

Search Overview

Search: search4
Date/Time done: Thu May 26 10:15:51 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: 18

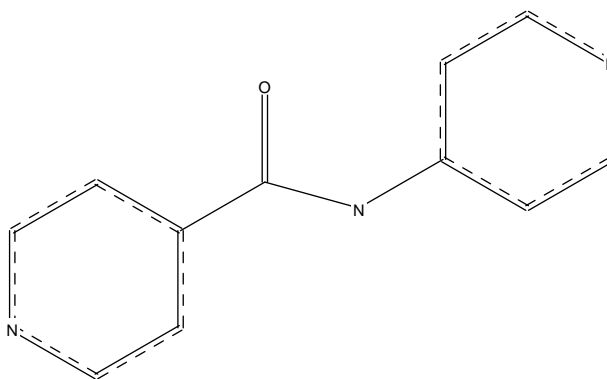
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

4M

Search: search4 (Thu May 26 10:15:51 2011): Hit 1

KAZTOV

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

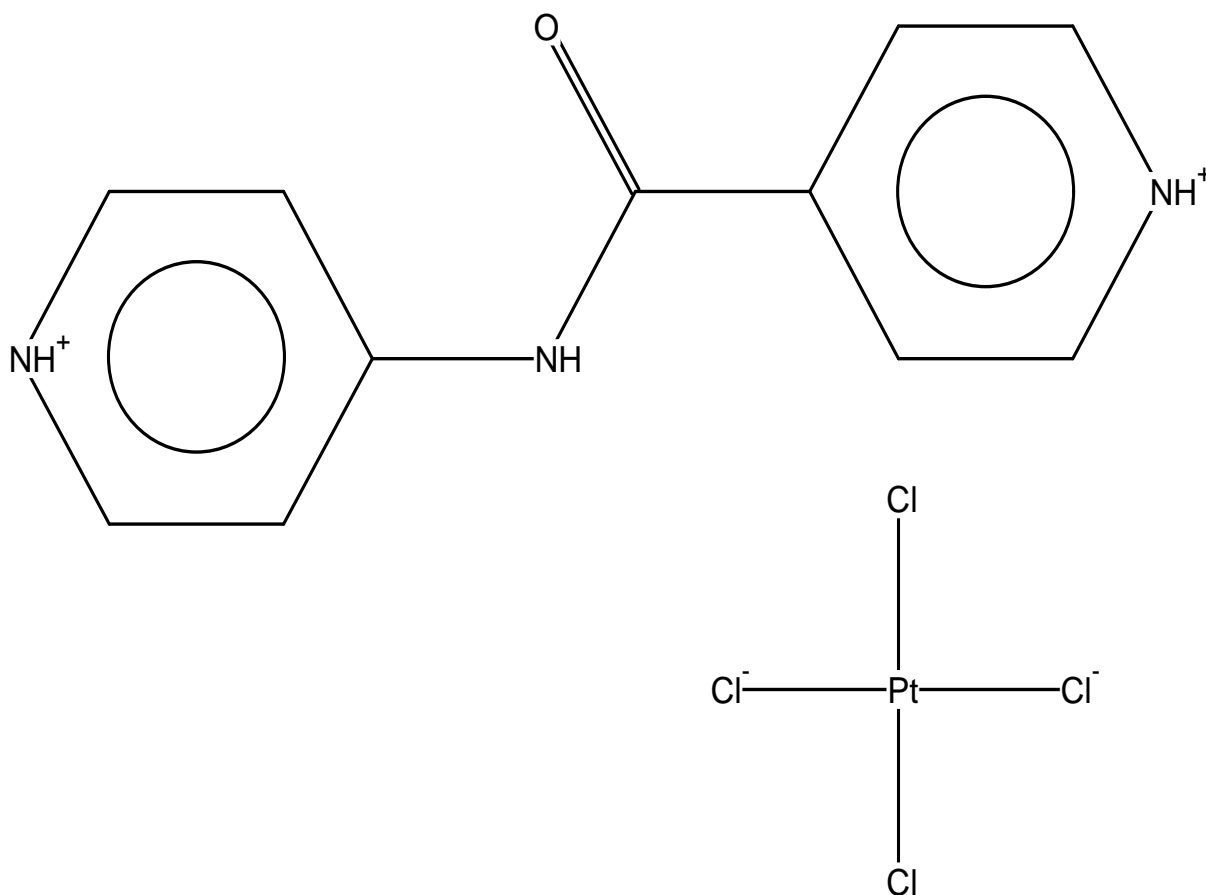
Formula: C₁₁ H₁₁ N₃ O₁²⁺, Cl₄ Pt₁²⁻

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

Space Group: P-1 **Cell:** **a** 7.021(1) **b** 9.280(2) **c** 11.633(3)

Space Group No.: 2 **(Å, °)** **α** 85.92(0) **β** 83.34(0) **γ** 76.84(0)

R-Factor (%): 3.87 **Temperature(K):** 298 **Density(g/cm³):** 2.441



Search: search4 (Thu May 26 10:15:51 2011): Hit 2

KAZTUB

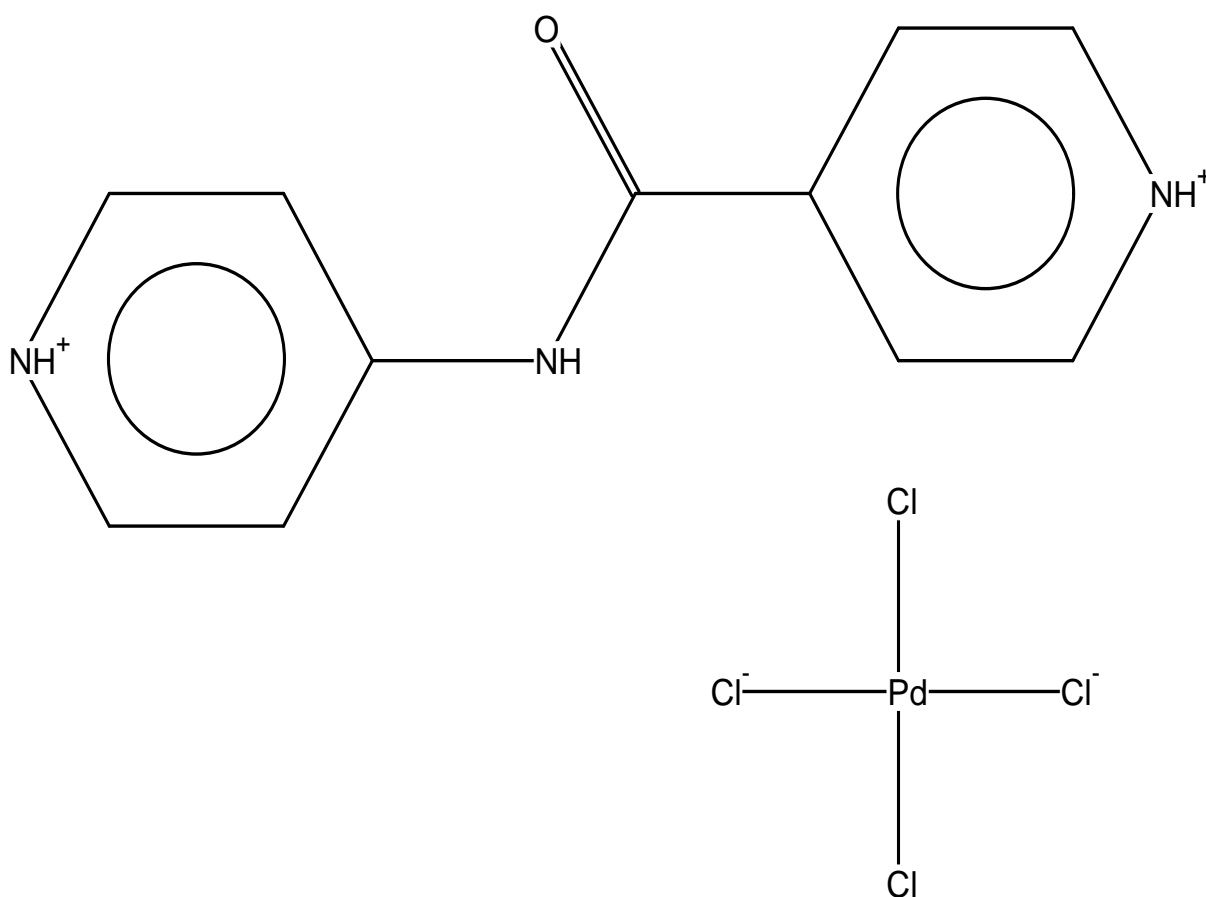
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *Cryst.Growth Des.* ,
6,216

Formula: C₁₁ H₁₁ N₃ O₁²⁺, Cl₄ Pd₁²⁻

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

Space Group: P-1 **Cell:** **a** 7.091(3) **b** 8.158(4) **c** 13.722(7)
Space Group No.: 2 **(Å, °)** α 102.42(0) β 95.69(0) γ 106.51(0)

