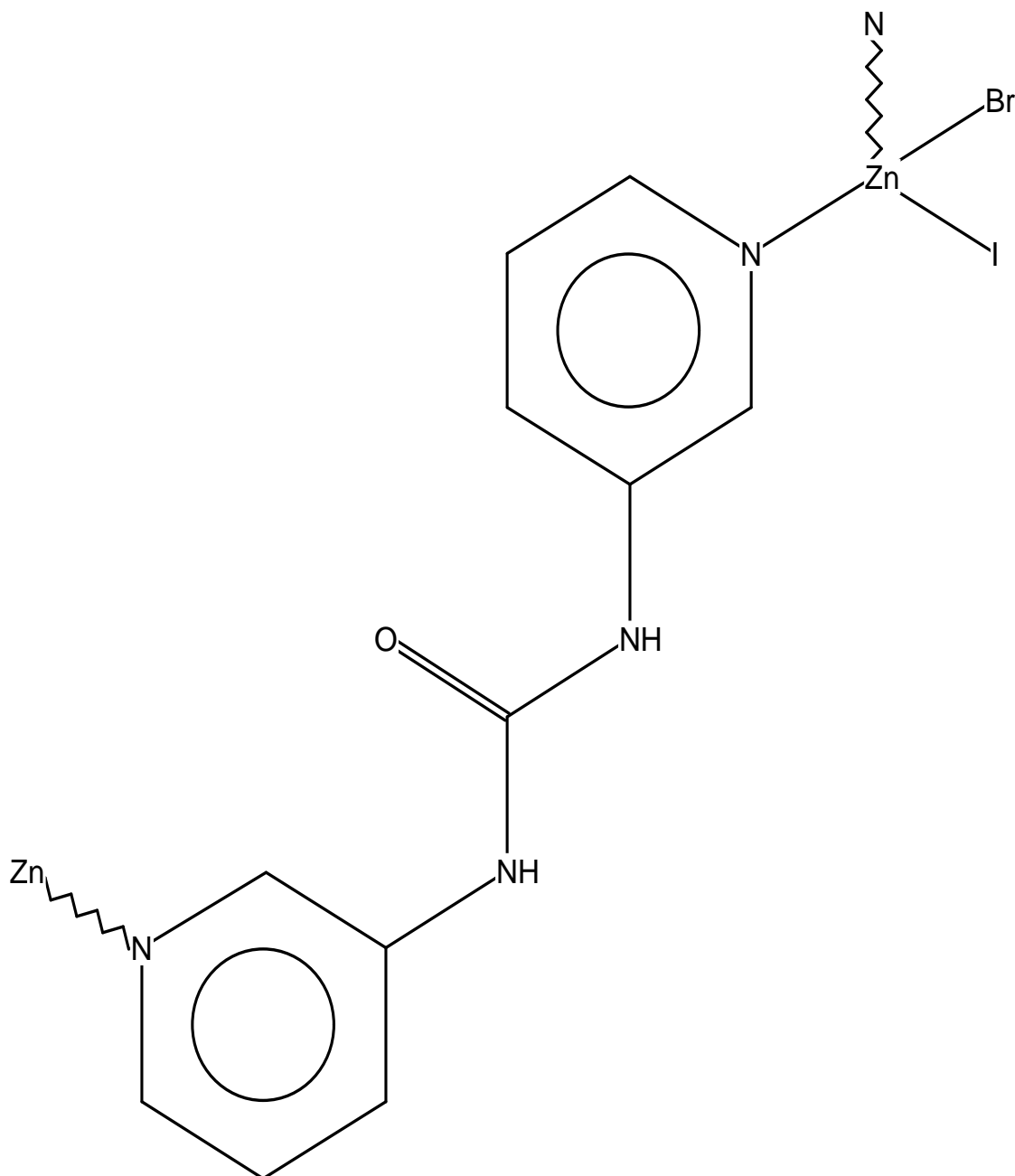
Reference: R.Custelcean, T.H.Haverlock, B.A.Moyer (2006)
Inorg.Chem. ,**45**,6446

Formula: (C₁₁ H₁₀ Br₁ I₁ N₄ O₁ Zn₁)_n

Compound Name: catena-((μ₂-N,N'-bis(3-pyridyl)urea)-bromo-iodo-zinc)

Space Group: P21/c **Cell:** **a** 10.094(0) **b** 17.029(1) **c** 8.585(0)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 104.66(0) **γ** 90.00

R-Factor (%): 2.78 **Temperature(K):** 173 **Density(g/cm³):** 2.263



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 24

NEMKOG

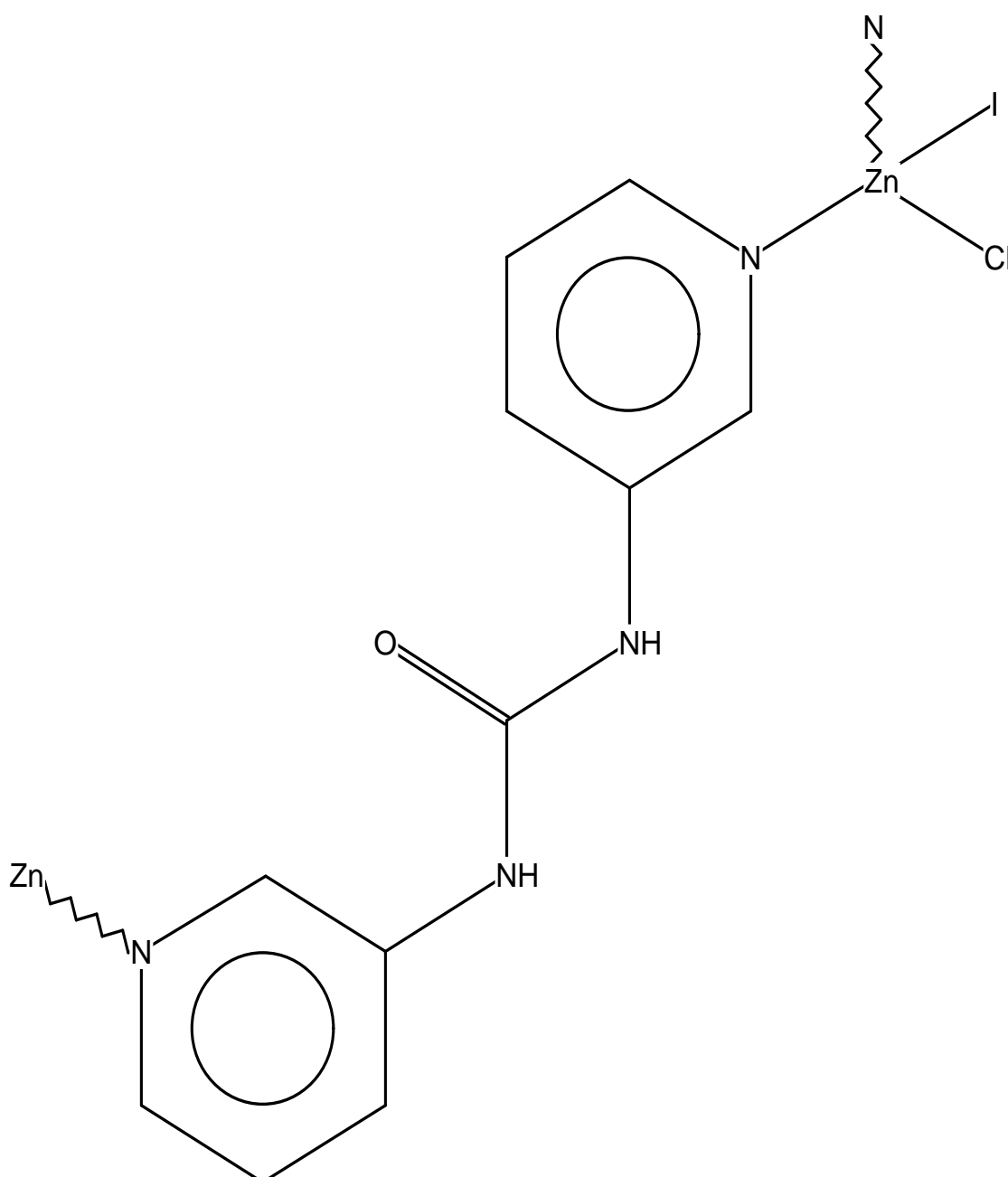
Reference: R.Custelcean, T.H.Haverlock, B.A.Moyer (2006)
Inorg.Chem. ,**45**,6446

Formula: (C₁₁ H₁₀ Cl₁ I₁ N₄ O₁ Zn₁)_n

Compound Name: catena-((μ₂-N,N'-bis(3-pyridyl)urea)-chloro-iodo-zinc)

Space Group: P21/c **Cell:** **a** 9.997(0) **b** 17.186(1) **c** 8.371(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 105.26(0) γ 90.00

R-Factor (%): 4.49 **Temperature(K):** 173 **Density(g/cm³):** 2.116



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 25

NERNOO

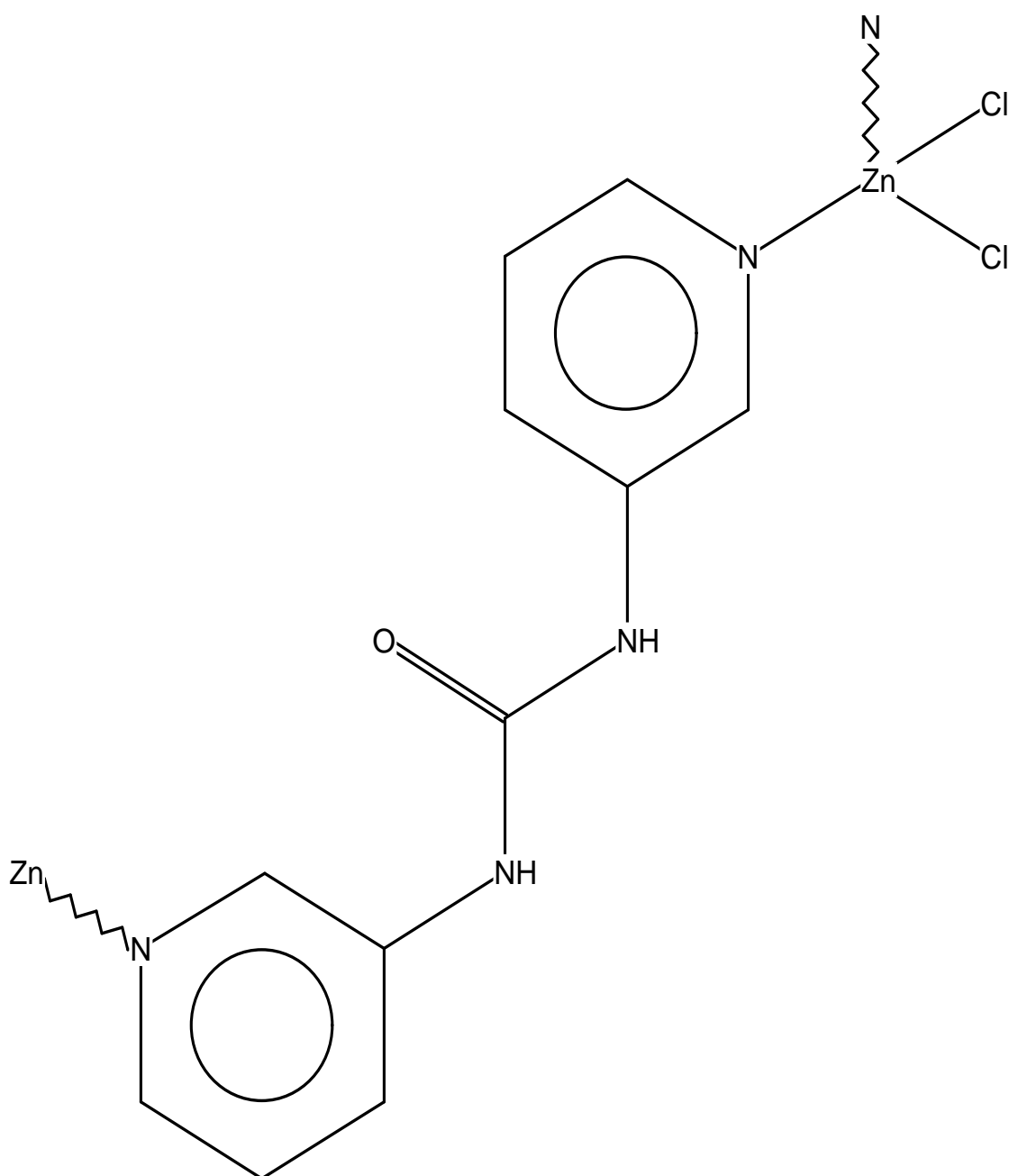
Reference: R.Custelcean, T.H.Haverlock, B.A.Moyer (2006)
Inorg.Chem. ,**45**,6446

Formula: (C₁₁ H₁₀ Cl₂ N₄ O₁ Zn₁)_n

Compound Name: catena-((μ₂-N,N'-bis(3-pyridyl)urea)-dichloro-zinc)

Space Group: Fdd2 **Cell:** **a** 18.367(1) **b** 9.878(0) **c** 15.937(1)
Space Group No.: 43 **(Å, °)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 1.55 **Temperature(K):** 173 **Density(g/cm³):** 1.610



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PEFGUD

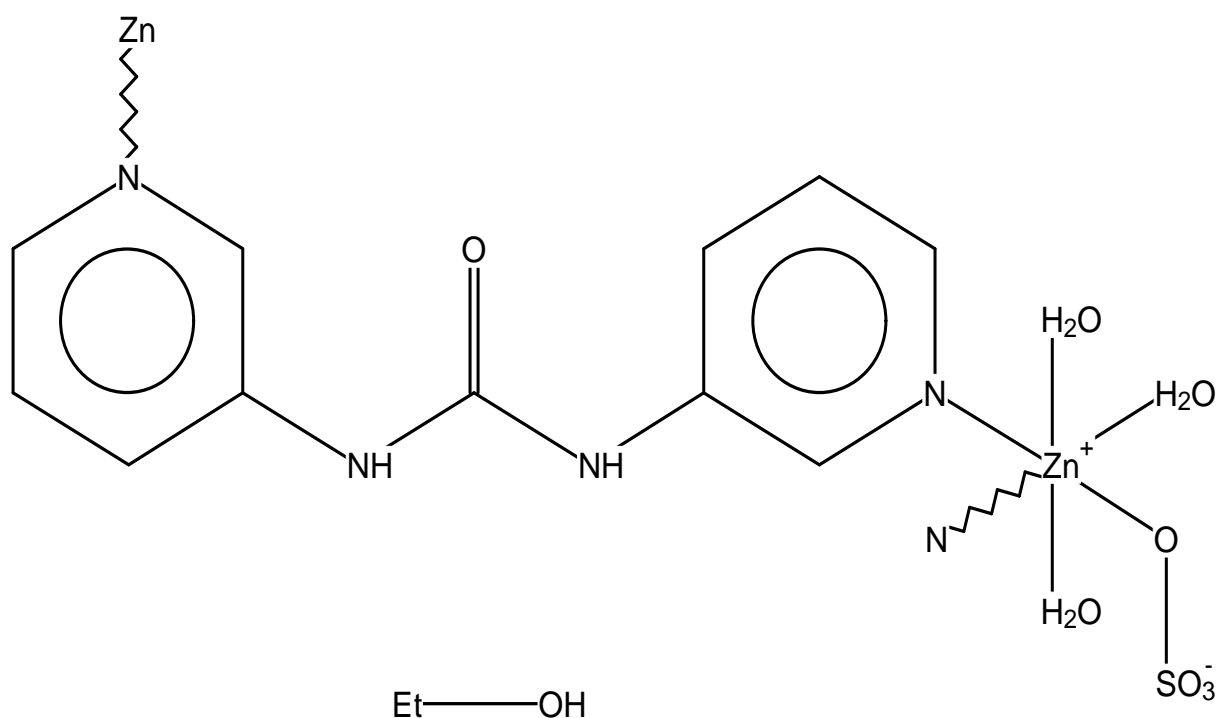
Reference: R.Custelcean, B.A.Moyer, V.S.Bryantsev, B.P.Hay (2006)
Cryst.Growth Des. ,6,555

Formula: (C₁₁ H₁₆ N₄ O₈ S₁ Zn₁)_n,n(C₂ H₆ O₁)

Compound Name: catena-((μ₂-N,N'-bis(3-Pyridyl)urea)-trihydrato-(sulfato-O)-zinc ethanol solvate)

Space Group: P21/n **Cell:** **a** 7.743(1) **b** 11.068(1) **c** 21.559(3)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 96.91(0) **γ** 90.00