R-Factor (%): 6.27 **Temperature(K):** 298 **Density(g/cm³):** 2.038



Search: search4 (Thu May 26 10:15:51 2011): Hit 3

KIFKUG

Reference: S.Ghosh, P.S.Mukherjee (2007) *Dalton Trans.* ,2542

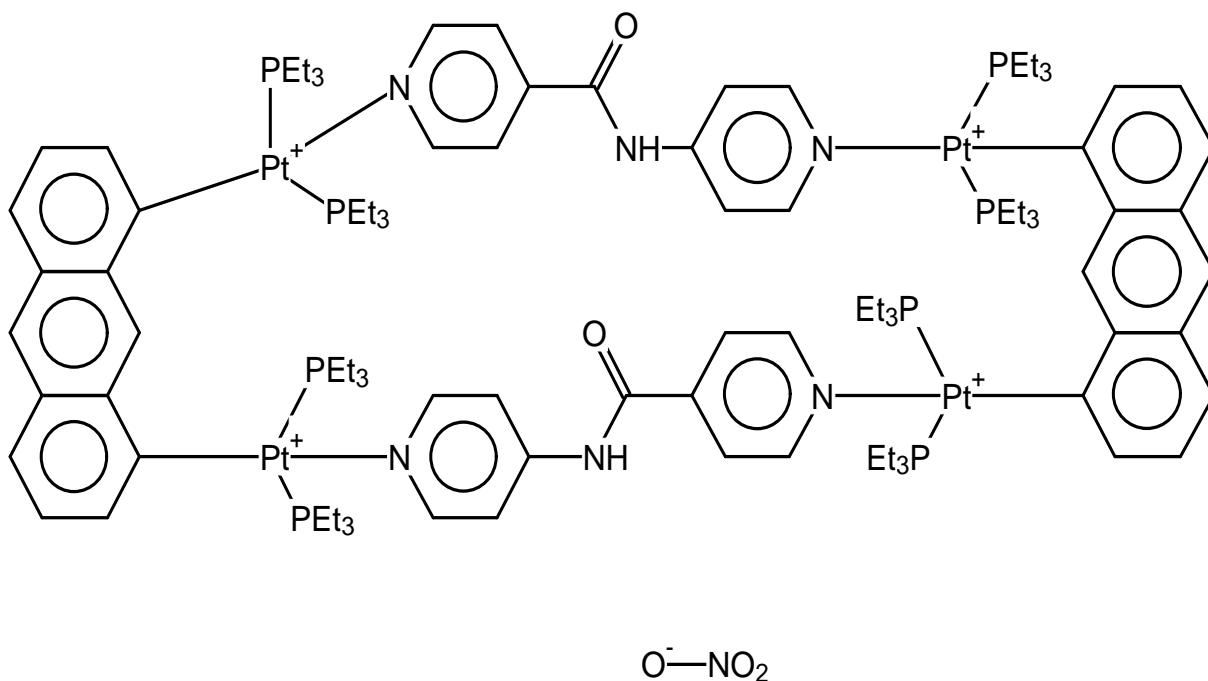
Formula: C₉₈ H₁₅₄ N₆ O₂ P₈ Pt₄⁴⁺,4(N₁ O₃¹⁻)

Compound Name: bis((μ₂-N-(4-Pyridyl)isonicotinamide-N,N')-(μ₂-anthracene-1,8-diyl))-octakis(triethylphosphine)-tetra-platinum tetranitrate unknown solvate

Space Group: C2/c **Cell:** **a** 40.612(1) **b** 14.795(0) **c** 20.004(0)

Space Group No.: 15 **(Å, °)** **α** 90.00 **β** 98.17(0) **γ** 90.00

R-Factor (%): 8.23 **Temperature(K):** 150 **Density(g/cm³):** 1.521



Search: search4 (Thu May 26 10:15:51 2011): Hit 4

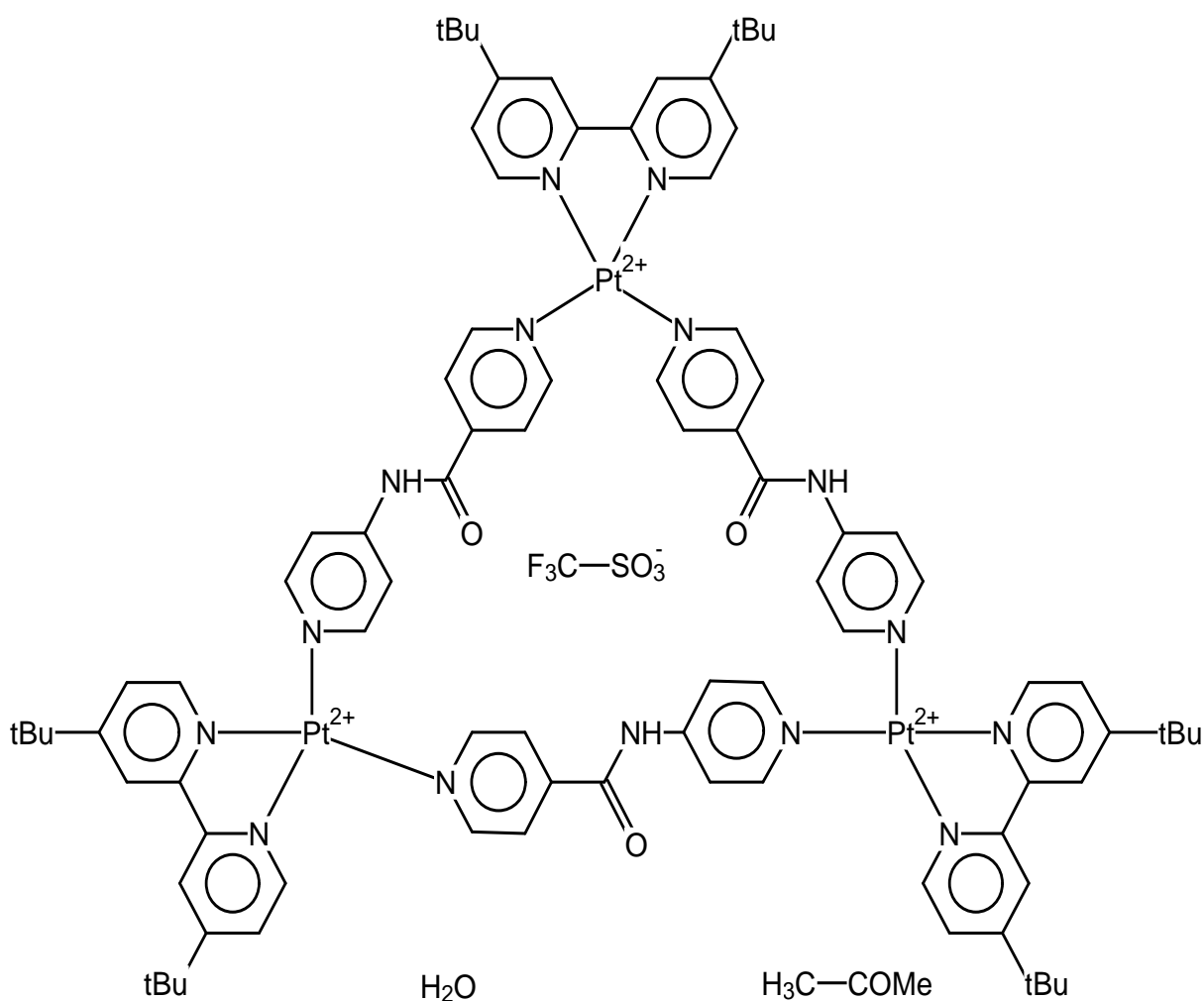
MEXBEW

Reference: Zengquan Qin, M.C.Jennings, R.J.Puddephatt (2001)
Chem.Commun. ,2676

Formula: $C_{87} H_{99} N_{15} O_3 Pt_3^{6+}, 6(C_1 F_3 O_3 S_1^{-}), C_3 H_6 O_1, 3(H_2 O_1)$

Compound Name: tris((μ_2 -N-(4-Pyridyl)isonicotinamide-N',N'')-(4,4'-di-t-butyl-2,2'-bipyridine-N,N')-platinum(ii) trifluoromethanesulfonate clathrate pentakis(trifluoromethanesulfonate) acetone solvate trihydrate

Space Group:	P-1	Cell:	a 15.240(0)	b 18.154(1)	c 23.462(1)
Space Group No.:	2	(Å, °)	α 79.11(0)	β 84.23(0)	γ 77.55(0)
R-Factor (%):	9.60	Temperature(K):	200	Density(g/cm³):	1.601



Search: search4 (Thu May 26 10:15:51 2011): Hit 5

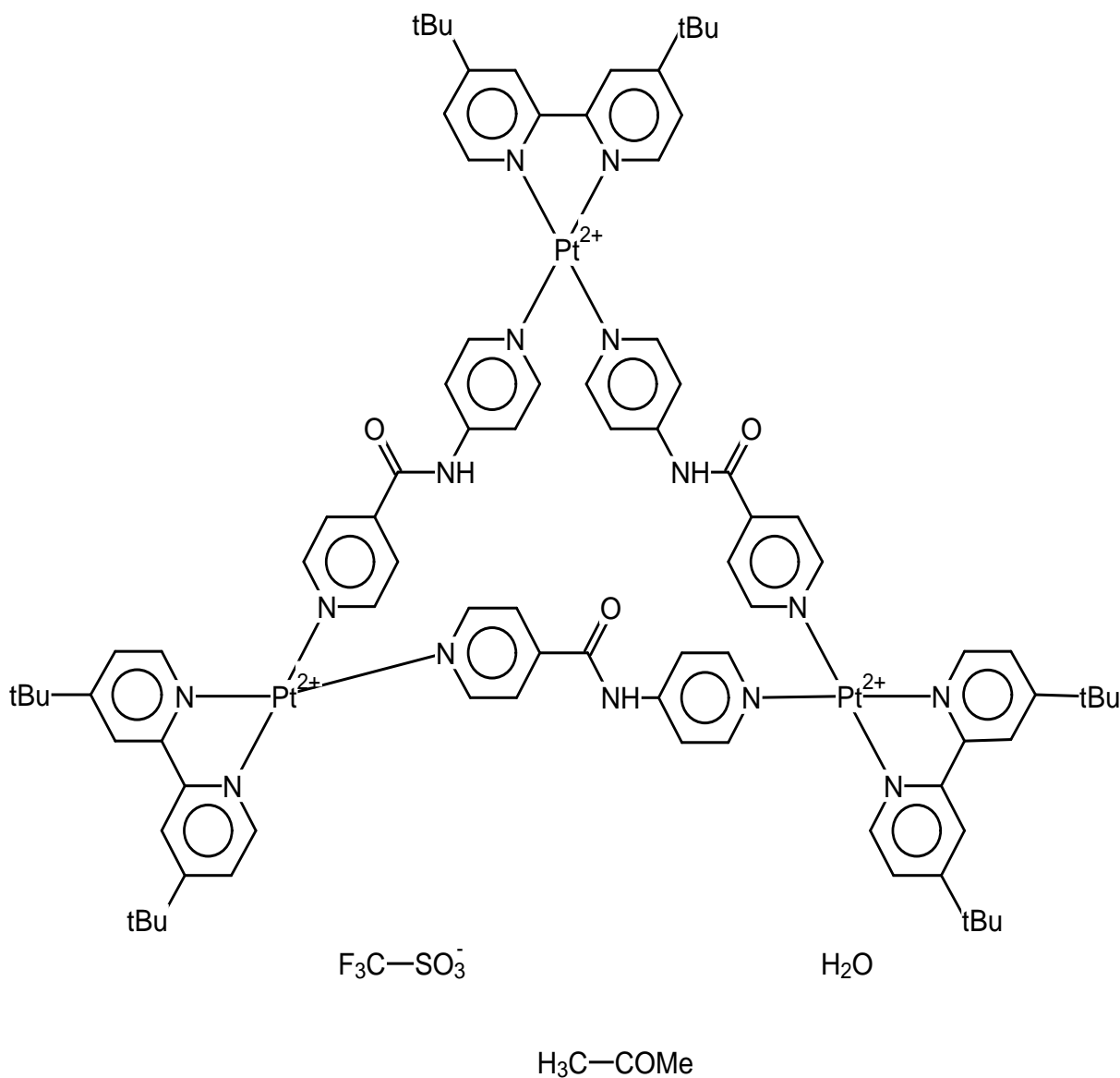
MEXBEW01

Reference: Zengquan Qin, M.C.Jennings, R.J.Puddephatt (2003)
Inorg.Chem. ,**42**,1956

Formula: $C_{87} H_{99} N_{15} O_3 Pt_3^{6+}, 6(C_1 F_3 O_3 S_1^{-1}), C_3 H_6 O_1, 3(H_2 O_1)$

Compound Name: tris((μ_2 -N-(4-Pyridyl)isonicotinamide-N',N'')-(4,4'-di-t-butyl-2,2'-bipyridine-N,N')-platinum(ii) trifluoromethanesulfonate clathrate pentakis(trifluoromethanesulfonate) acetone solvate trihydrate

Space Group:	P-1	Cell:	a 15.240(0)	b 18.154(1)	c 23.462(1)
Space Group No.:	2	(Å, °)	α 79.11(0)	β 84.23(0)	γ 77.55(0)
R-Factor (%):	9.60	Temperature(K):	200	Density(g/cm³):	1.601



Search: search4 (Thu May 26 10:15:51 2011): Hit 6

OHOROT

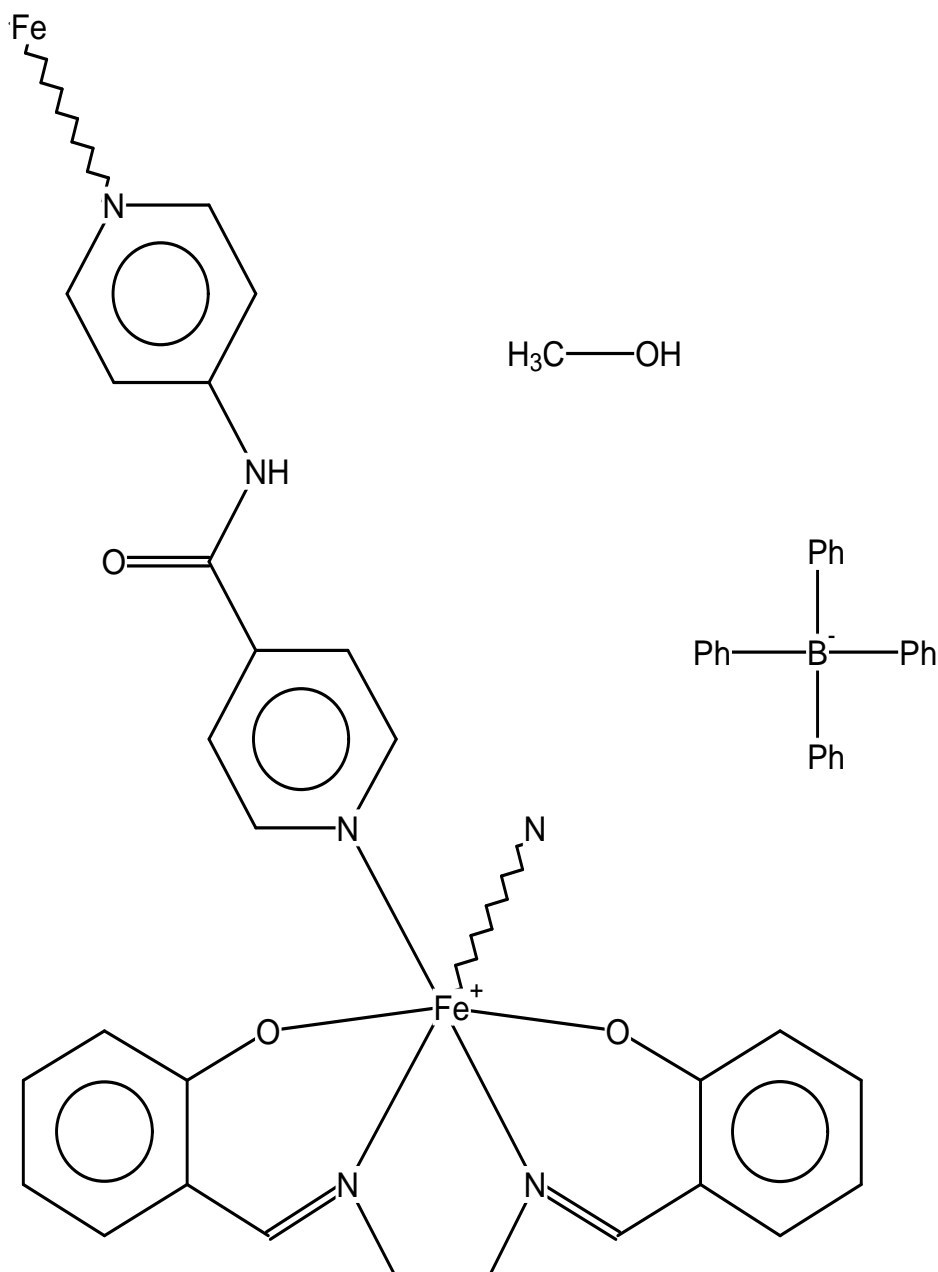
Reference: T.M.Ross, S.M.Neville, D.S.Innes, D.R.Turner,
B.Moubaraki, K.S.Murray (2010) *Dalton Trans.* ,**39**,149

Formula: $(C_{27} H_{23} Fe_1 N_5 O_3^{1+})_n, n(C_{24} H_{20} B_1^{1-})_n, 2n(C_1 H_4 O_1)$

Compound Name: catena-((μ_2 -N-(4-pyridyl)isonicotinamide)-(N,N'-bis(salicylidene) ethylenediamine)-iron(iii) tetraphenylborate methanol solvate)

Space Group: P21/n **Cell:** **a** 13.709(1) **b** 14.501(1) **c** 22.956(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 96.14(0) γ 90.00

R-Factor (%): 11.75 **Temperature(K):** 123 **Density(g/cm³):** 1.324



Search: search4 (Thu May 26 10:15:51 2011): Hit 7

PAQLAV

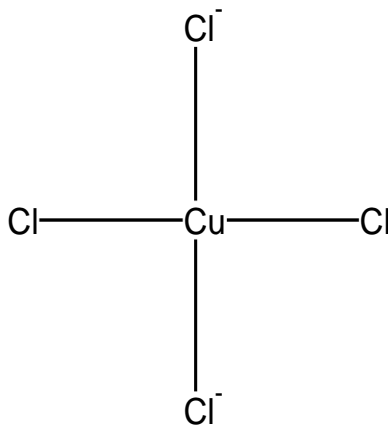
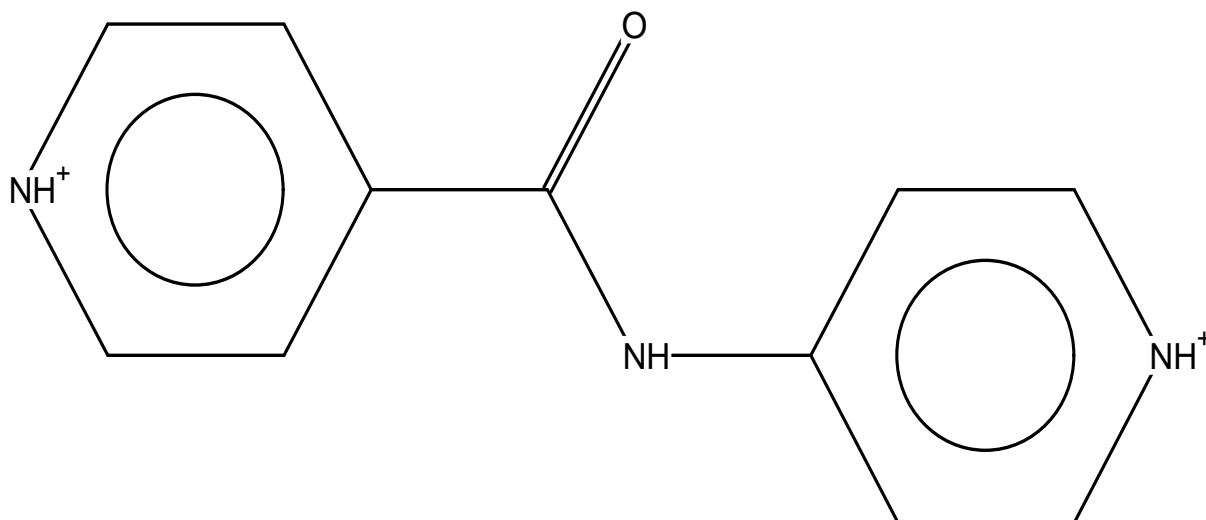
Reference: D.K.Kumar, A.Ballabh, D.A.Jose, P.Dastidar, A.Das
(2005) *Cryst.Growth Des.* ,5,651

Formula: $C_{11} H_{11} N_3 O_1^{2+}, Cl_4 Cu_1^{2-}$

Compound Name: N-(4-Pyridinio)isonicotinamidinium tetrachloro-copper

Space Group: P-1 **Cell:** **a** 7.341(2) **b** 7.401(7) **c** 14.620(7)
Space Group No.: 2 **(Å, °)** α 104.60(5) β 98.24(3) γ 90.69(5)