R-Factor (%): 4.86 **Temperature(K):** 173 **Density(g/cm³):** 1.723



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 27

PEFHAK

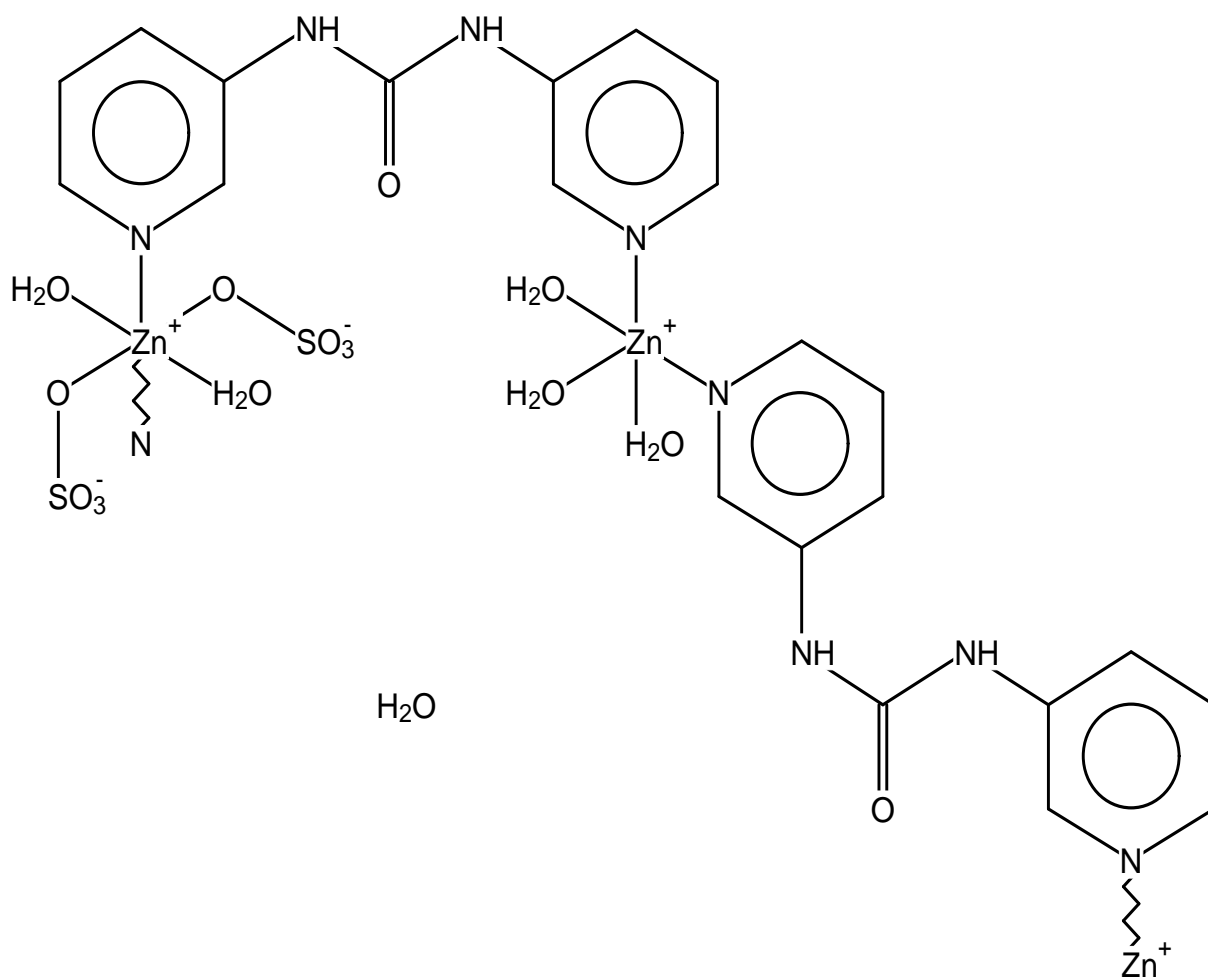
Reference: R.Custelcean, B.A.Moyer, V.S.Bryantsev, B.P.Hay (2006)
Cryst.Growth Des. ,6,555

Formula: $(C_{22} H_{30} N_8 O_{15} S_2 Zn_2)_n \cdot 7n(H_2 O)_1$

Compound Name: catena-(bis(μ_2 -N,N'-bis(3-Pyridyl)urea-N,N')-penta-aqua-bis(sulfato-O)-di-zinc heptahydrate)

Space Group: P2/c **Cell:** **a** 8.489(1) **b** 10.584(1) **c** 20.733(4)
Space Group No.: 13 **(Å, °)** α 90.00 β 96.62(0) γ 90.00

R-Factor (%): 3.81 **Temperature(K):** 173 **Density(g/cm³):** 1.737



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 28

PEFHEO

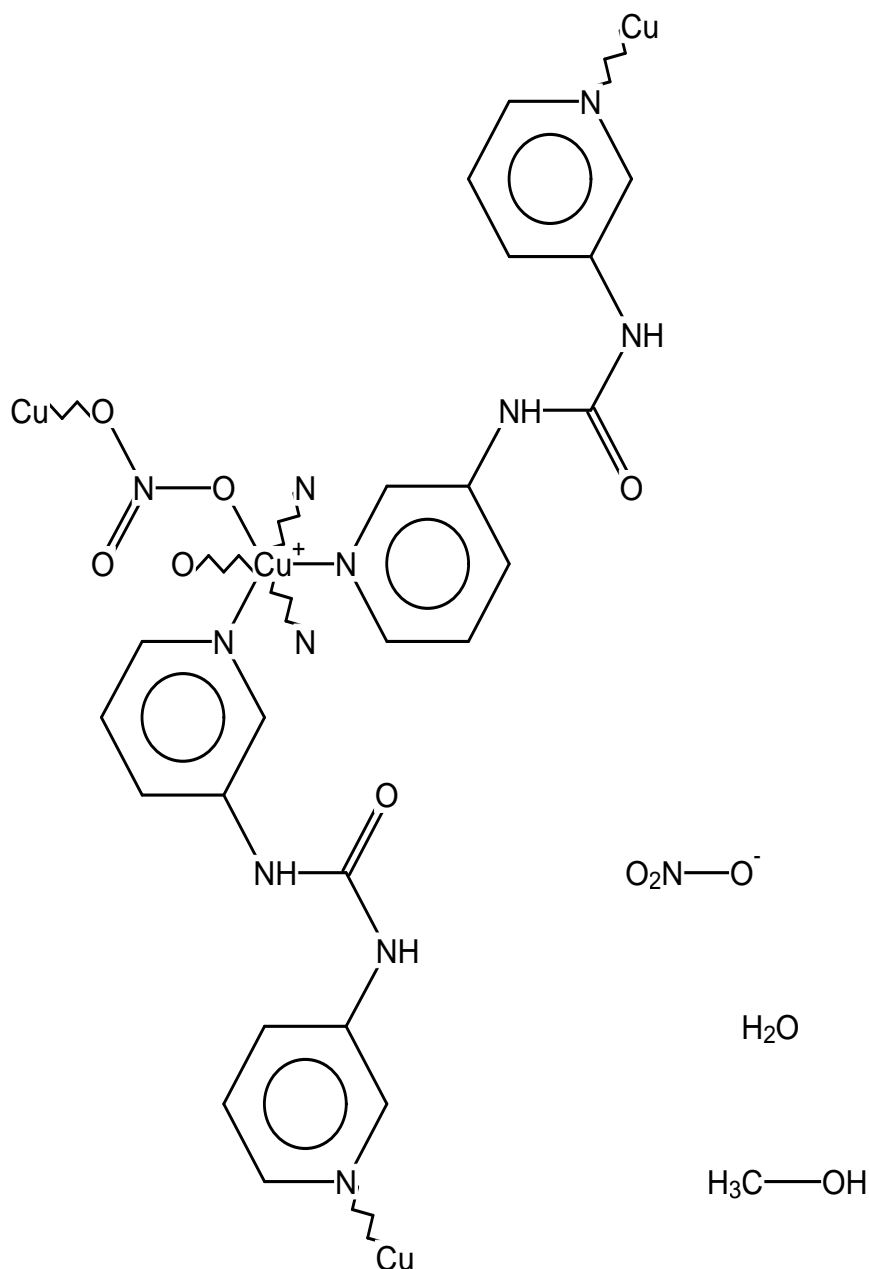
Reference: R.Custelcean, B.A.Moyer, V.S.Bryantsev, B.P.Hay (2006)
Cryst.Growth Des. ,6,555

Formula: $(C_{22} H_{20} Cu_1 N_9 O_5^{1+})_n, n(N_1 O_3^{1-}), 0.5n(C_1 H_4 O_1), 2.5n(H_2 O_1)$

Compound Name: catena-(bis(μ_2 -N,N'-bis(3-Pyridyl)urea)-(μ_2 -nitrate-O,O')-copper(i) nitrate methanol solvate hydrate)

Space Group: P21/c **Cell:** **a** 6.722(0) **b** 26.649(4) **c** 17.515(2)
Space Group No.: 14 **(Å, °)** α 90.00 β 92.45(0) γ 90.00

R-Factor (%): 6.79 **Temperature(K):** 173 **Density(g/cm³):** 1.435



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 29

PEFHIS

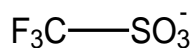
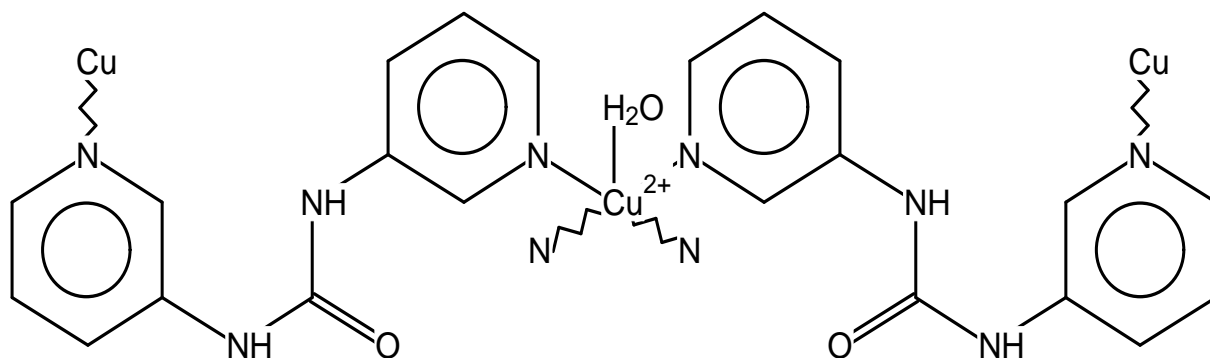
Reference: R.Custelcean, B.A.Moyer, V.S.Bryantsev, B.P.Hay (2006)
Cryst.Growth Des. ,6,555

Formula: $(C_{22} H_{22} Cu_1 N_8 O_3^{2+})_n, 2n(C_1 F_3 O_3 S_1^{-1}), n(H_2 O_1)$

Compound Name: catena-(bis(μ_2 -N,N'-bis(3-Pyridyl)urea-N,N')-aqua-copper(i)
bis(trifluoromethanesulfonate) monohydrate)

Space Group: P21/c **Cell:** **a** 9.124(0) **b** 18.127(1) **c** 19.586(2)
Space Group No.: 14 **(Å, °)** α 90.00 β 94.71(0) γ 90.00

R-Factor (%): 4.50 **Temperature(K):** 173 **Density(g/cm³):** 1.700



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 30

PEFHIS01

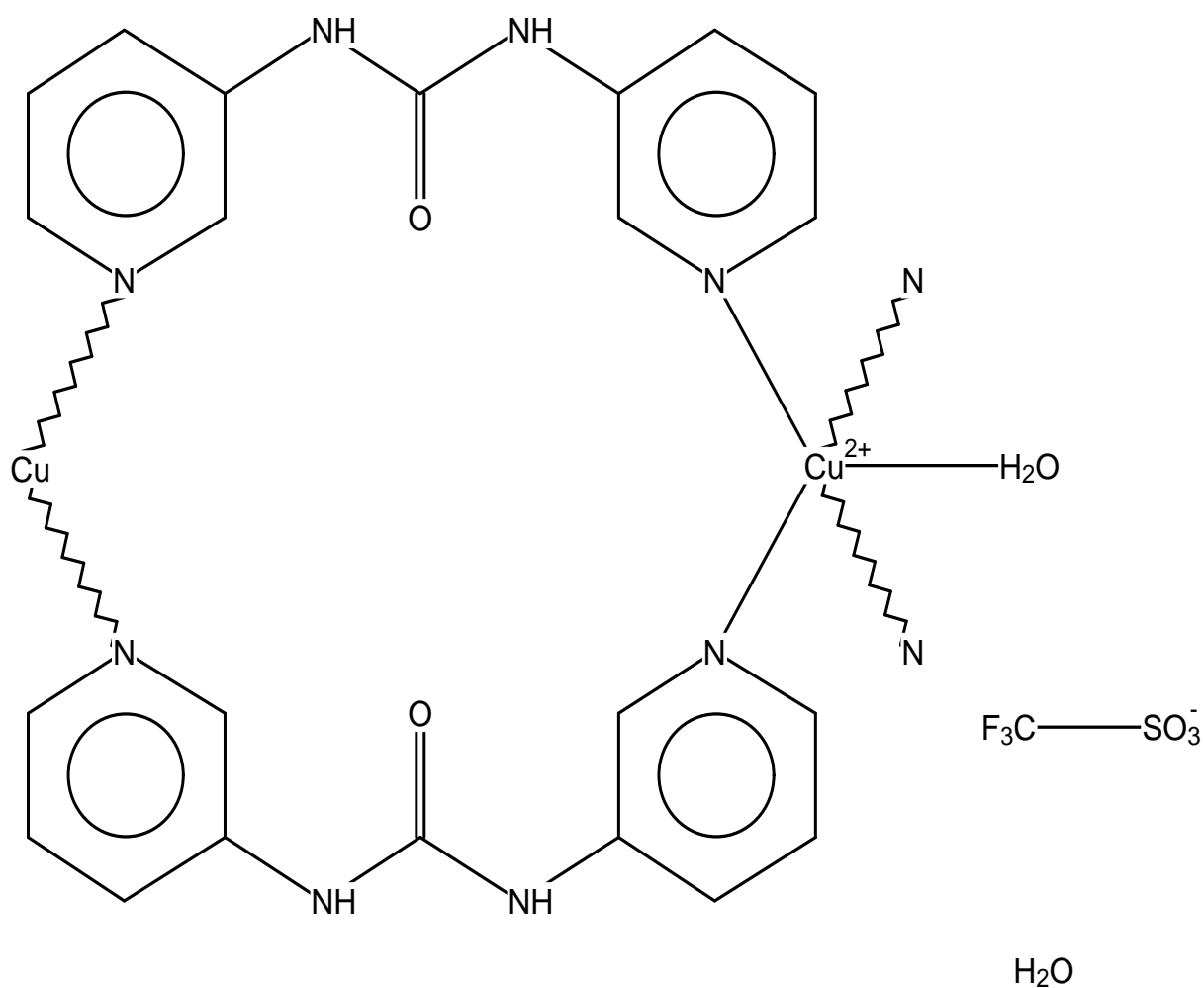
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *New J.Chem.* ,**30**, 1267

Formula: $(C_{22}H_{22}Cu_1N_8O_3^{2+})_n, 2n(C_1F_3O_3S_1^{-1}), n(H_2O_1)$

Compound Name: catena-(bis(μ_2 -N,N'-bis(3-Pyridyl)urea)-aqua-copper(ii) bis(trifluoromethanesulfonate) monohydrate)

Space Group: P21/c **Cell:** **a** 9.052(0) **b** 18.099(1) **c** 19.554(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 95.29(0) γ 90.00