R-Factor (%): 5.51 **Temperature(K):** 293 **Density(g/cm³):** 1.777



Search: search4 (Thu May 26 10:15:51 2011): Hit 8

PAQLAV01

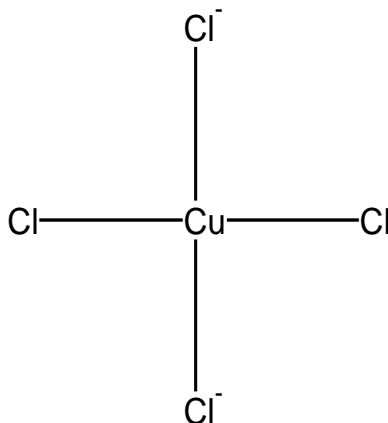
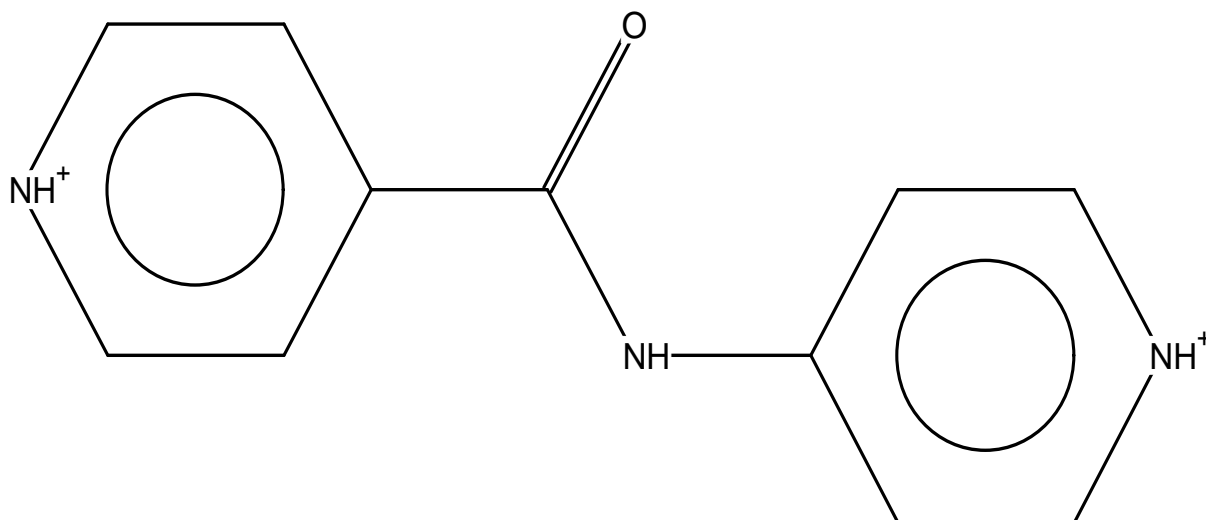
Reference: D.K.Kumar, A.Ballabh, D.A.Jose, P.Dastidar, A.Das
(2005) *Cryst.Growth Des.* ,5,651

Formula: C₁₁ H₁₁ N₃ O₁²⁺, Cl₄ Cu₁²⁻

Compound Name: N-(4-Pyridinio)isonicotinamidinium tetrachloro-copper

Space Group: P-1 **Cell:** **a** 7.242(1) **b** 7.400(1) **c** 14.848(2)
Space Group No.: 2 **(Å, °)** **α** 77.77(0) **β** 76.10(0) **γ** 83.13(0)

R-Factor (%): 5.56 **Temperature(K):** 273 **Density(g/cm³):** 1.793



Search: search4 (Thu May 26 10:15:51 2011): Hit 9

POJYUJ

Reference: K.Uemura, Y.Kumamoto, S.Kitagawa (2008)
Chem.-Eur.J. ,**14**,9565

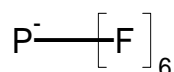
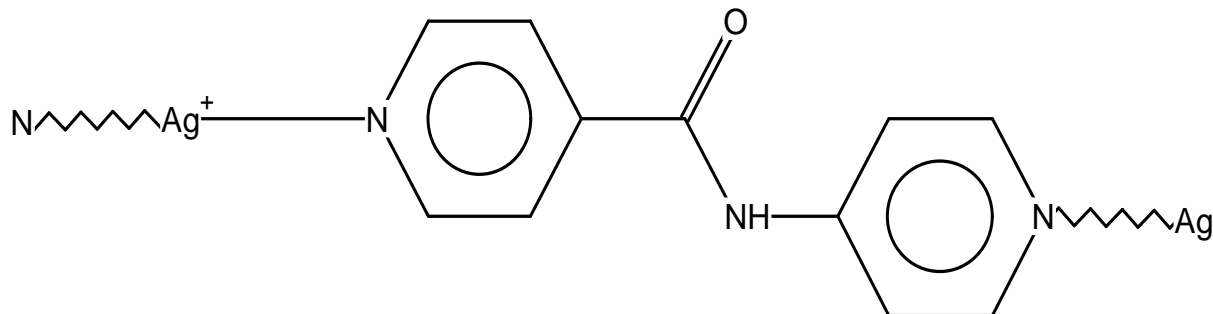
Formula: (C₁₁ H₉ Ag₁ N₃ O₁ 1⁺)_n,n(F₆ P₁ 1⁻)

Compound Name: catena-((μ₂-N-(Pyridin-4-yl)pyridine-4-carboxamide-N,N')-silver(i) hexafluorophosphate)

Synonym: catena-((μ₂-N-(Pyridin-4-yl)isonicotinamide-N,N')-silver(i) hexafluorophosphate)

Space Group: C2/c **Cell:** **a** 20.222(8) **b** 8.652(3) **c** 16.482(6)
Space Group No.: 15 **(Å, °)** **α** 90.00 **β** 92.28(0) **γ** 90.00

R-Factor (%): 7.03 **Temperature(K):** 293 **Density(g/cm³):** 2.084



Search: search4 (Thu May 26 10:15:51 2011): Hit 10

POJZAQ

Reference: K.Uemura, Y.Kumamoto, S.Kitagawa (2008)
Chem.-Eur.J. ,**14**,9565

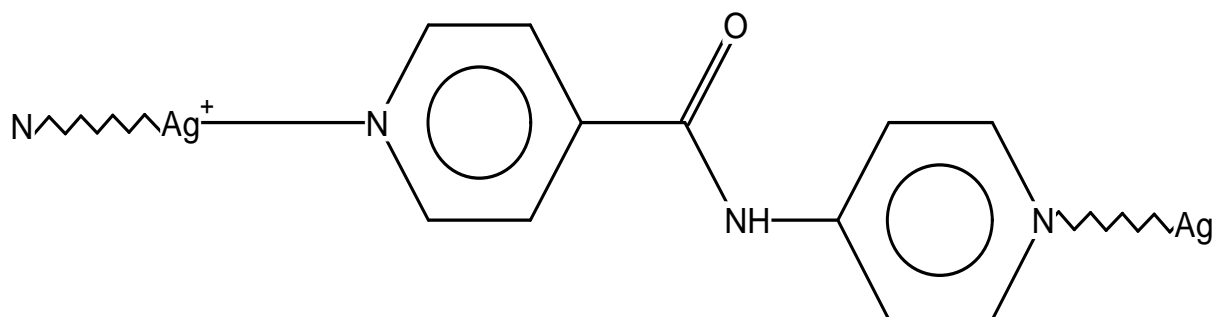
Formula: (C₁₁ H₉ Ag₁ N₃ O₁¹⁺)_n,n(Cl₁ O₄¹⁻)

Compound Name: catena-((μ₂-N-(Pyridin-4-yl)pyridine-4-carboxamide-N,N')-silver(i) perchlorate)

Synonym: catena-((μ₂-N-(Pyridin-4-yl)isonicotinamide-N,N')-silver(i) perchlorate)

Space Group: C2/c **Cell:** **a** 19.760(10) **b** 8.112(3) **c** 16.797(8)
Space Group No.: 15 **(Å, °)** **α** 90.00 **β** 93.52(0) **γ** 90.00

R-Factor (%): 10.37 **Temperature(K):** 293 **Density(g/cm³):** 2.010



Search: search4 (Thu May 26 10:15:51 2011): Hit 11

POJZEU

Reference: K.Uemura, Y.Kumamoto, S.Kitagawa (2008)
Chem.-Eur.J. ,**14**,9565

Formula: (C₁₁ H₉ Ag₁ N₃ O₁¹⁺)_n,n(B₁ F₄¹⁻)

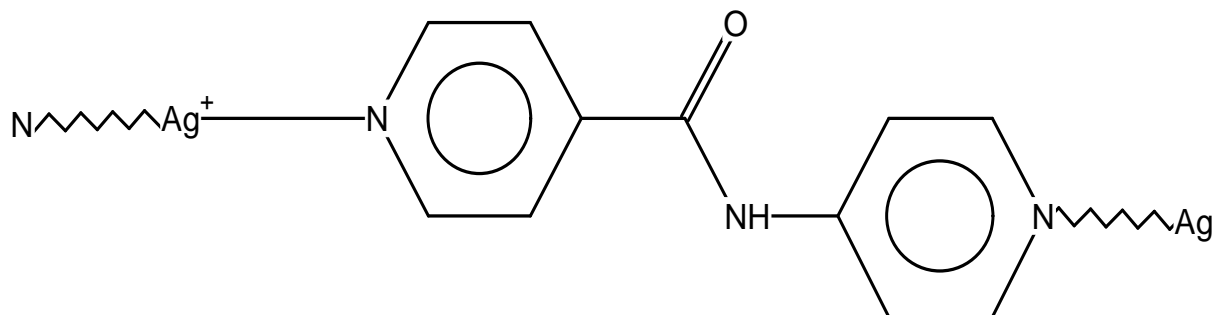
Compound Name: catena-((μ₂-N-(Pyridin-4-yl)pyridine-4-carboxamide-N,N')-silver(i) tetrafluoroborate)

Synonym: catena-((μ₂-N-(Pyridin-4-yl)isonicotinamide-N,N')-silver(i) tetrafluoroborate)

Space Group: C2/c **Cell:** **a** 19.670(8) **b** 7.908(3) **c** 16.980(7)

Space Group No.: 15 **(Å, °)** **α** 90.00 **β** 92.94(0) **γ** 90.00

R-Factor (%): 4.99 **Temperature(K):** 293 **Density(g/cm³):** 1.984



BF₄⁻

Search: search4 (Thu May 26 10:15:51 2011): Hit 12

POJZIY

Reference: K.Uemura, Y.Kumamoto, S.Kitagawa (2008)
Chem.-Eur.J. ,**14**,9565

Formula: (C₁₁ H₉ Ag₁ N₃ O₁¹⁺)_n,n(N₁ O₃¹⁻)

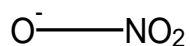
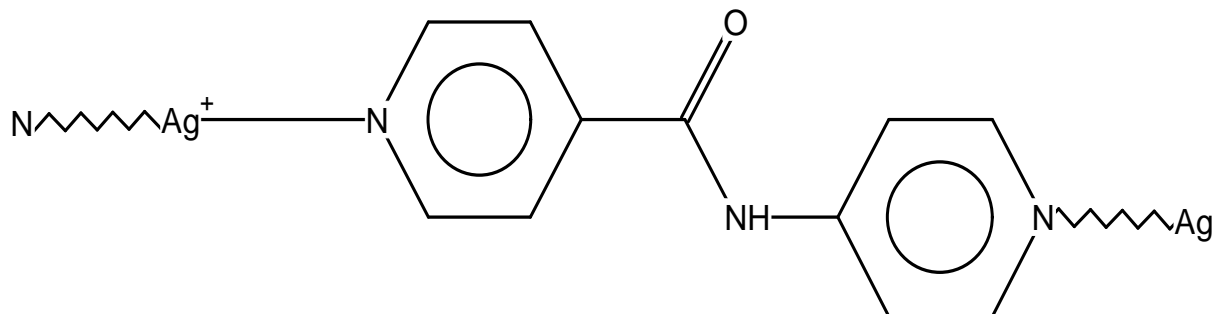
Compound Name: catena-((μ₂-N-(Pyridin-4-yl)pyridine-4-carboxamide-N,N')-silver(i) nitrate)

Synonym: catena-((μ₂-N-(Pyridin-4-yl)isonicotinamide-N,N')-silver(i) nitrate)

Space Group: C2/c **Cell:** **a** 19.670(10) **b** 6.728(4) **c** 18.670(10)

Space Group No.: 15 **(Å, °)** **α** 90.00 **β** 91.66(0) **γ** 90.00

R-Factor (%): 4.39 **Temperature(K):** 293 **Density(g/cm³):** 1.985



Search: search4 (Thu May 26 10:15:51 2011): Hit 13

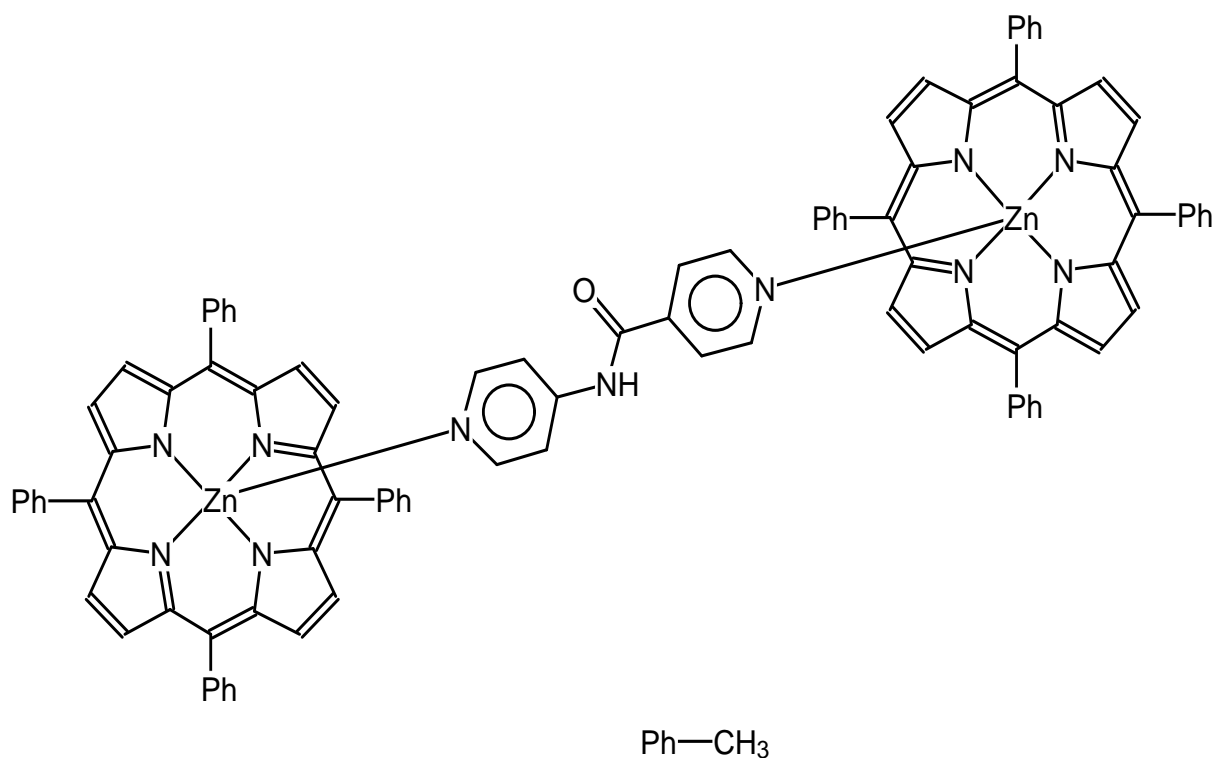
VIMZOH

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

Formula: C₉₉ H₆₅ N₁₁ O₁ Zn₂,4(C₇ H₈)

Compound Name: (μ₂-N-(4-Pyridyl)isonicotinamide)-bis(5,10,15,20-tetraphenylporphyrinato)-di-zinc(ii) bis(toluene) clathrate toluene solvate

Space Group:	P-1	Cell:	a 11.170(3)	b 11.284(3)	c 22.556(6)
Space Group No.:	2	(Å, °)	α 80.64(0)	β 86.85(0)	γ 73.52(0)
R-Factor (%):	8.19	Temperature(K):	100	Density(g/cm³):	1.188



Search: search4 (Thu May 26 10:15:51 2011): Hit 14

VIMZUN

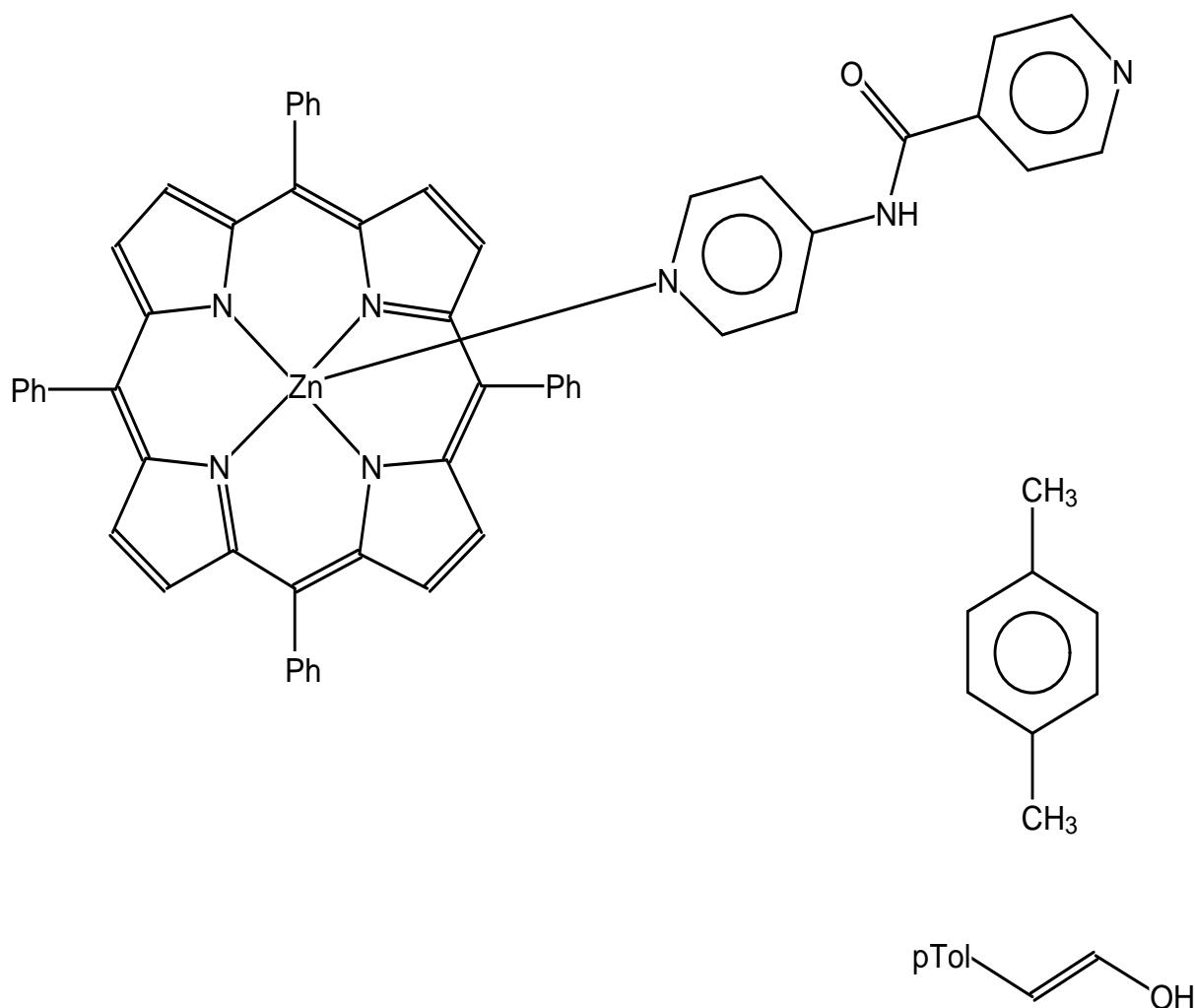
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *Inorg.Chem.* ,**46**, 7351

Formula: C₅₅ H₃₇ N₇ O₁ Zn₁, C₈ H₁₀, C₉ H₁₀ O₁

Compound Name: (N-(4-Pyridyl)isonicotinamide)-(5,10,15,20-tetraphenylporphyrinato)-zinc(ii) p-xylene 2-(p-tolyl)ethenol clathrate

Space Group: P21/c **Cell:** **a** 11.682(2) **b** 23.694(5) **c** 22.016(4)
Space Group No.: 14 **(Å, °)** α 90.00 β 104.75(0) γ 90.00