R-Factor (%): 4.27 **Temperature(K):** 100 **Density(g/cm³):** 1.720



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 31

PEFH0Y

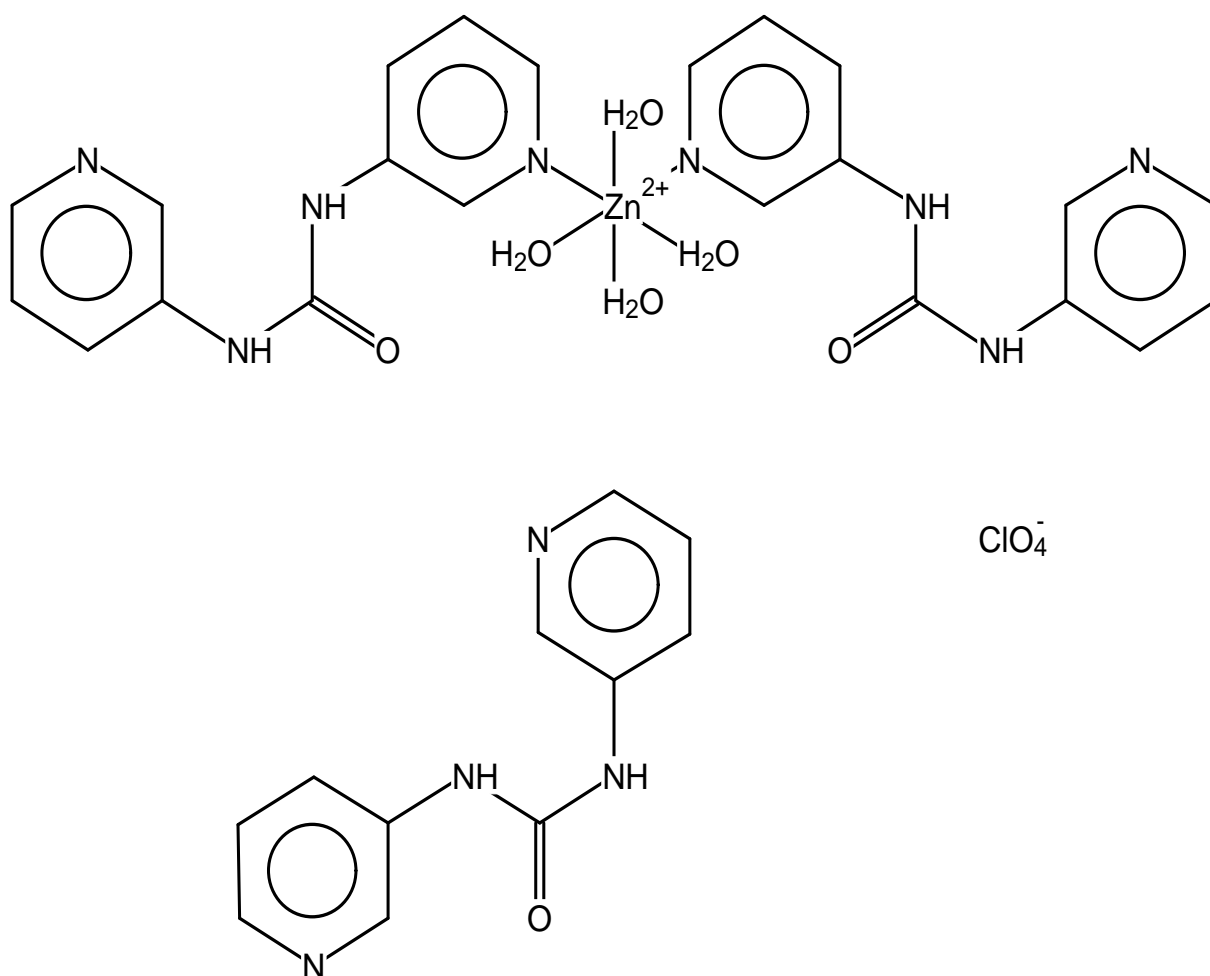
Reference: R.Custelcean, B.A.Moyer, V.S.Bryantsev, B.P.Hay (2006)
Cryst.Growth Des. ,6,555

Formula: $C_{22} H_{28} N_8 O_6 Zn_1^{2+}, 2(Cl_1 O_4^{1-}), 2(C_{11} H_{10} N_4 O_1)$

Compound Name: Tetra-aqua-bis(N,N'-bis(3-pyridyl)urea-N)-zinc diperchlorate N,N'-bis(3-pyridyl)urea solvate

Space Group: C2/c **Cell:** **a** 23.905(5) **b** 13.712(3) **c** 15.538(3)
Space Group No.: 15 **(Å, °)** α 90.00 β 99.54(0) γ 90.00

R-Factor (%): 4.61 **Temperature(K):** 173 **Density(g/cm³):** 1.578



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 32

SEQHAY

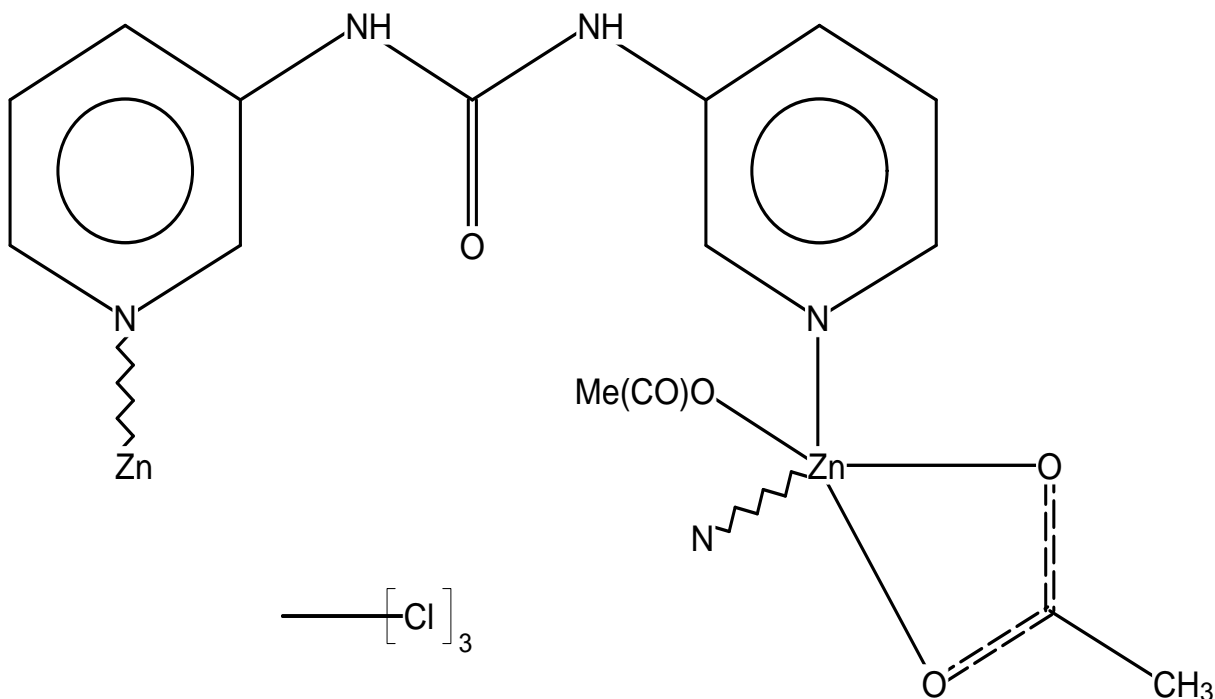
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *CrystEngComm*, **8**, 805

Formula: (C₁₅ H₁₆ N₄ O₅ Zn₁)_n,n(C₁ H₁ Cl₃)

Compound Name: catena-((μ₂-N,N'-bis(3-Pyridyl)urea)-(acetato-O)-(acetato-O,O')-zinc(ii) chloroform solvate)

Space Group: P21/c **Cell:** **a** 9.213(1) **b** 12.441(2) **c** 19.292(3)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 95.45(0) **γ** 90.00

R-Factor (%): 6.86 **Temperature(K):** 100 **Density(g/cm³):** 1.560



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 33

SETKIM

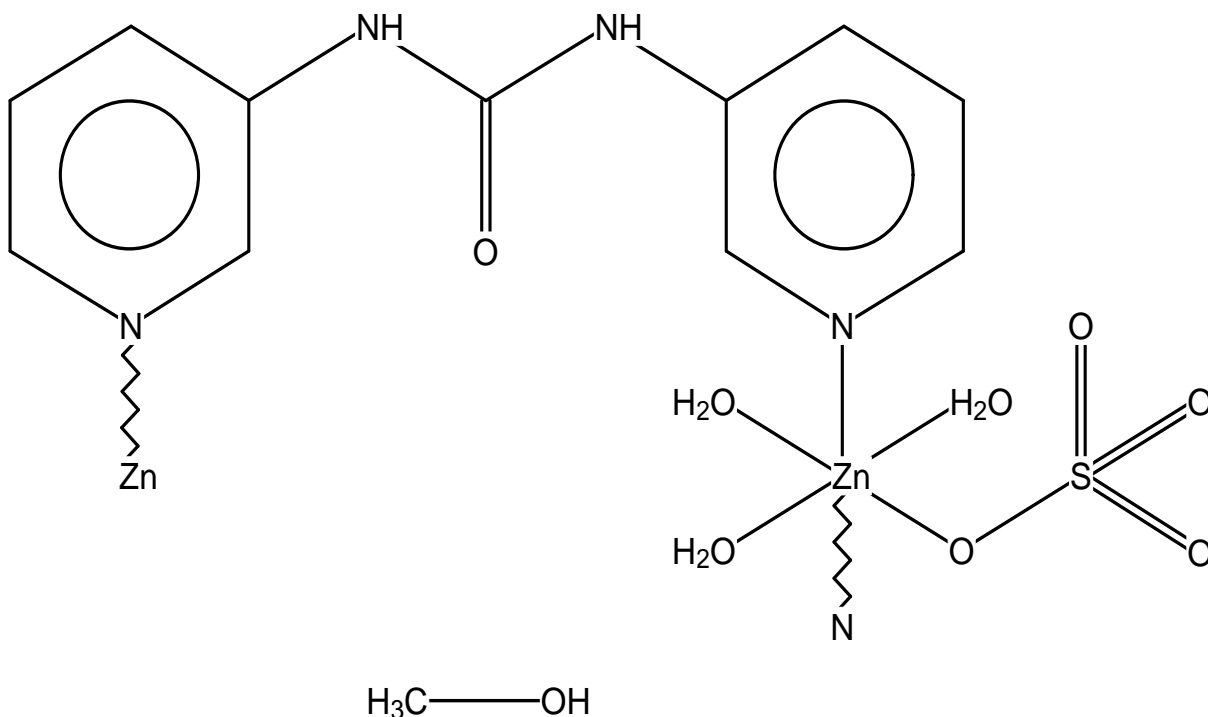
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *CrystEngComm*, **8**, 805

Formula: (C₁₁ H₁₆ N₄ O₈ S₁ Zn₁)_n,n(C₁ H₄ O₁)

Compound Name: catena-((μ₂-N,N'-bis(3-Pyridyl)urea)-(sulfato-O)-triaqua-zinc(ii) methanol solvate)

Space Group: P21/n **Cell:** **a** 7.736(1) **b** 10.898(1) **c** 21.528(4)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 96.73(0) **γ** 90.00

R-Factor (%): 5.68 **Temperature(K):** 298 **Density(g/cm³):** 1.702



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 34

VIMZEX

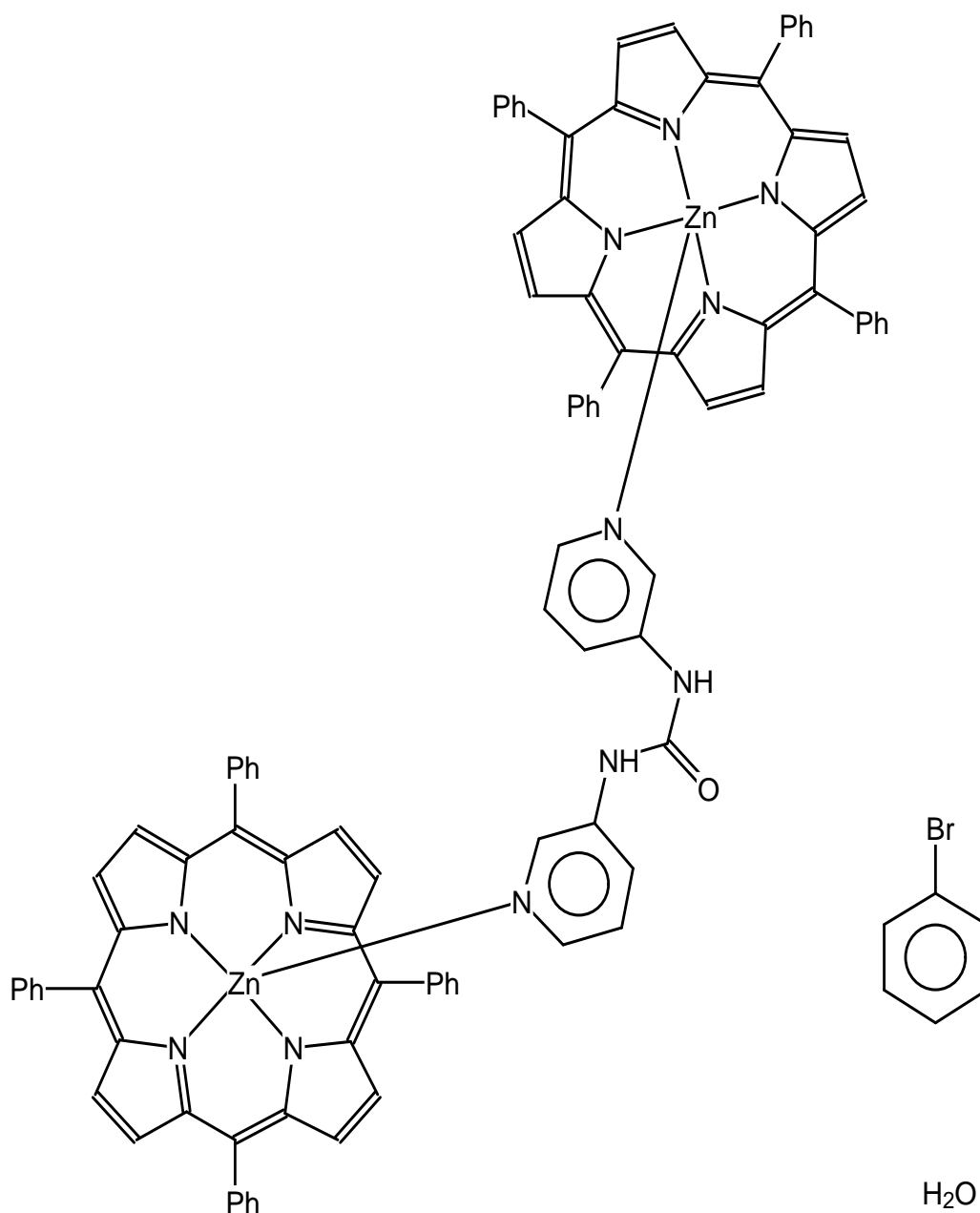
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *Inorg.Chem.* ,**46**, 7351

Formula: $C_{99} H_{66} N_{12} O_1 Zn_2 \cdot 4(C_6 H_5 Br)_1, H_2 O_1$

Compound Name: (μ_2 -N,N'-bis(3-Pyridyl)urea)-bis(5,10,15,20-tetraphenylporphyrinato)-di-zinc(ii) tetrakis(bromobenzene) clathrate monohydrate

Space Group: C2 **Cell:** **a** 18.541(1) **b** 11.909(1) **c** 23.836(2)
Space Group No.: 5 **(Å, °)** α 90.00 β 110.05(0) γ 90.00