R-Factor (%): 5.79 **Temperature(K):** 150 **Density(g/cm³):** 1.260



Search: search4 (Thu May 26 10:15:51 2011): Hit 15

VIPTUK

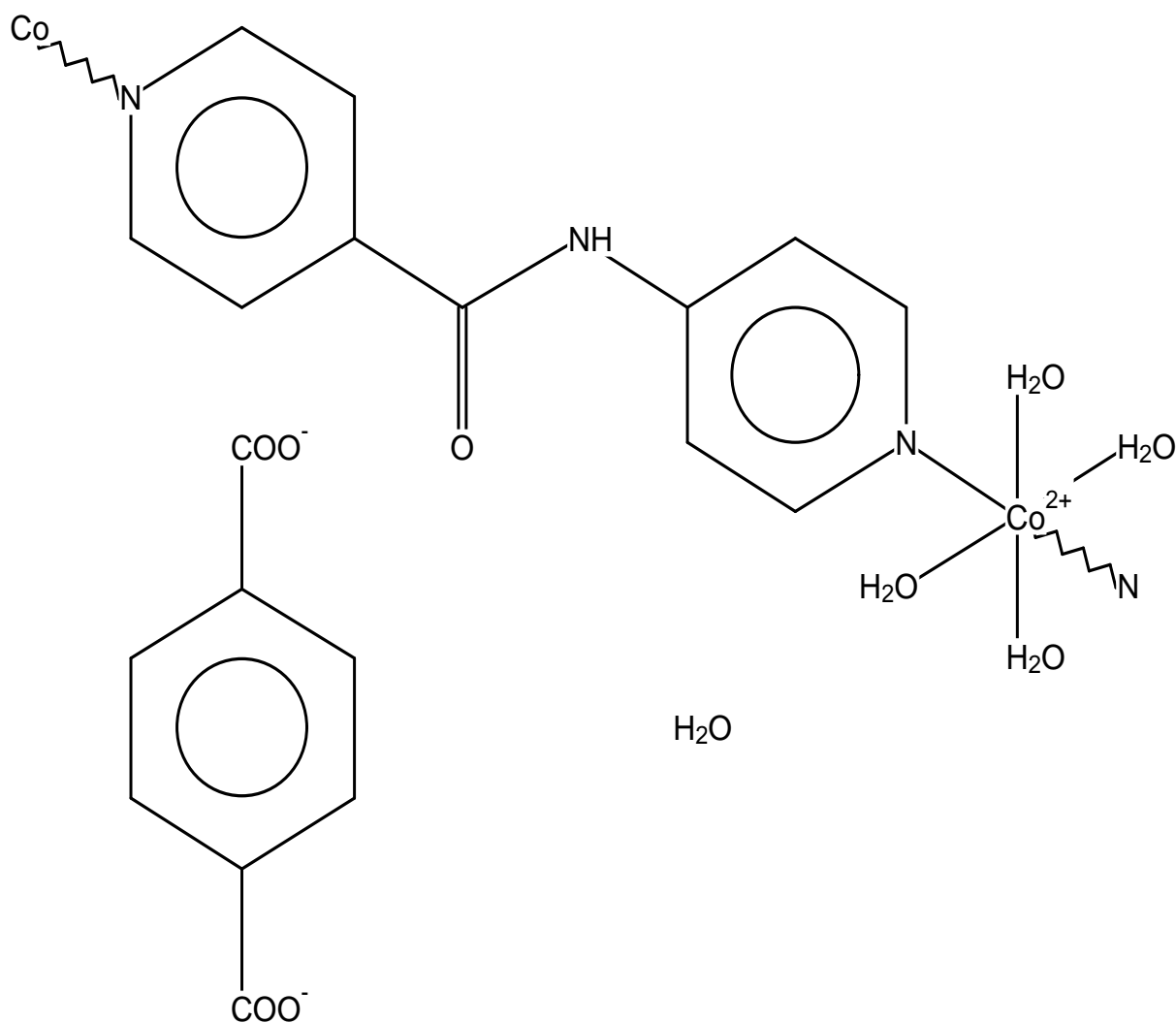
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *CrystEngComm*, **9**, 895

Formula: $(C_{11}H_{17}Co_1N_3O_5^{2+})_n, n(C_8H_4O_4^{2-})_n, 3n(H_2O)_1$

Compound Name: catena-((μ_2 -N-(4-Pyridyl)isonicotinamide)-tetraqua-cobalt(ii) terephthalate trihydrate)

Space Group: P21/c **Cell:** **a** 14.887(1) **b** 11.860(1) **c** 13.946(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 115.34(0) γ 90.00

R-Factor (%): 4.51 **Temperature(K):** 100 **Density(g/cm³):** 1.637



Search: search4 (Thu May 26 10:15:51 2011): Hit 16

VIPVAS

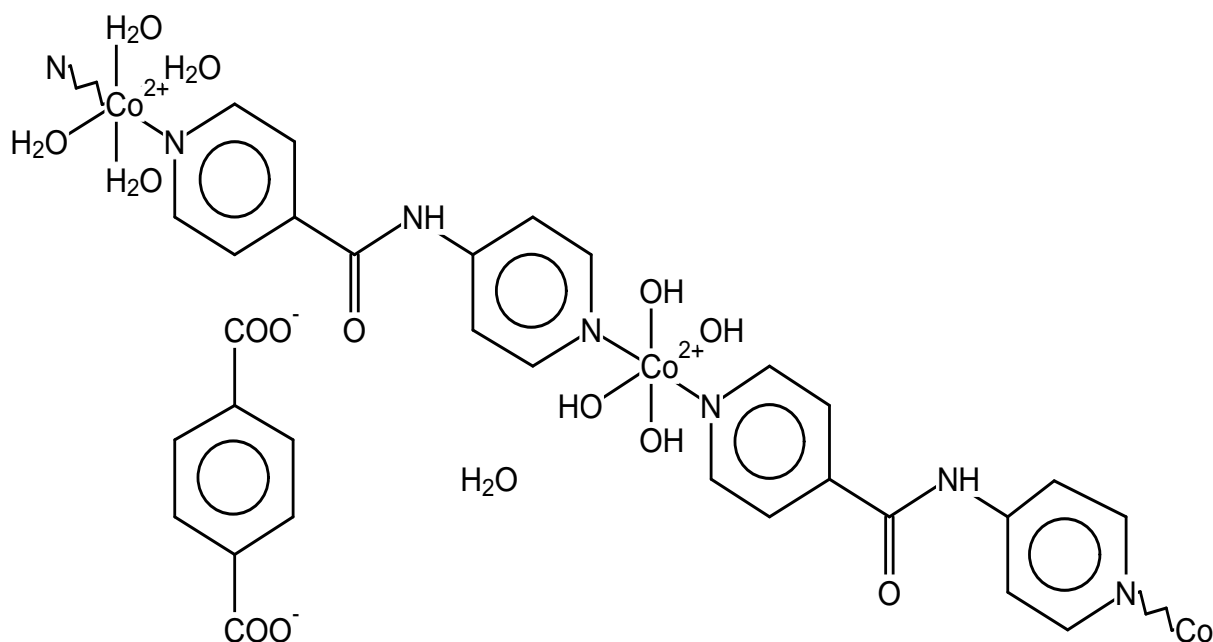
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *CrystEngComm* ,9, 895

Formula: $(C_{22} H_{30} Co_2 N_6 O_{10}^{4+})_n, 2n(C_8 H_4 O_4^{2-}), 10n(H_2 O_1)$

Compound Name: catena-(bis(μ_2 -N-(4-Pyridyl)isonicotinamide)-octaaqua-di-cobalt(ii) bis(terephthalate) decahydrate)

Space Group: P-1 **Cell:** **a** 14.228(2) **b** 14.831(3) **c** 14.954(3)
Space Group No.: 2 (**Å, °**) α 61.24(0) β 79.34(0) γ 66.12(0)

R-Factor (%): 9.13 **Temperature(K):** 298 **Density(g/cm³):** 1.529



Search: search4 (Thu May 26 10:15:51 2011): Hit 17

YEPDIH

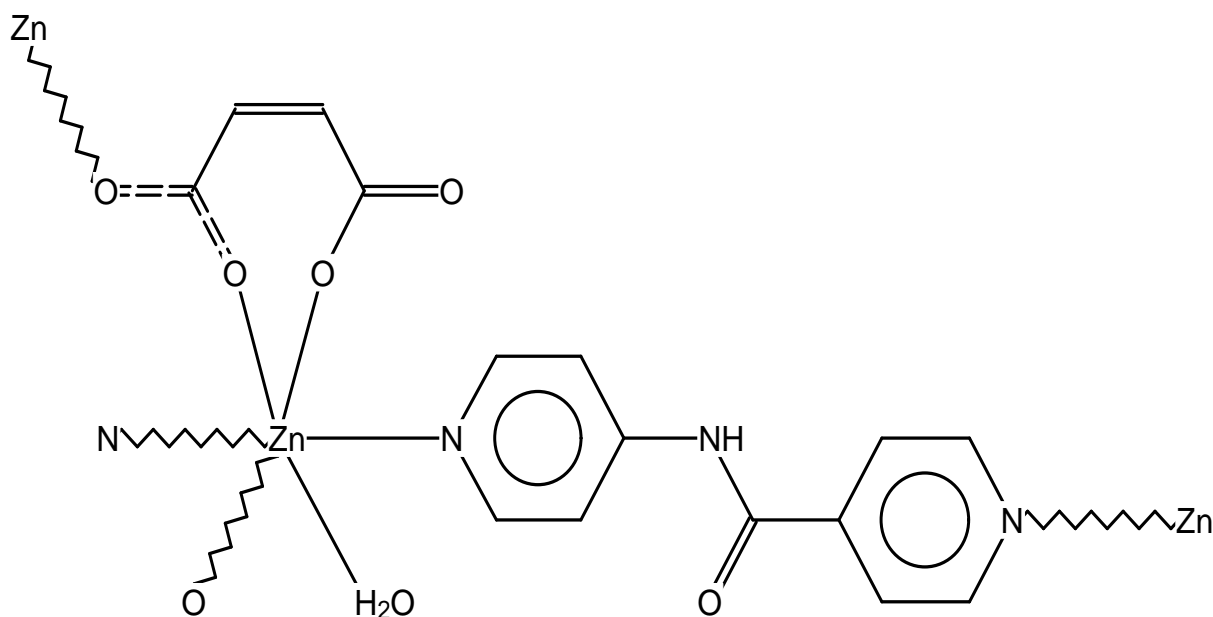
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *Cryst.Growth Des.* ,
6,1903

Formula: (C₁₅ H₁₃ N₃ O₆ Zn₁)_n

Compound Name: catena-((μ₂-Maleato-O,O',O'')-(μ₂-N-(4-pyridyl)isonicotinamide-N,N')-
aqua-zinc(ii))

Space Group: P21/c **Cell:** **a** 9.194(0) **b** 8.804(0) **c** 19.555(2)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 91.11(0) **γ** 90.00