R-Factor (%): 3.78 **Temperature(K):** 100 **Density(g/cm³):** 1.489



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 35

VIMZIB

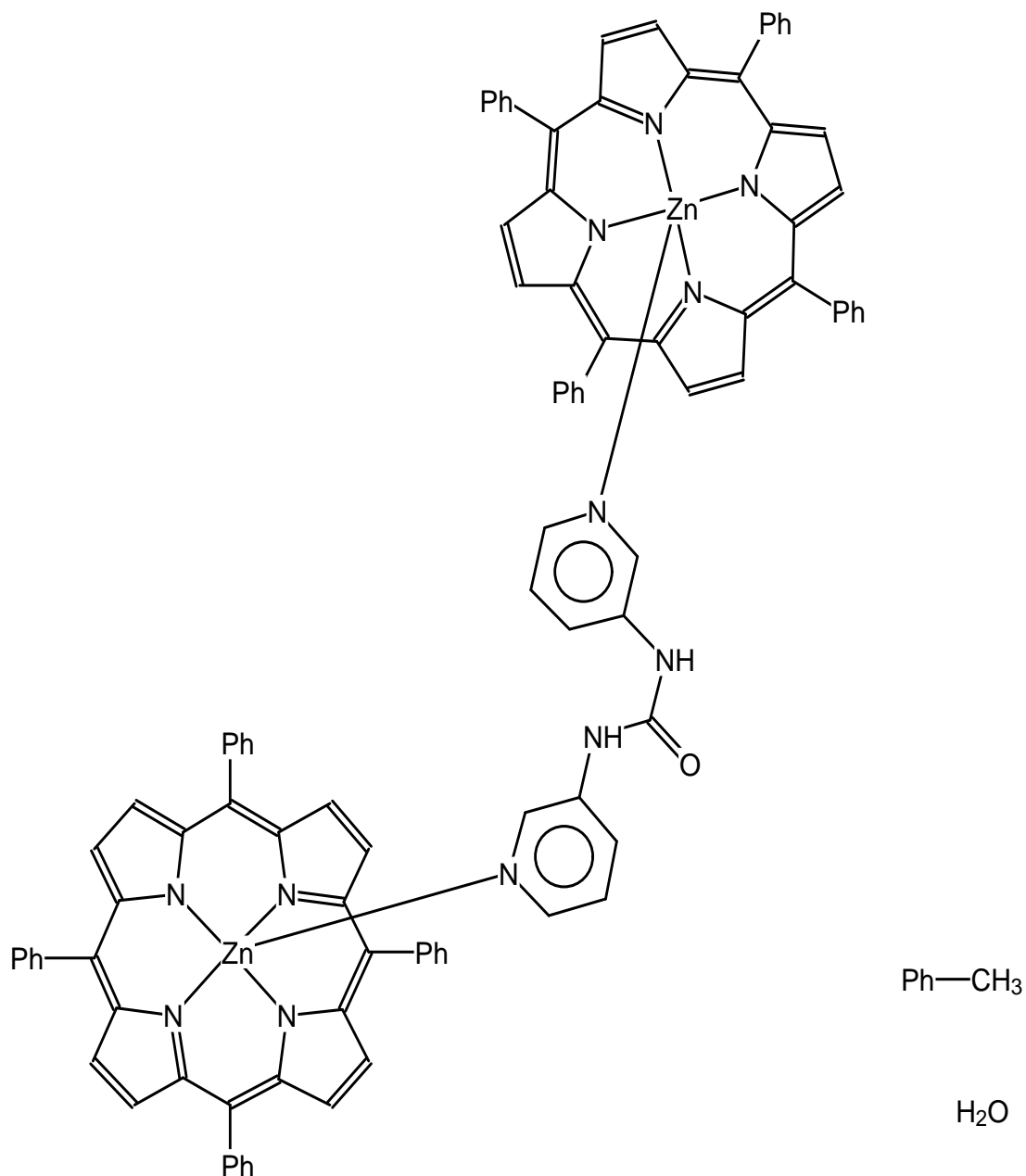
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *Inorg.Chem.* ,**46**, 7351

Formula: C₉₉ H₆₆ N₁₂ O₁ Zn₂,4(C₇ H₈),H₂ O₁

Compound Name: (μ_2 -N,N'-bis(3-Pyridyl)urea)-bis(5,10,15,20-tetraphenylporphyrinato)-di-zinc(ii) tetrakis(toluene) monohydrate clathrate

Space Group: C2 **Cell:** **a** 18.528(1) **b** 11.884(0) **c** 23.815(1)
Space Group No.: 5 **(Å, °)** α 90.00 β 109.56(0) γ 90.00

R-Factor (%): 3.51 **Temperature(K):** 100 **Density(g/cm³):** 1.315



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 36

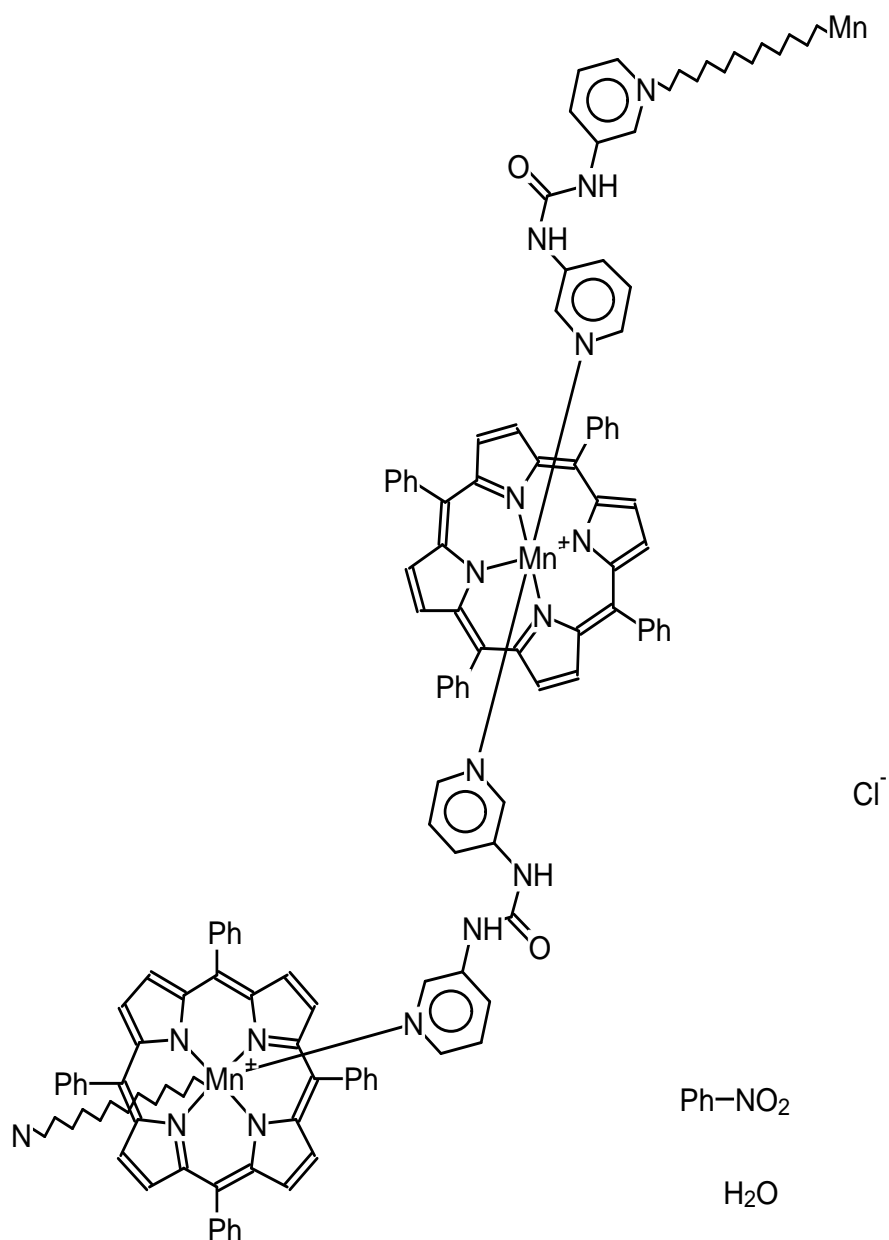
VINBAW

Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *Inorg.Chem.* ,**46**, 7351

Formula: $(C_{110} H_{76} Mn_2 N_{16} O_2^{2+})_n, 2n(Cl_1^{-1-}), 4n(C_6 H_5 N_1 O_2), 4n(H_2 O_1)$

Compound Name: catena-(bis(μ_2 -N,N'-bis(3-Pyridyl)urea)-bis(5,10,15,20-tetraphenylporphyrinato)-di-manganese(ii) dichloride tetrakis(nitrobenzene) dihydrate clathrate dihydrate)

Space Group:	P-1	Cell:	a 12.920(1)	b 13.906(1)	c 16.053(1)
Space Group No.:	2	(Å, °)	α 93.85(0)	β 94.52(0)	γ 96.53(0)
R-Factor (%):	9.64	Temperature(K):	100	Density(g/cm³):	1.399



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 37

VINBEA

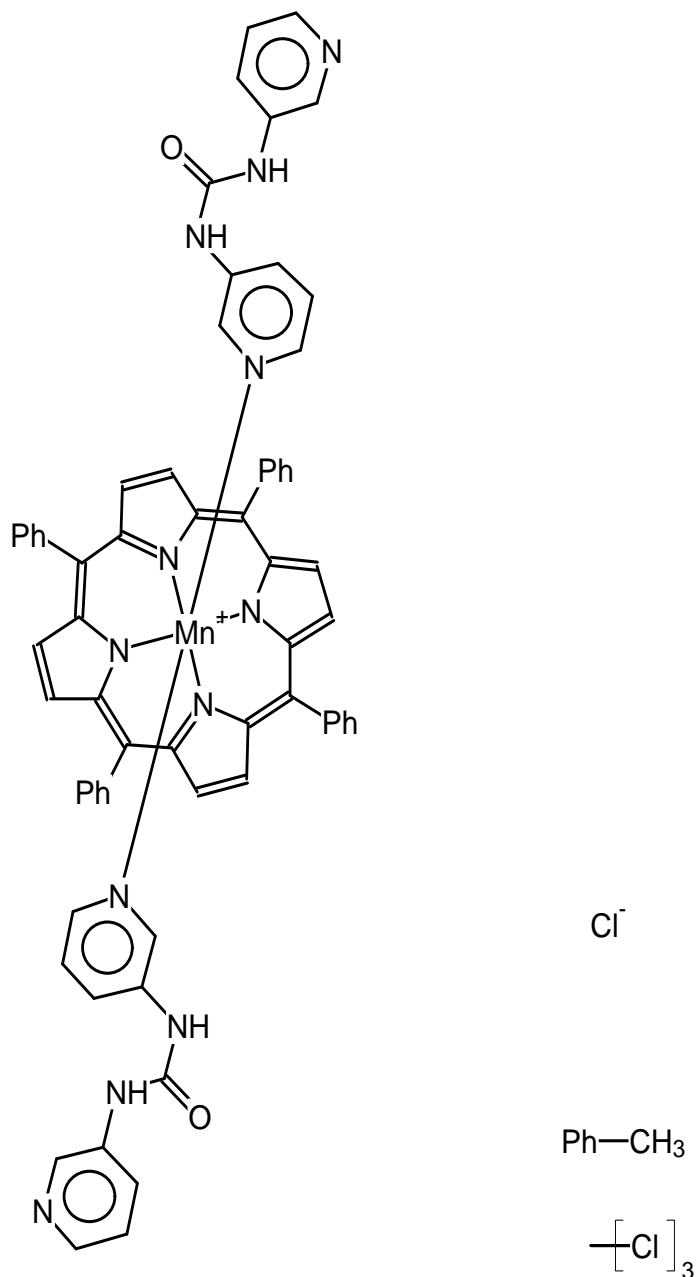
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *Inorg.Chem.* ,**46**, 7351

Formula: $C_{66} H_{48} Mn_1 N_{12} O_2^{1+}, Cl_1^{1-}, C_7 H_8, C_1 H_1 Cl_3$

Compound Name: bis(N,N'-bis(3-Pyridyl)urea)-(5,10,15,20-tetraphenylporphyrinato)-manganese(ii) chloride toluene chloroform clathrate

Space Group: P-1 **Cell:** **a** 12.915(1) **b** 15.739(2) **c** 17.626(2)
Space Group No.: 2 **(Å, °)** α 92.63(0) β 110.36(0) γ 105.79(0)

R-Factor (%): 6.86 **Temperature(K):** 150 **Density(g/cm³):** 1.397



Search: search2 (Sun Nov 20 19:30:17 2011): Hit 38

VINBIE

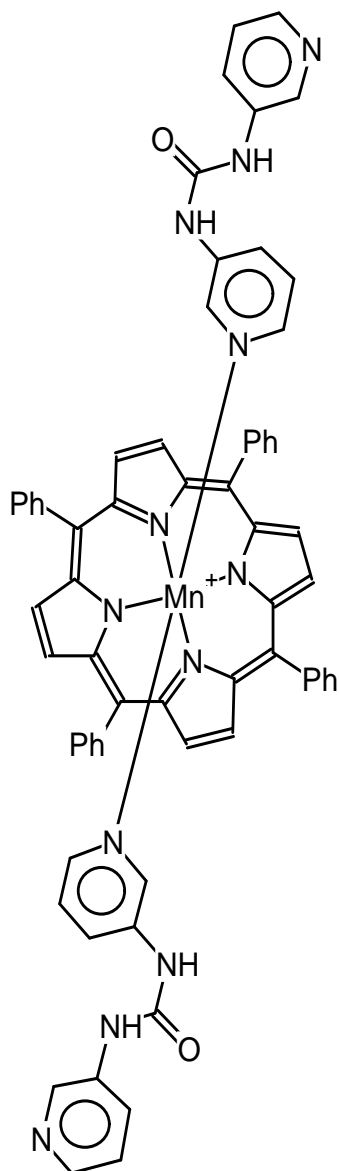
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *Inorg.Chem.* ,**46**, 7351

Formula: $C_{66} H_{48} Mn_1 N_{12} O_2^{1+}, Cl_1^{1-}, 1.5(C_8 H_{10}), H_2 O_1$

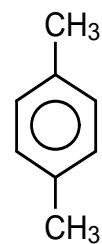
Compound Name: bis(N,N'-bis(3-Pyridyl)urea)-(5,10,15,20-tetraphenylporphyrinato)-manganese(ii) chloride sesquikis(p-xylene) monohydrate clathrate

Space Group: P-1 **Cell:** **a** 12.873(1) **b** 13.071(1) **c** 20.029(1)
Space Group No.: 2 **(Å, °)** α 82.51(0) β 84.05(0) γ 78.27(0)

R-Factor (%): 5.75 **Temperature(K):** 100 **Density(g/cm³):** 1.333



Cl⁻



H₂O

Search Overview

Search: search3
Date/Time done: Sun Nov 20 19:32:00 2011
Database(s): CSD version 5.32 (November 2010)
CSD version 5.32 updates (Nov 2010)
Restriction Info: No refcode restrictions applied
Filters: None
Percentage Completed: 100%
Number of Hits: 10

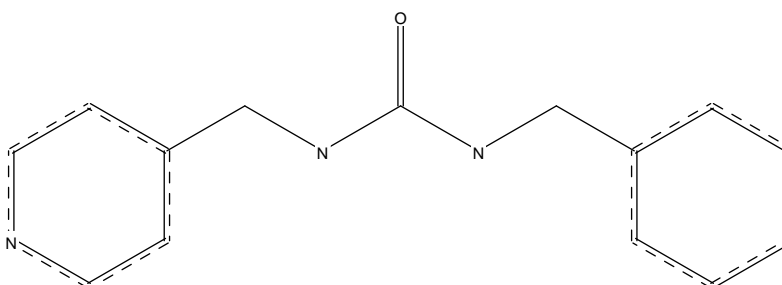
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

4M

Search: search3 (Sun Nov 20 19:32:00 2011): Hit 1

HEYDEV

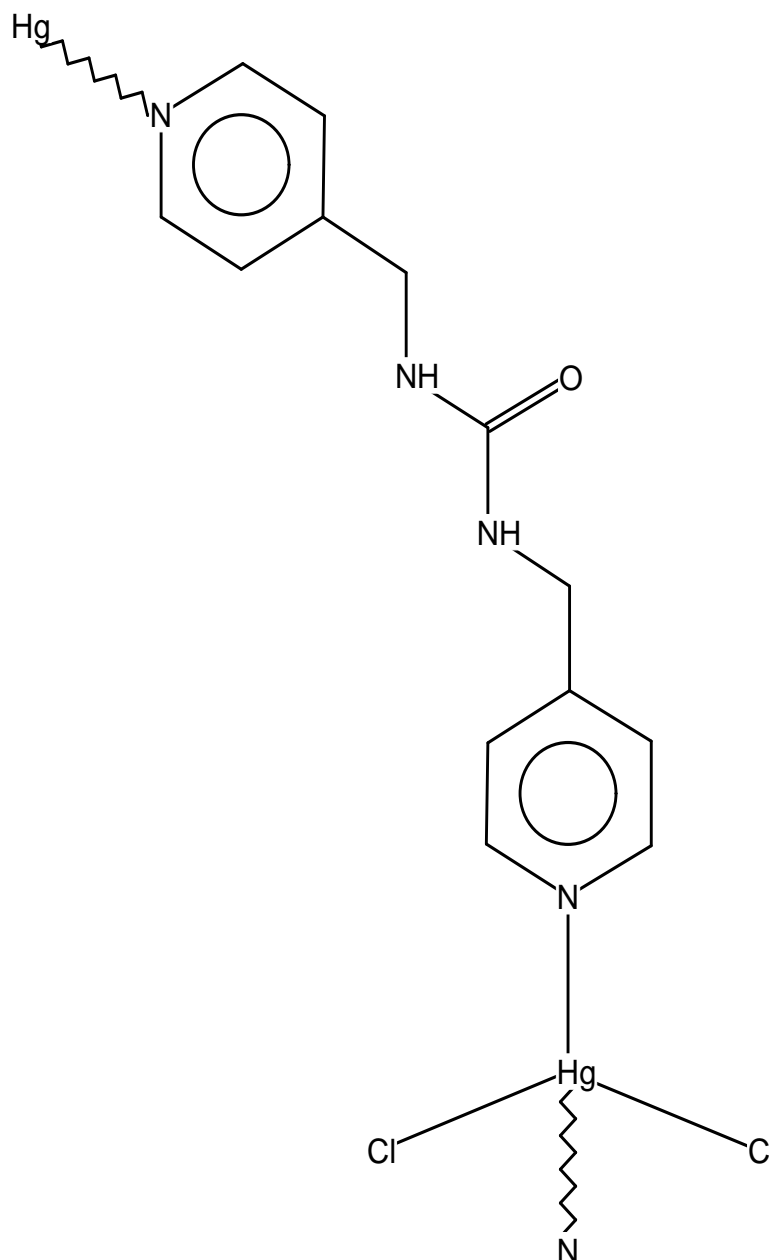
Reference: Biing-Chiau Tzeng, Yung-Chi Huang, Bo-So Chen, Wan-Min Wu, Shih-Yang Lee, Gene-Hsiang Lee, Shie-Ming Peng (2007) *Inorg.Chem.* ,**46**,186

Formula: (C₁₃ H₁₄ Cl₂ Hg₁ N₄ O₁)_n

Compound Name: catena-((μ₂-1,3-bis(4-Pyridylmethyl)urea)-dichloro-mercury(ii))

Space Group: P2/n **Cell:** **a** 14.609(1) **b** 4.471(0) **c** 15.142(1)
Space Group No.: 13 **(Å, °)** **α** 90.00 **β** 106.78(0) **γ** 90.00

R-Factor (%): 4.63 **Temperature(K):** 273 **Density(g/cm³):** 1.802



Search: search3 (Sun Nov 20 19:32:00 2011): Hit 2

HEYDUL

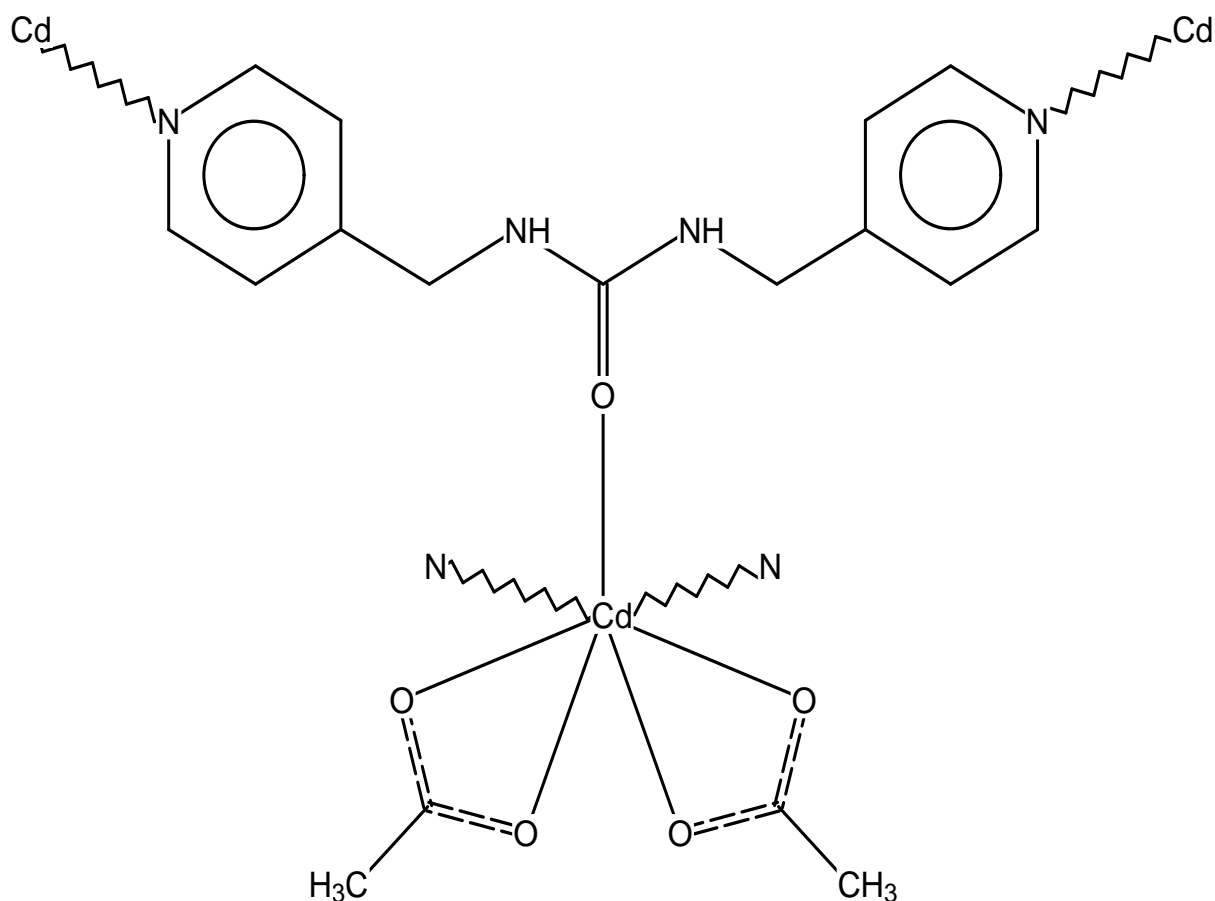
Reference: Biing-Chiau Tzeng, Yung-Chi Huang, Bo-So Chen, Wan-Min Wu, Shih-Yang Lee, Gene-Hsiang Lee, Shie-Ming Peng (2007) *Inorg.Chem.* ,**46**,186

Formula: (C₁₇ H₂₀ Cd₁ N₄ O₅)_n

Compound Name: catena-((μ₃-1,3-bis(4-Pyridylmethyl)urea)-bis(acetato)-cadmium(ii))

Space Group: Pn **Cell:** **a** 9.393(1) **b** 8.962(1) **c** 11.080(2)
Space Group No.: 7 **(Å, °)** α 90.00 β 95.57(0) γ 90.00

R-Factor (%): 3.01 **Temperature(K):** 273 **Density(g/cm³):** 1.691



Search: search3 (Sun Nov 20 19:32:00 2011): Hit 3

NOGROQ

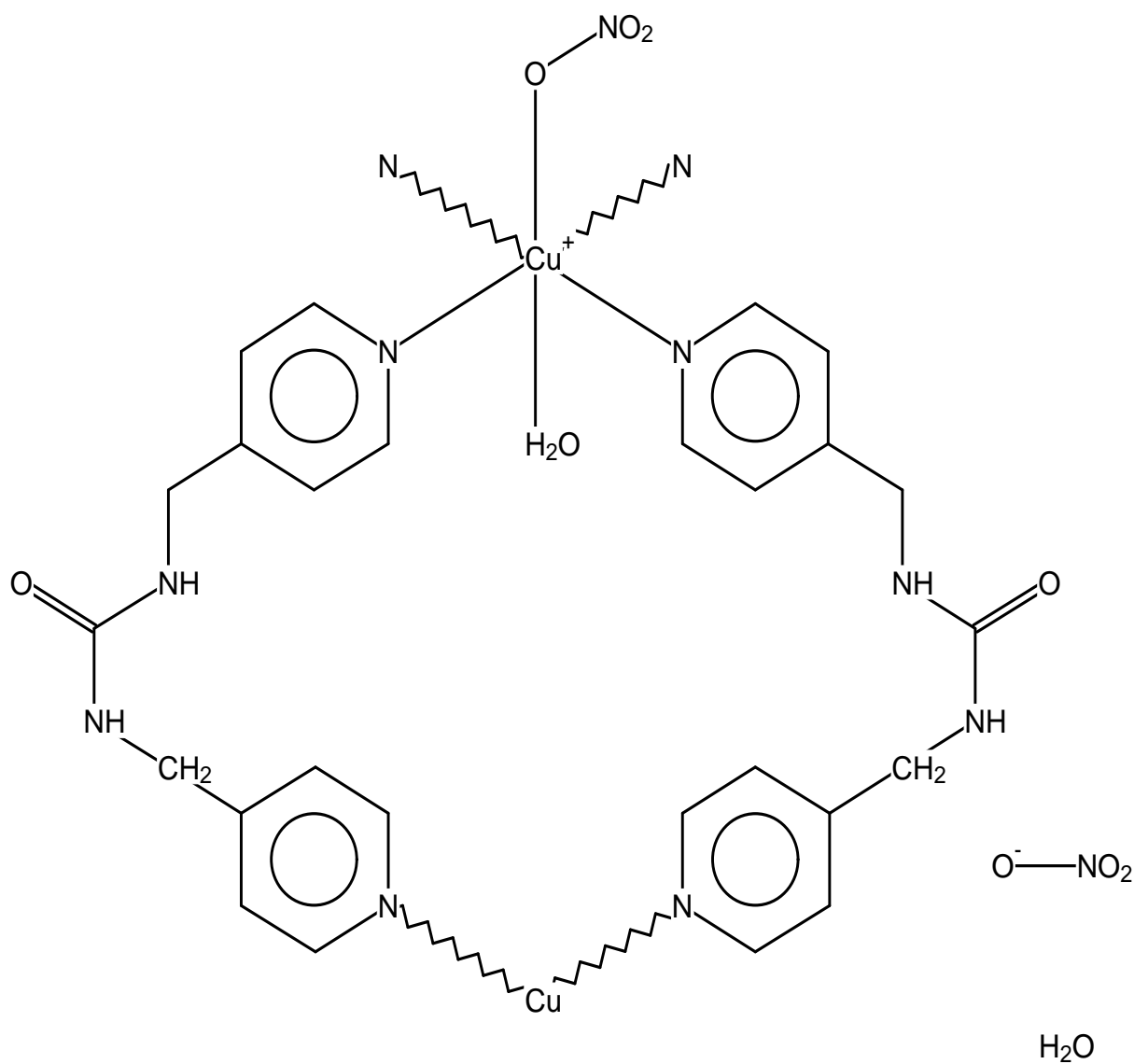
Reference: M.J.Plater, B.M.de Silva, J.M.S.Skakle, R.A.Howie, A.Riffat, T.Gelbrich, M.B.Hursthouse (2001) *Inorg.Chim.Acta* ,**325**,141

Formula: (C₂₆ H₃₀ Cu₁ N₉ O₆¹⁺)_n,n(N₁ O₃¹⁻),n(H₂ O₁)

Compound Name: catena-(bis(μ₂-N,N'-bis(4-pyridylmethyl)urea)-aqua-nitrato-copper(ii) nitrate monohydrate)

Space Group: P21/n **Cell:** **a** 13.539(0) **b** 17.772(0) **c** 13.585(0)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 107.83(0) **γ** 90.00

R-Factor (%): 4.83 **Temperature(K):** 293 **Density(g/cm³):** 1.511



Search: search3 (Sun Nov 20 19:32:00 2011): Hit 4

NOGXAI

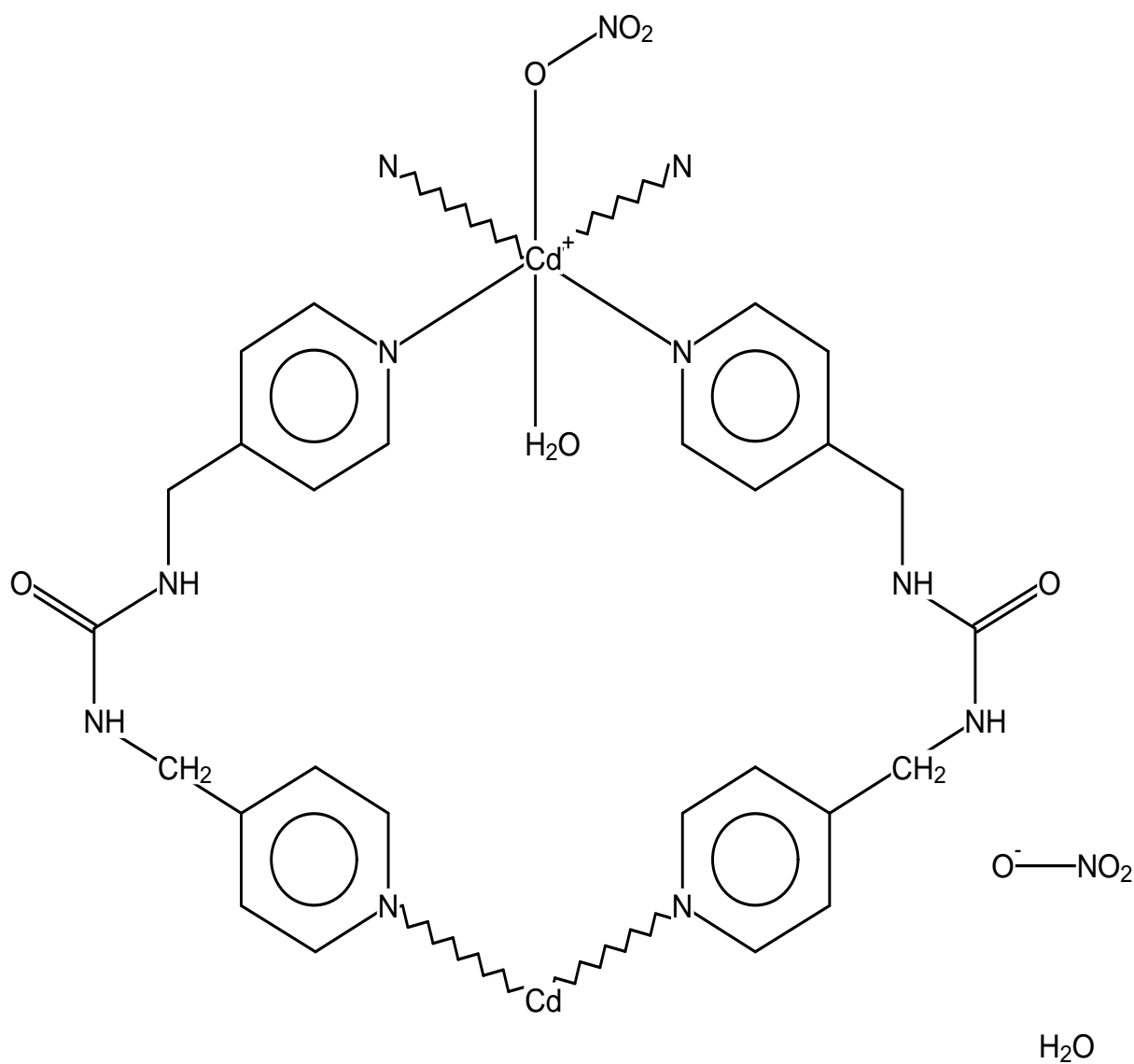
Reference: M.J.Plater, B.M.de Silva, J.M.S.Skakle, R.A.Howie, A.Riffat, T.Gelbrich, M.B.Hursthouse (2001) *Inorg.Chim.Acta* ,**325**,141

Formula: (C₂₆ H₃₀ Cd₁ N₉ O₆¹⁺)_n,n(N₁ O₃¹⁻),n(H₂ O₁)

Compound Name: catena-(bis(μ₂-N,N'-bis(4-pyridylmethyl)urea)-aqua-nitrato-cadmium(ii) nitrate monohydrate)

Space Group: P21/n **Cell:** **a** 13.410(0) **b** 17.642(0) **c** 14.005(0)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 106.90(0) **γ** 90.00