R-Factor (%): 2.65 **Temperature(K):** 100 **Density(g/cm³):** 1.665



Search: search4 (Thu May 26 10:15:51 2011): Hit 18

YEPFOP

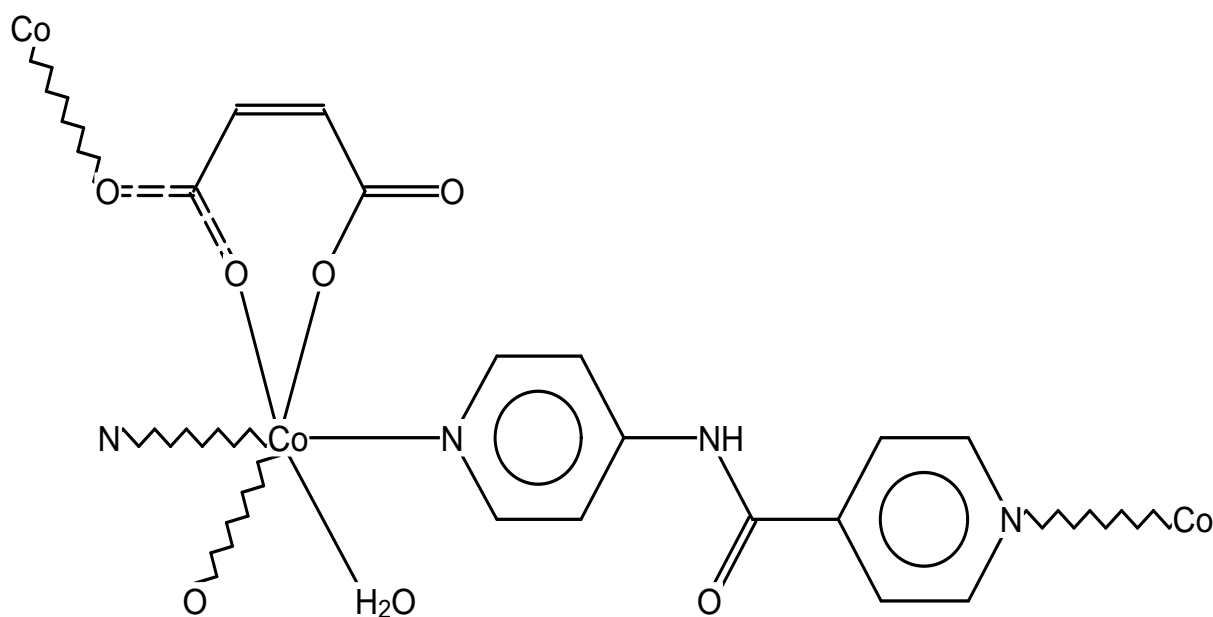
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *Cryst.Growth Des.* ,
6,1903

Formula: (C₁₅ H₁₃ Co₁ N₃ O₆)_n

Compound Name: catena-((μ₂-Maleato-O,O',O'')-(μ₂-N-(4-pyridyl)isonicotinamide-N,N')-
aqua-cobalt(ii))

Space Group: P21/c **Cell:** **a** 9.179(0) **b** 8.730(0) **c** 19.481(1)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 91.31(0) **γ** 90.00

R-Factor (%): 4.75 **Temperature(K):** 100 **Density(g/cm³):** 1.661



Search Overview

Search: search5
Date/Time done: Thu May 26 10:17:05 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

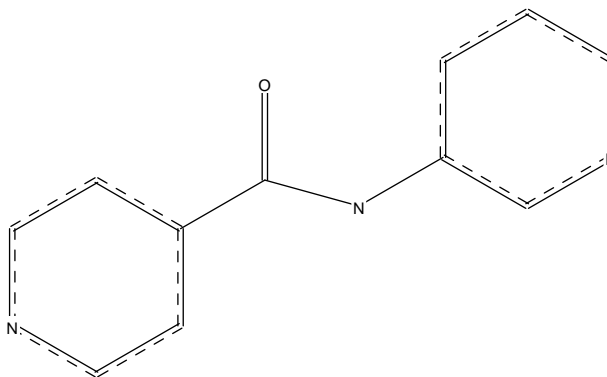
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

4M

Search: search5 (Thu May 26 10:17:05 2011): Hit 1

DEPSUN

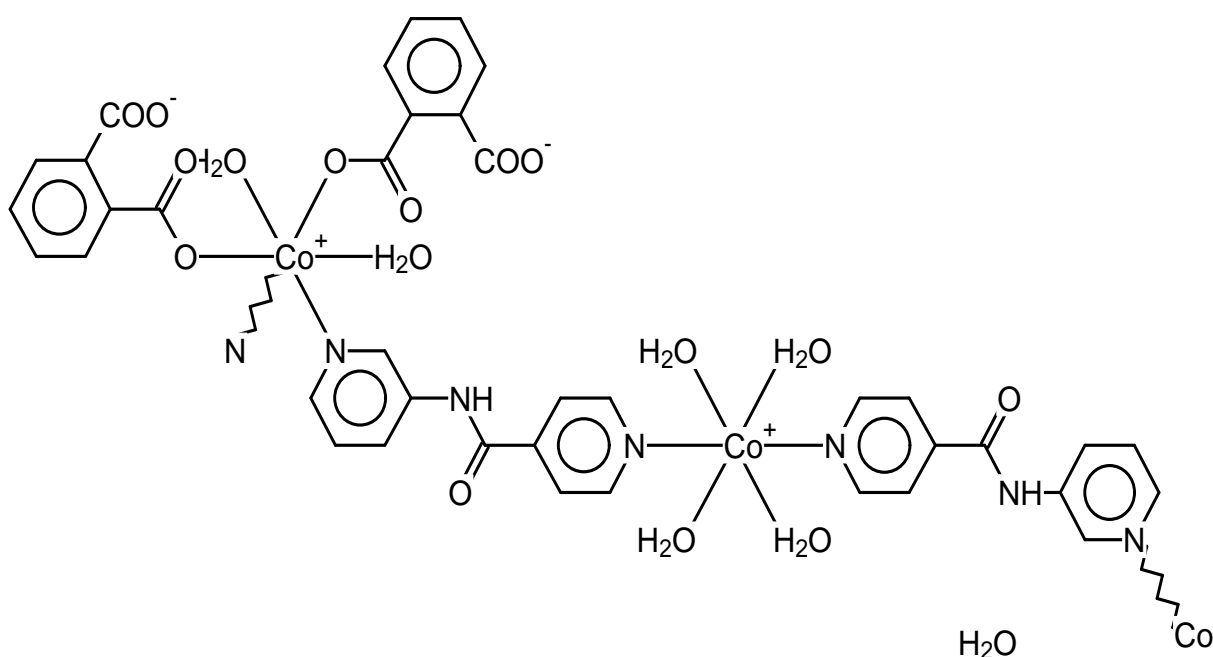
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *J.Mol.Struct.* ,**796**, 139

Formula: $(C_{38} H_{38} Co_2 N_6 O_{16})_n \cdot 2n(H_2 O)_1$

Compound Name: catena-(bis(μ_2 -N-(3-pyridyl)isonicotinamide)-bis(phthalato)-hexaaqua-di-cobalt(ii) dihydrate)

Space Group: P21/n **Cell:** **a** 10.665(0) **b** 7.995(0) **c** 24.744(1)
Space Group No.: 14 (**Å, °**) α 90.00 β 102.38(0) γ 90.00

R-Factor (%): 3.35 **Temperature(K):** 100 **Density(g/cm³):** 1.593



Search: search5 (Thu May 26 10:17:05 2011): Hit 2

KAZVIR

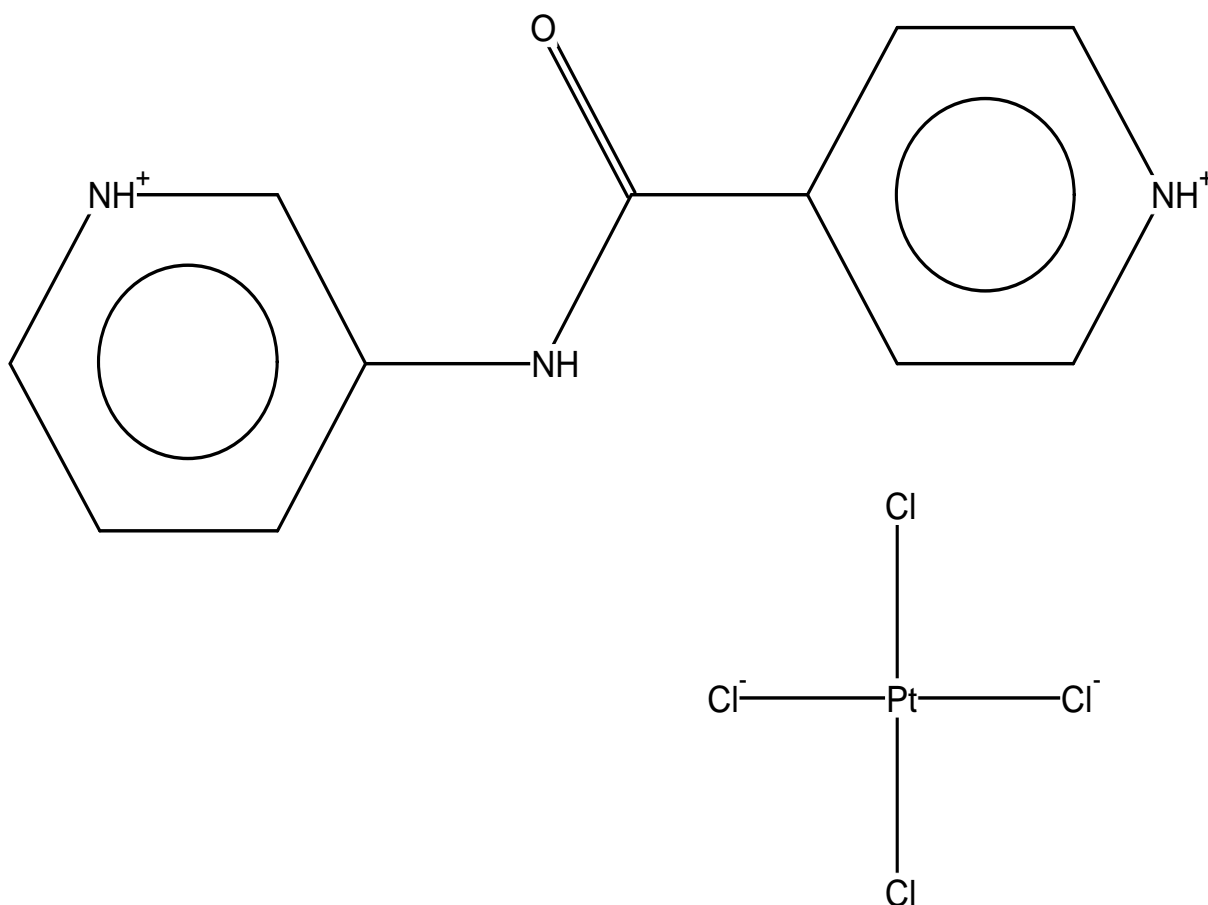
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *Cryst.Growth Des.* ,
6,216