R-Factor (%): 3.65 **Temperature(K):** 150 **Density(g/cm³):** 1.586



Search: search3 (Sun Nov 20 19:32:00 2011): Hit 5

VEDYAF

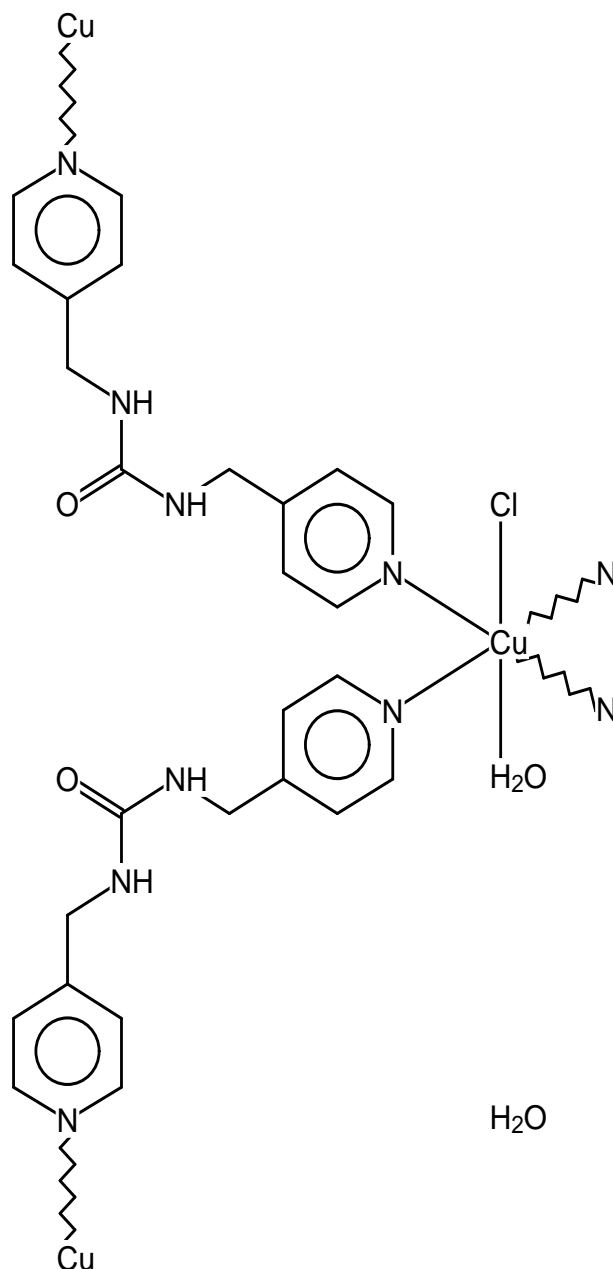
Reference: P.Diaz, J.Benet-Buchholz, R.Vilar, A.J.P.White (2006)
Inorg.Chem. ,**45**,1617

Formula: (C₂₆ H₃₀ Cl₁ Cu₁ N₈ O₃)_n,₁0.92n(H₂ O₁)

Compound Name: catena-(bis(μ₂-1,3-bis(4-Pyridylmethyl)urea-N,N')-aqua-chloro-copper(ii) hydrate)

Space Group: P21/n **Cell:** **a** 9.107(0) **b** 23.983(0) **c** 18.080(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 97.56(0) γ 90.00

R-Factor (%): 8.36 **Temperature(K):** 90 **Density(g/cm³):** 1.354



Search: search3 (Sun Nov 20 19:32:00 2011): Hit 6

VEDYEJ

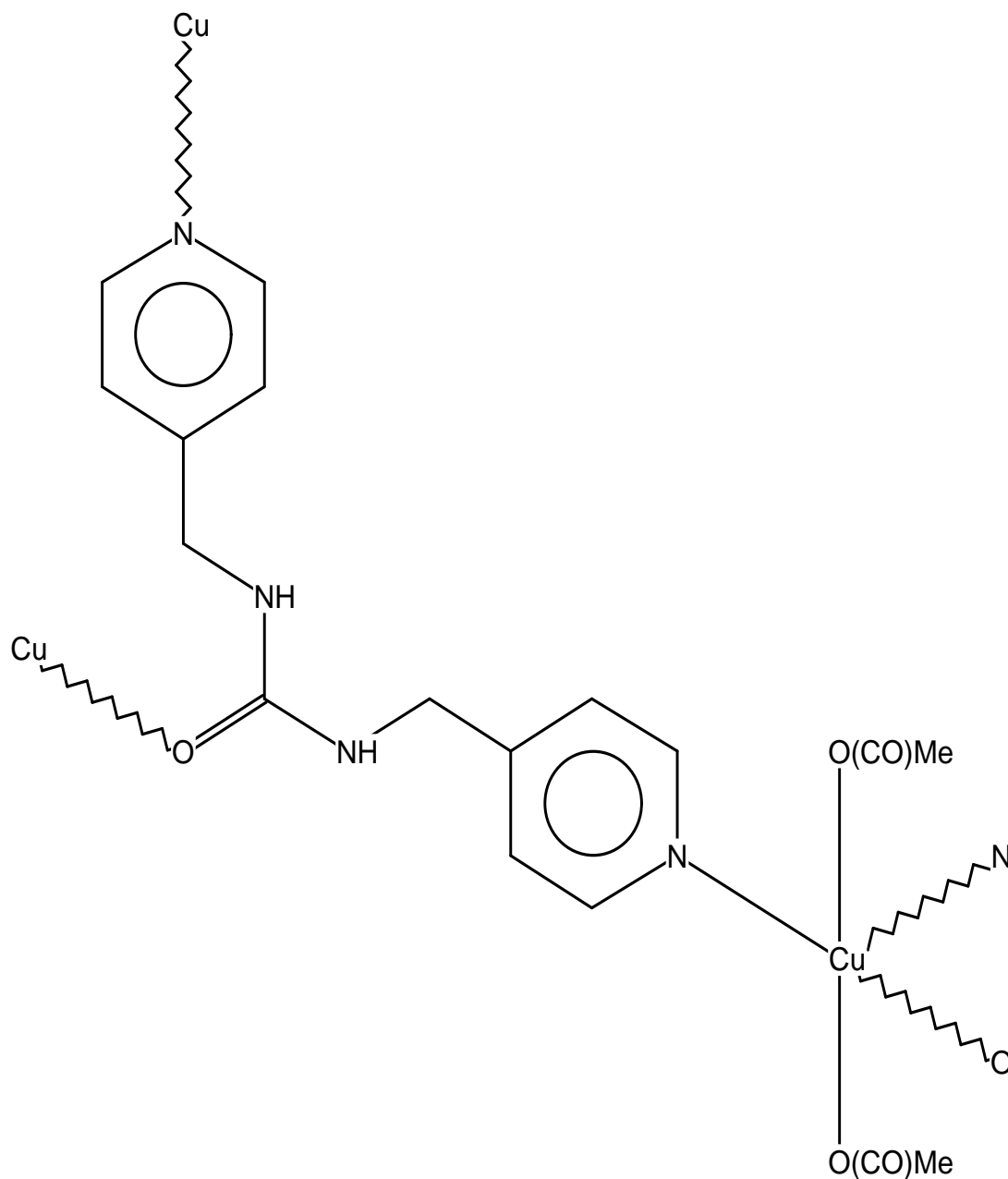
Reference: P.Diaz, J.Benet-Buchholz, R.Vilar, A.J.P.White (2006)
Inorg.Chem. ,**45**,1617

Formula: (C₁₇ H₂₀ Cu₁ N₄ O₅)_n

Compound Name: catena-((μ₃-1,3-bis(4-Pyridylmethyl)urea-N,N',O)-bis(acetato-O)-copper(ii))

Space Group: P21/n **Cell:** **a** 9.205(0) **b** 18.367(1) **c** 10.837(0)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 93.80(0) **γ** 90.00

R-Factor (%): 4.48 **Temperature(K):** 293 **Density(g/cm³):** 1.540



Search: search3 (Sun Nov 20 19:32:00 2011): Hit 7

VEDYIN

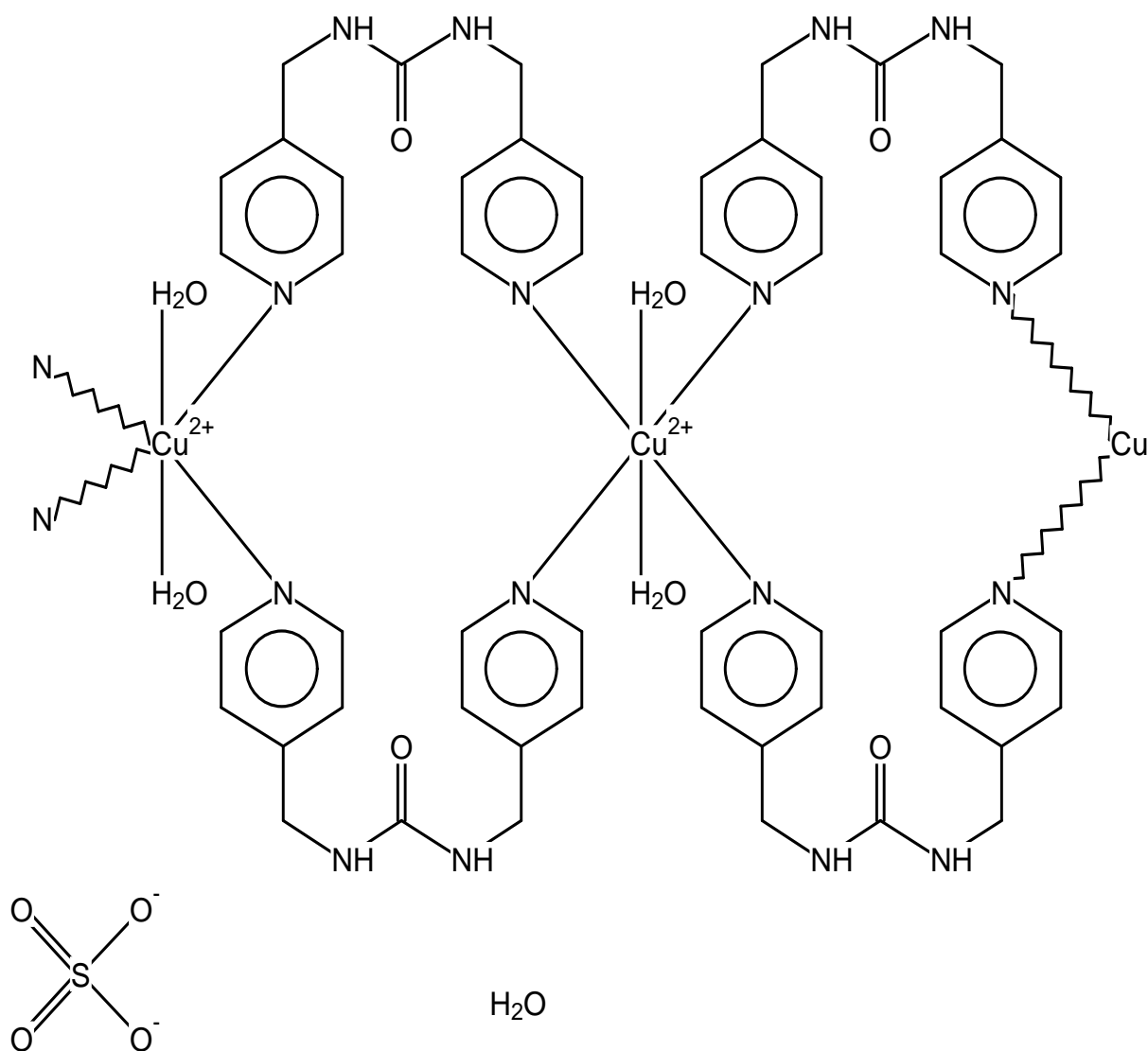
Reference: P.Diaz, J.Benet-Buchholz, R.Vilar, A.J.P.White (2006)
Inorg.Chem. ,**45**,1617

Formula: $(C_{52}H_{64}Cu_2N_{16}O_8^{4+})_n, 2n(O_4S_1^{2-}), 4n(H_2O_1)$

Compound Name: catena-(tetrakis(μ_2 -1,3-bis(4-Pyridylmethyl)urea-N,N')-tetra-aqua-di-copper(ii) bis(sulfate) tetrahydrate)

Space Group: C2/c **Cell:** **a** 13.693(0) **b** 47.613(2) **c** 14.311(0)
Space Group No.: 15 **(Å, °)** α 90.00 β 105.69(0) γ 90.00

R-Factor (%): 6.22 **Temperature(K):** 173 **Density(g/cm³):** 1.589



Search: search3 (Sun Nov 20 19:32:00 2011): Hit 8

XEGXOX

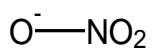
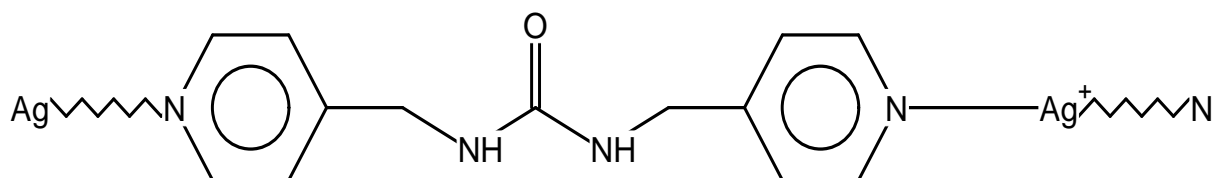
Reference: C.L.Schauer, E.Matwey, F.W.Fowler, J.W.Lauher (1998)
Crystal Engineering, 1, 213

Formula: $(C_{13}H_{14}Ag_1N_4O_1^{1+})_n, n(N_1O_3^{1-}), n(H_2O_1)$

Compound Name: catena-((μ_2 -N,N'-bis(4-Pyridylmethyl)urea-N,N')-silver(i) nitrate monohydrate)

Space Group: P21/n **Cell:** **a** 7.822(0) **b** 14.753(0) **c** 14.626(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 104.40(0) γ 90.00

R-Factor (%): 4.63 **Temperature(K):** 295 **Density(g/cm³):** 1.748



Search: search3 (Sun Nov 20 19:32:00 2011): Hit 9

YIJBOJ

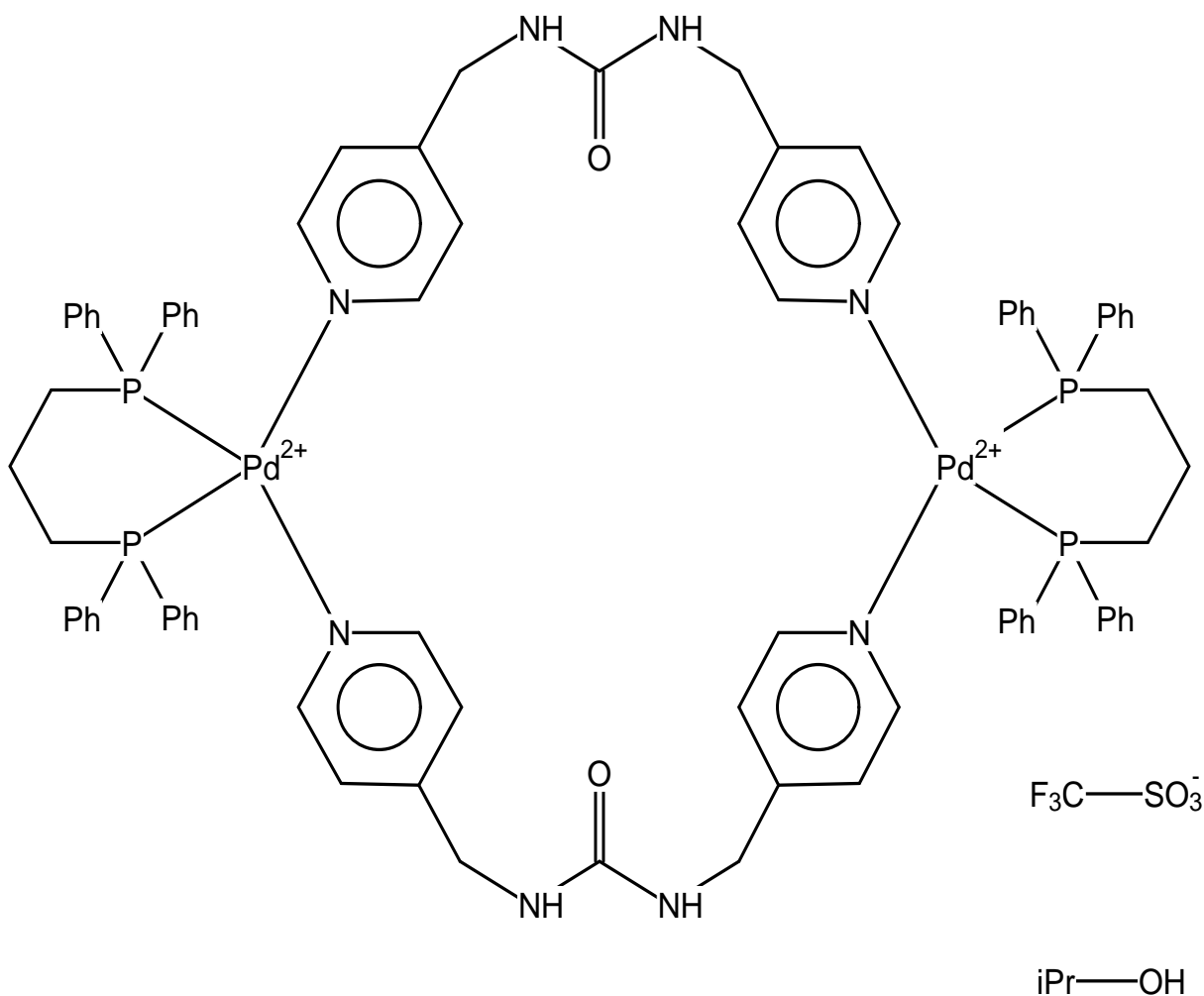
Reference: P.Diaz, J.A.Tovilla, P.Ballester, J.Benet-Buchholz, R.Vilar
(2007) *Dalton Trans.* ,3516

Formula: C₈₀ H₈₀ N₈ O₂ P₄ Pd₂ 4+,4(C₁ F₃ O₃ S₁ 1-),1.25(C₃ H₈ O₁)

Compound Name: bis((μ₂-N,N'-bis(4-Pyridylmethyl)urea)-(1,3-bis(diphenylphosphino)propane)-palladium(ii)) tetrakis(trifluoromethanesulfonate) isopropanol solvate

Space Group: P212121 **Cell:** **a** 18.606(1) **b** 21.536(1) **c** 27.110(1)
Space Group No.: 19 **(Å, °)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 8.54 **Temperature(K):** 100 **Density(g/cm³):** 1.341



Search: search3 (Sun Nov 20 19:32:00 2011): Hit 10

YIJCAW

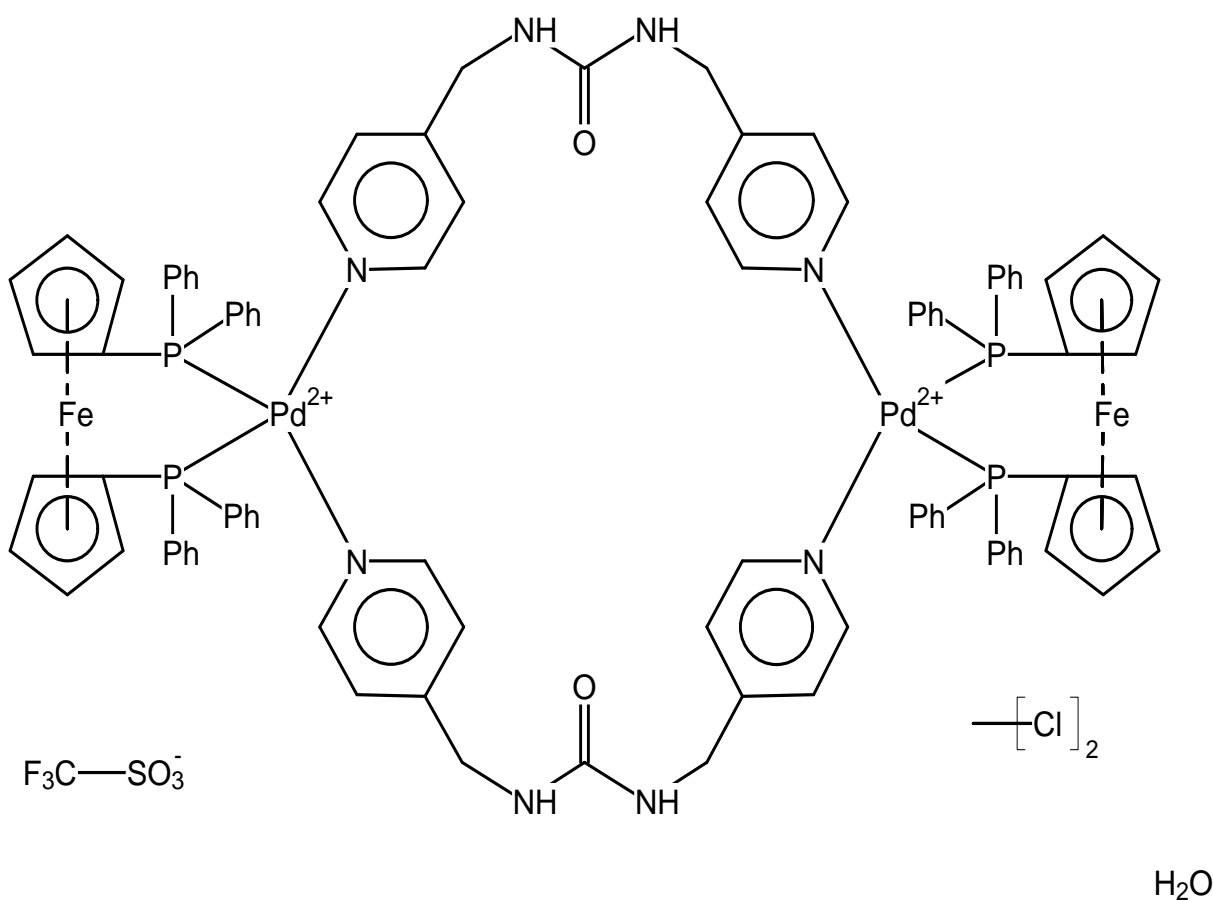
Reference: P.Diaz, J.A.Tovilla, P.Ballester, J.Benet-Buchholz, R.Vilar
(2007) *Dalton Trans.* ,3516

Formula: $C_{94} H_{84} Fe_2 N_8 O_2 P_4 Pd_2^{4+}, 4(C_1 F_3 O_3 S_1^{-}), C_1 H_2 Cl_2, 3(H_2 O_1)$

Compound Name: bis(μ_2 -N,N'-bis(4-Pyridylmethyl)urea)-(1,1'-bis(diphenylphosphino)ferrocene)-palladium(ii) tetrakis(trifluoromethanesulfonate) dichloromethane solvate trihydrate

Space Group: P-1 **Cell:** **a** 15.828(3) **b** 16.901(3) **c** 20.704(4)
Space Group No.: 2 (**Å, °**) α 71.94(0) β 86.14(0) γ 87.92(0)

R-Factor (%): 9.73 **Temperature(K):** 100 **Density(g/cm³):** 1.607



Search Overview

Search: search4
Date/Time done: Sun Nov 20 19:32:48 2011
Database(s): CSD version 5.32 (November 2010)
CSD version 5.32 updates (Nov 2010)
Restriction Info: No refcode restrictions applied
Filters: None
Percentage Completed: 100%
Number of Hits: 7

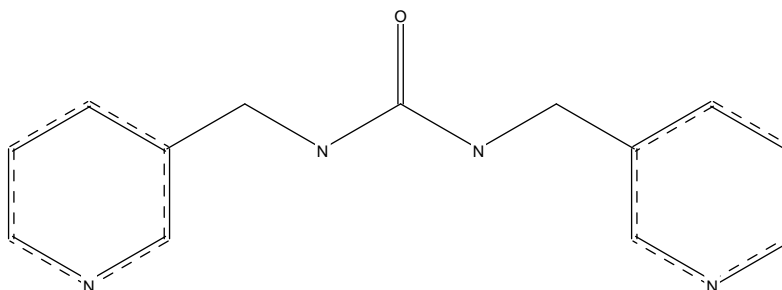
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

4M

Search: search4 (Sun Nov 20 19:32:48 2011): Hit 1

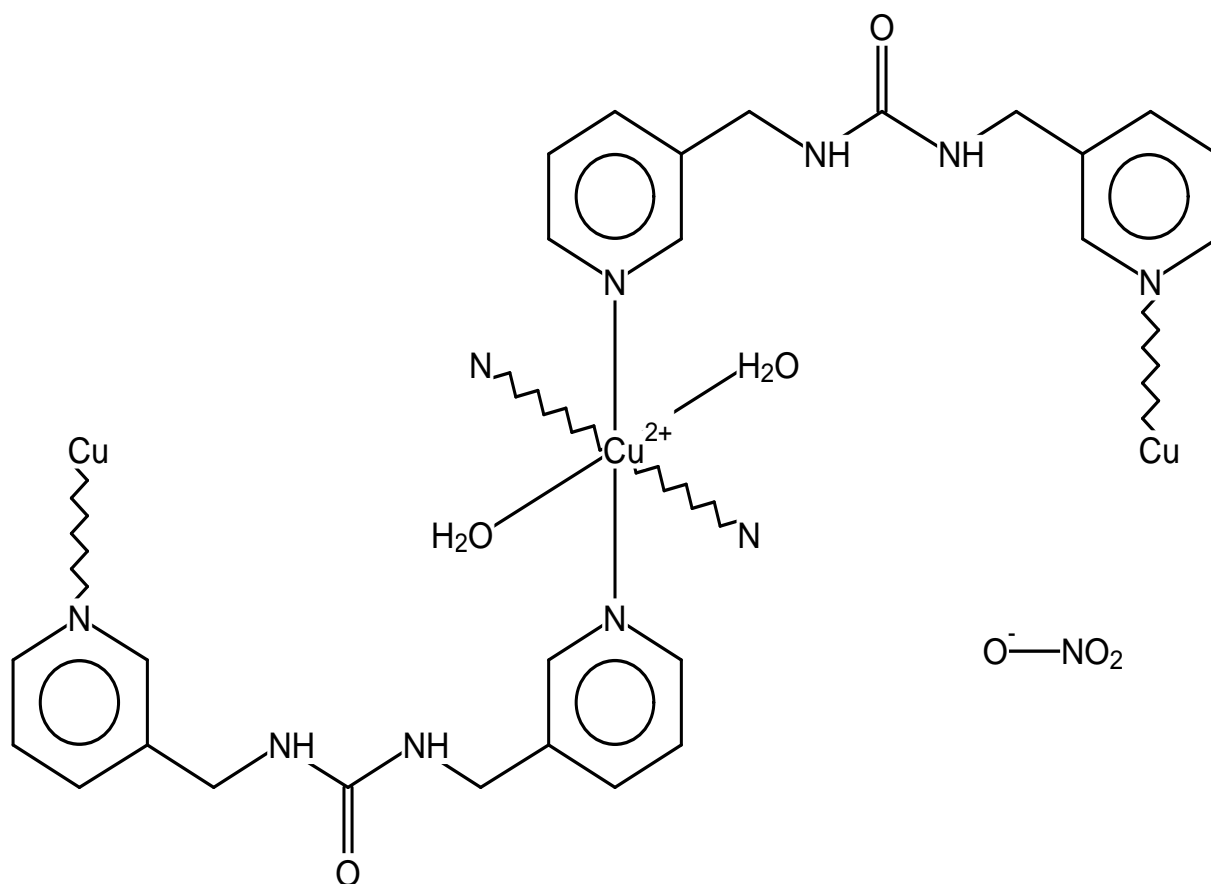
IPONOQ

Reference: M.B.Hursthouse, T.Gelbrich, M.J.Plater (2003)
Private Communication,

Formula: $(C_{26}H_{32}Cu_1N_8O_4^{2+})_n, 2n(N_1O_3^{1-})$

Compound Name: catena-(bis(μ_2 -N,N'-bis(Pyrid-3-ylmethyl)urea-N'',N''')-diaqua-copper dinitrate)

Space Group:	P-1	Cell:	a 7.835(0)	b 9.835(0)	c 10.284(0)
Space Group No.:	2	(Å, °)	α 81.65(0)	β 75.35(0)	γ 86.90(0)
R-Factor (%):	3.06	Temperature(K):	150	Density(g/cm³):	1.551



Search: search4 (Sun Nov 20 19:32:48 2011): Hit 2

NOGSIL

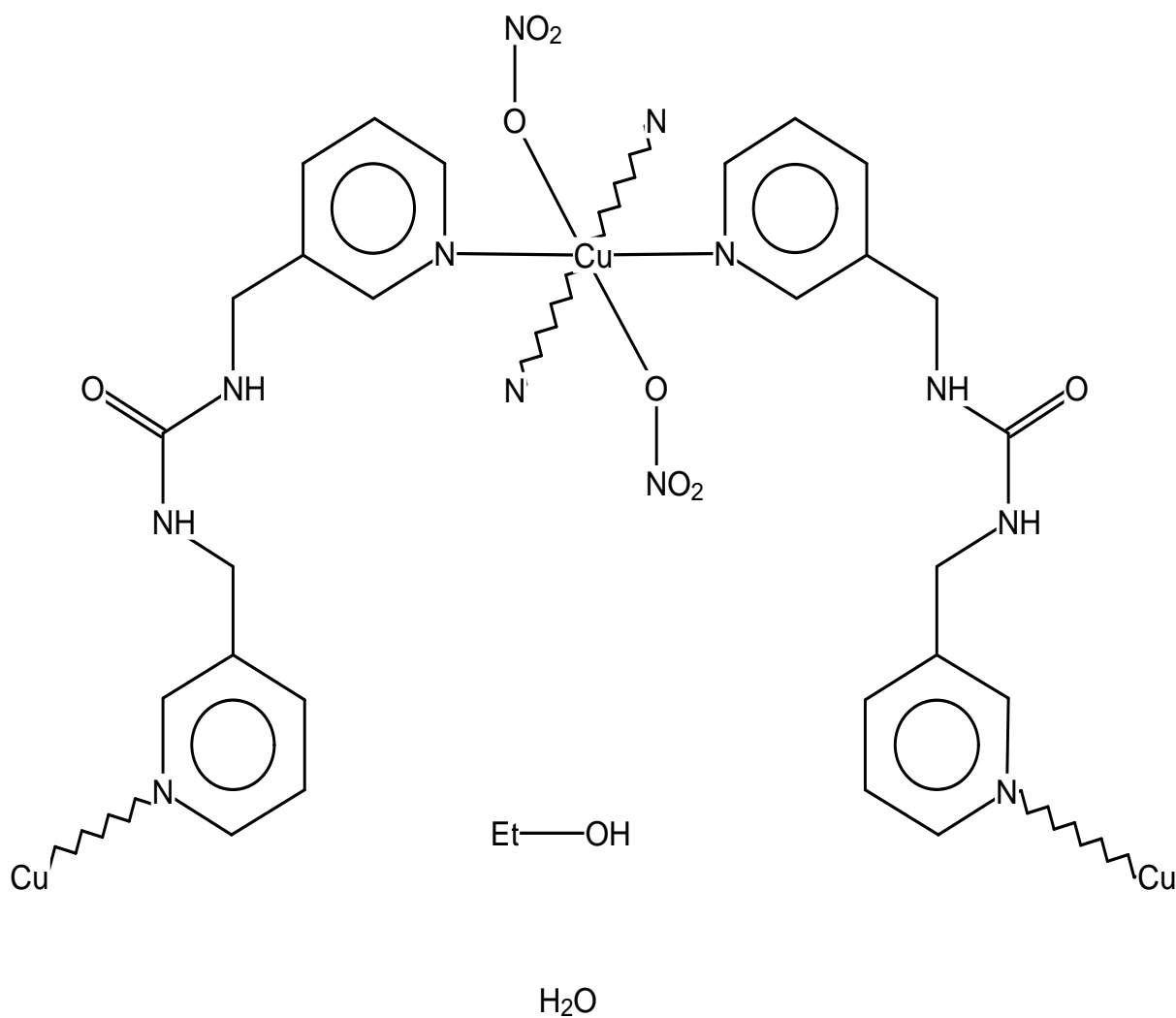
Reference: M.J.Plater, B.M.de Silva, J.M.S.Skakle, R.A.Howie, A.Riffat, T.Gelbrich, M.B.Hursthouse (2001) *Inorg.Chim.Acta* ,**325**,141

Formula: $(C_{26} H_{28} Cu_1 N_{10} O_8)_n, 2n(C_2 H_6 O_1), 2n(H_2 O_1)$

Compound Name: catena-(bis(μ_2 -N,N'-bis(3-pyridylmethyl)urea)-bis(nitrato)-copper(ii) ethanol solvate dihydrate)

Space Group: P21/c **Cell:** **a** 9.117(0) **b** 21.558(1) **c** 9.122(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 96.27(1) γ 90.00

R-Factor (%): 4.51 **Temperature(K):** 150 **Density(g/cm³):** 1.491



Search: search4 (Sun Nov 20 19:32:48 2011): Hit 3

NOGXEM

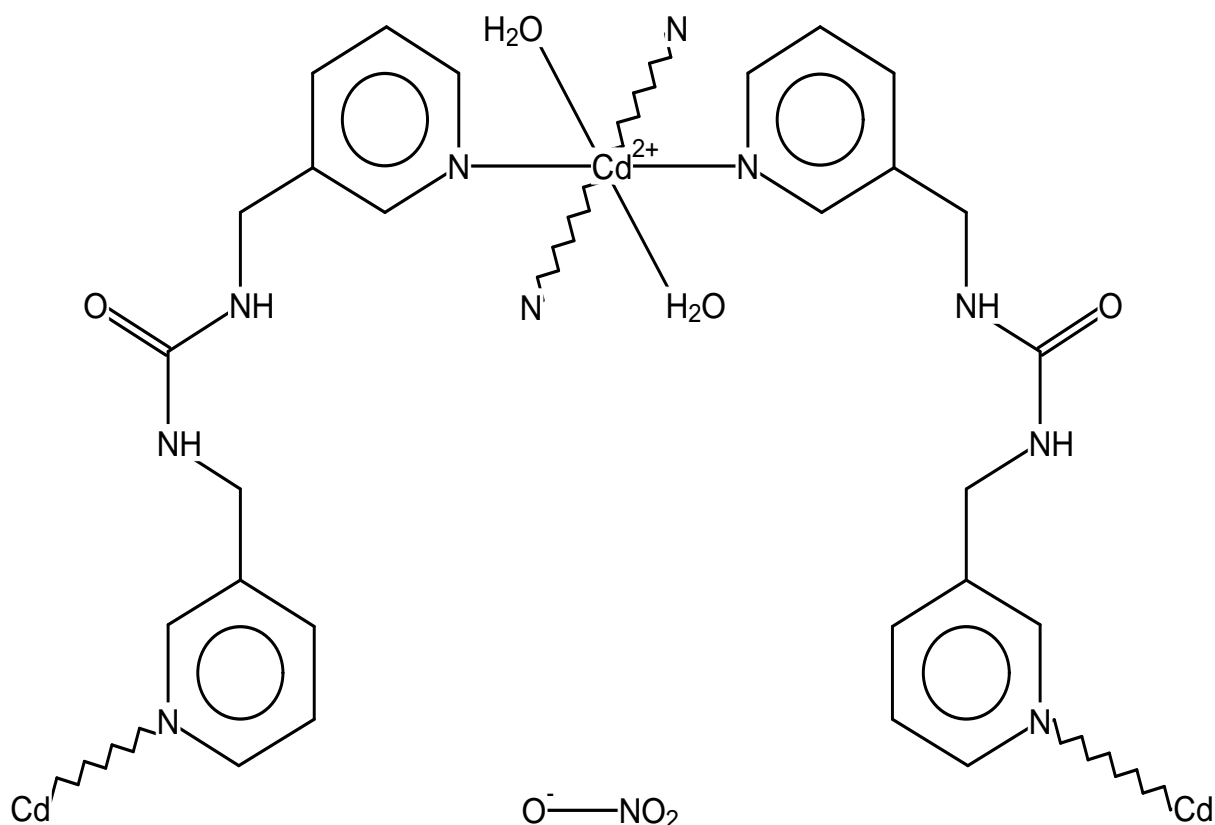
Reference: M.J.Plater, B.M.de Silva, J.M.S.Skakle, R.A.Howie, A.Riffat, T.Gelbrich, M.B.Hursthouse (2001) *Inorg.Chim.Acta* ,**325**,141

Formula: (C₂₆ H₃₂ Cd₁ N₈ O₄ ²⁺)_n,2n(N₁ O₃ ¹⁻)

Compound Name: catena-(bis(μ₂-N,N'-bis(3-pyridylmethyl)urea)-diaqua-cadmium(ii) dinitrate)

Space Group: P-1 **Cell:** **a** 7.838(0) **b** 10.044(0) **c** 10.287(0)
Space Group No.: 2 **(Å, °)** **α** 80.37(0) **β** 75.84(0) **γ** 83.93(0)

R-Factor (%): 2.84 **Temperature(K):** 150 **Density(g/cm³):** 1.628



Search: search4 (Sun Nov 20 19:32:48 2011): Hit 4

NOQSOB

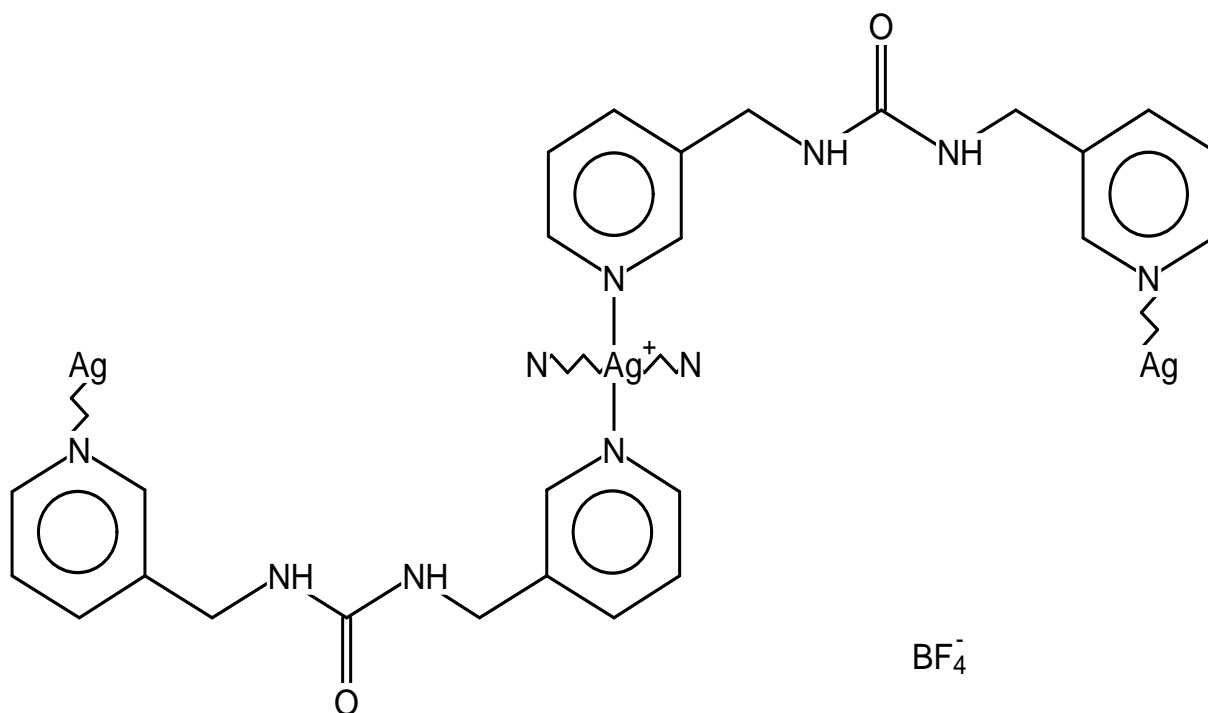
Reference: C.L.Schauer, E.Matwey, F.W.Fowler, J.W.Lauher (1997)
J.Am.Chem.Soc. ,**119**,10245

Formula: (C₂₆ H₂₈ Ag₁ N₈ O₂ 1⁺)_n,n(B₁ F₄ 1⁻)

Compound Name: catena(bis(μ₂-N,N'-bis(3-Pyridylmethyl)-urea)-silver tetrafluoroborate)

Space Group: P-4 **Cell:** **a** 11.984(2) **b** 11.984(2) **c** 4.625(1)
Space Group No.: 81 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.20 **Temperature(K):** 295 **Density(g/cm³):** 1.698



Search: search4 (Sun Nov 20 19:32:48 2011): Hit 5

TAPFAS

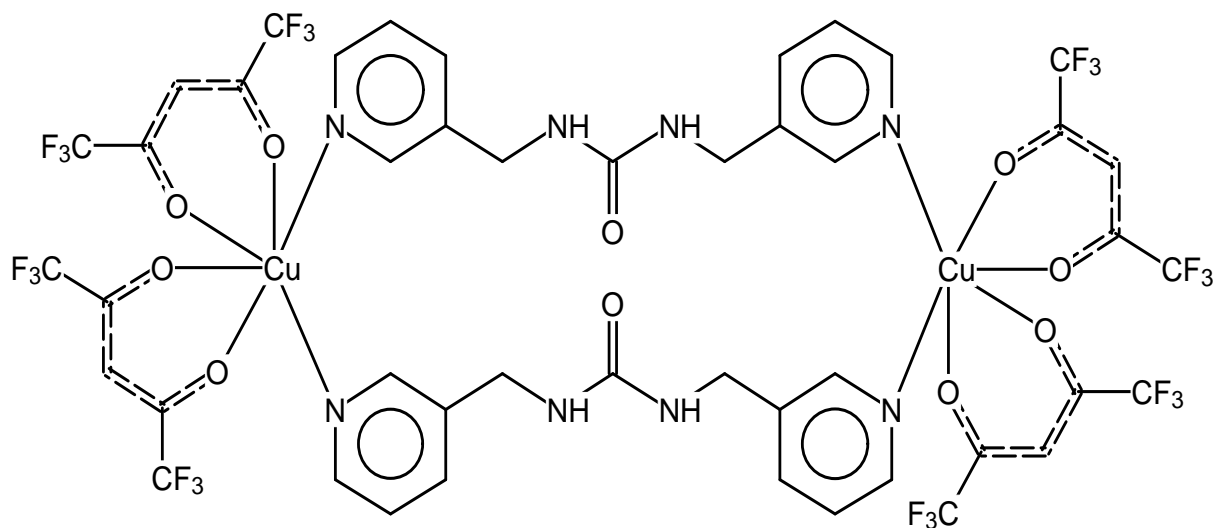
Reference: J.Granifo, M.T.Garland, R.Baggio (2005)
Inorg.Chem.Commun. ,**8**,568

Formula: C₄₆ H₃₂ Cu₂ F₂₄ N₈ O₁₀

Compound Name: bis(μ_2 -N,N'-bis(3-Pyridylmethyl)urea)-tetrakis(hexafluoroacetylacetonato)-di-copper(ii)

Space Group: C2/c **Cell:** **a** 24.524(3) **b** 9.042(0) **c** 27.253(3)
Space Group No.: 15 **(Å, °)** α 90.00 β 108.90(0) γ 90.00

R-Factor (%): 5.75 **Temperature(K):** 299 **Density(g/cm³):** 1.673



Search: search4 (Sun Nov 20 19:32:48 2011): Hit 6

VEDYOT

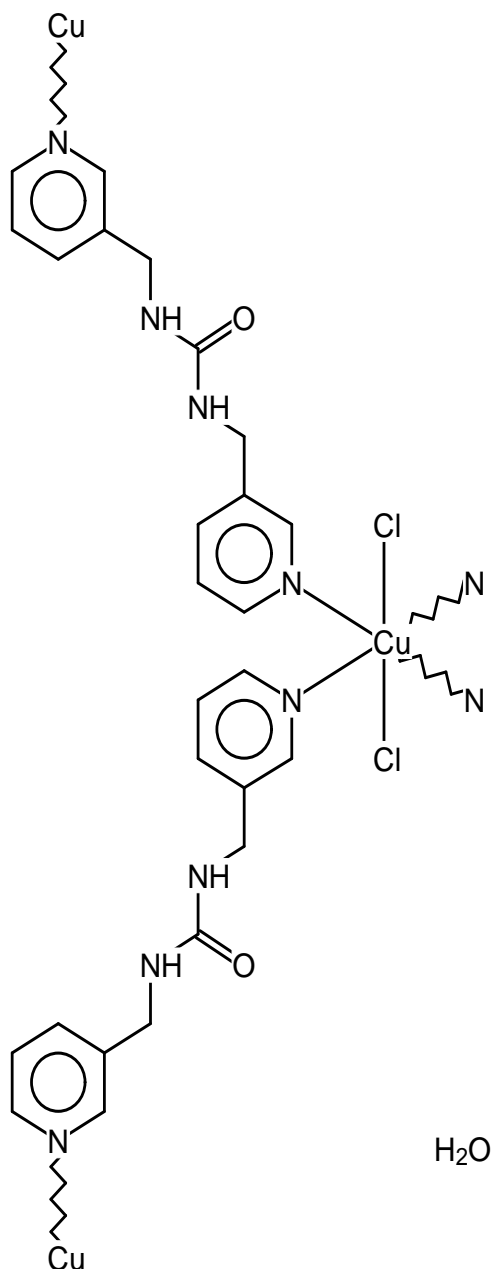
Reference: P.Diaz, J.Benet-Buchholz, R.Vilar, A.J.P.White (2006)
Inorg.Chem. ,**45**,1617

Formula: (C₂₆ H₂₈ Cl₂ Cu₁ N₈ O₂)_n,7n(H₂ O₁)

Compound Name: catena-(bis(μ₂-1,3-bis(3-Pyridylmethyl)urea-N,N')-dichloro-copper(ii) heptahydrate)

Space Group: P21/c **Cell:** **a** 11.055(0) **b** 21.402(0) **c** 15.442(1)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 105.12(0) **γ** 90.00

R-Factor (%): 5.75 **Temperature(K):** 173 **Density(g/cm³):** 1.403



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VEDYUZ

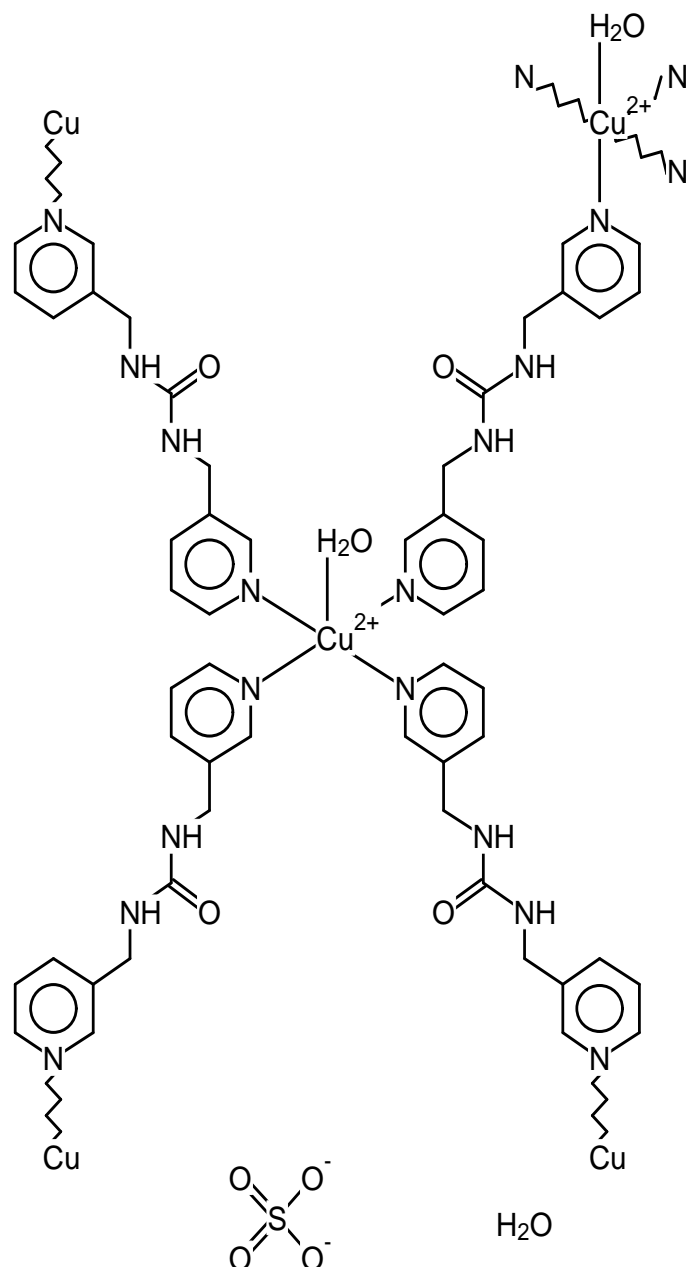
Reference: P.Diaz, J.Benet-Buchholz, R.Vilar, A.J.P.White (2006)
Inorg.Chem. ,**45**,1617

Formula: $(C_{52} H_{60} Cu_2 N_{16} O_6^{4+})_n, 2n(O_4 S_1^{2-}), 11n(H_2 O_1)$

Compound Name: catena-(tetrakis(μ_2 -1,3-bis(3-Pyridylmethyl)urea-N,N')-diaqua-di-copper(ii) disulfate undecahydrate)

Space Group: Pba2 **Cell:** **a** 18.419(1) **b** 20.412(1) **c** 8.938(0)
Space Group No.: 32 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.67 **Temperature(K):** 100 **Density(g/cm³):** 1.505



L44 and L45: 2HITS

1

Reference: S. Banerjee, N. N. Adarsh and P. Dastidar, *Eur. J. Inorg. Chem.* **2010**, 3770–3779.

Formula: C₁₃H₂₀CdN₄O₈S

Cell: a = 8.5328(5), b = 8.9113(5), c = 23.9587(14)

Space Group: P2₁2₁2₁

2

Reference: S. Banerjee, N. N. Adarsh and P. Dastidar, *Eur. J. Inorg. Chem.* **2010**, 3770–3779.

Formula: C₂₄H₂₈CdN₈O₈S

Cell: a = 8.9312(9), b = 12.6841(13), c = 13.7130(13); $\alpha = 87.699(2)$; $\beta = 81.445(2)$; $\gamma = 82.031(2)$

Space Group: P-1