Formula: C₁₁ H₁₁ N₃ O₁ 2⁺, Cl₄ Pt₁ 2⁻

Compound Name: N-(3-Pyridinio)isonicotinamidinium tetrachloro-platinum(ii)

Space Group: P21/n **Cell:** **a** 10.624(0) **b** 11.190(0) **c** 12.922(1)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 97.60(0) **γ** 90.00

R-Factor (%): 2.59 **Temperature(K):** 298 **Density(g/cm³):** 2.347



Search: search5 (Thu May 26 10:17:05 2011): Hit 3

KAZVOX

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

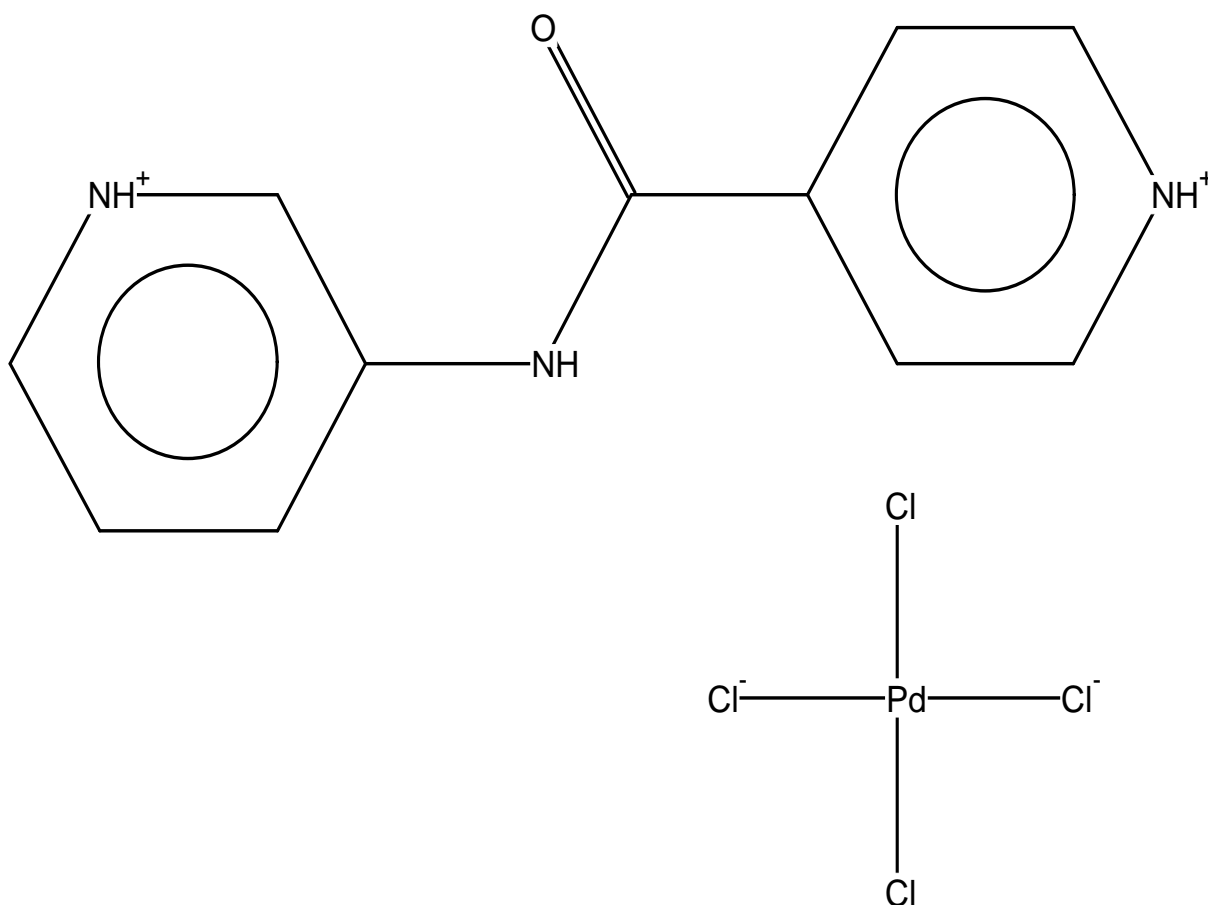
Formula: C₁₁ H₁₁ N₃ O₁ 2⁺, Cl₄ Pd₁ 2⁻

Compound Name: N-(3-Pyridinio)isonicotinamidinium tetrachloro-palladium(ii)

Space Group: C2/c **Cell:** **a** 24.166(1) **b** 7.974(0) **c** 15.287(1)

Space Group No.: 15 **(Å, °)** **α** 90.00 **β** 92.70(0) **γ** 90.00

R-Factor (%): 3.39 **Temperature(K):** 100 **Density(g/cm³):** 2.029



Search: search5 (Thu May 26 10:17:05 2011): Hit 4

MOVPAO

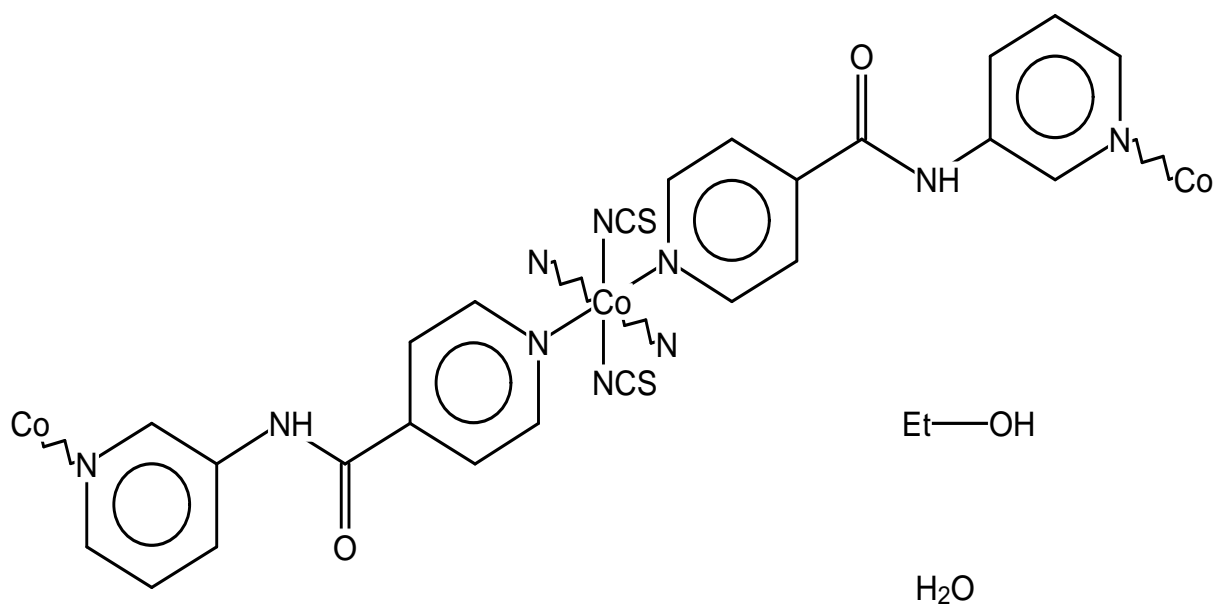
Reference: K.Uemura, S.Kitagawa, M.Kondo, K.Fukui, R.Kitaura,
Ho-Chol Chang, T.Mizutani (2002) *Chem.-Eur.J.* ,**8**,3586

Formula: (C₂₄ H₁₈ Co₁ N₈ O₂ S₂)_n,2n(C₂ H₆ O₁),11n(H₂ O₁)

Compound Name: catena-(bis(μ₂-N-(3-Pyridyl)isonicotinamide)-bis(isothiocyanato)-cobalt ethanol solvate undecahydrate)

Space Group: C2/c **Cell:** **a** 19.730(3) **b** 18.329(0) **c** 14.988(0)
Space Group No.: 15 **(Å, °)** α 90.00 β 115.21(0) γ 90.00

R-Factor (%): 8.10 **Temperature(K):** 293 **Density(g/cm³):** 1.170



Search: search5 (Thu May 26 10:17:05 2011): Hit 5

MOVPEs

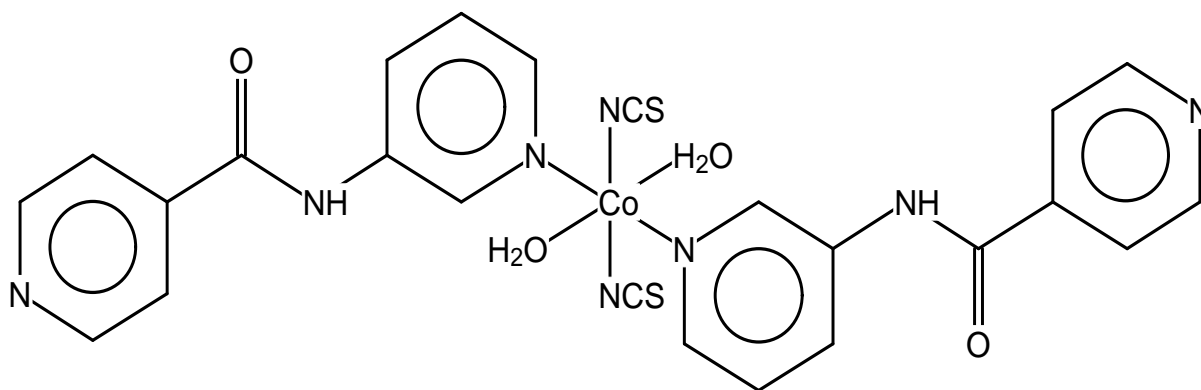
Reference: K.Uemura, S.Kitagawa, M.Kondo, K.Fukui, R.Kitaura,
Ho-Chol Chang, T.Mizutani (2002) *Chem.-Eur.J.* ,**8**,3586

Formula: C₂₄ H₂₂ Co₁ N₈ O₄ S₂

Compound Name: Diaqua-bis(isothiocyanato)-bis(N-(3-pyridyl)isonicotinamide)-cobalt

Space Group: P21/c **Cell:** **a** 8.727(0) **b** 12.271(2) **c** 13.301(2)
Space Group No.: 14 **(Å, °)** α 90.00 β 110.13(0) γ 90.00

R-Factor (%): 3.84 **Temperature(K):** 293 **Density(g/cm³):** 1.514



Search: search5 (Thu May 26 10:17:05 2011): Hit 6

MOVPIW

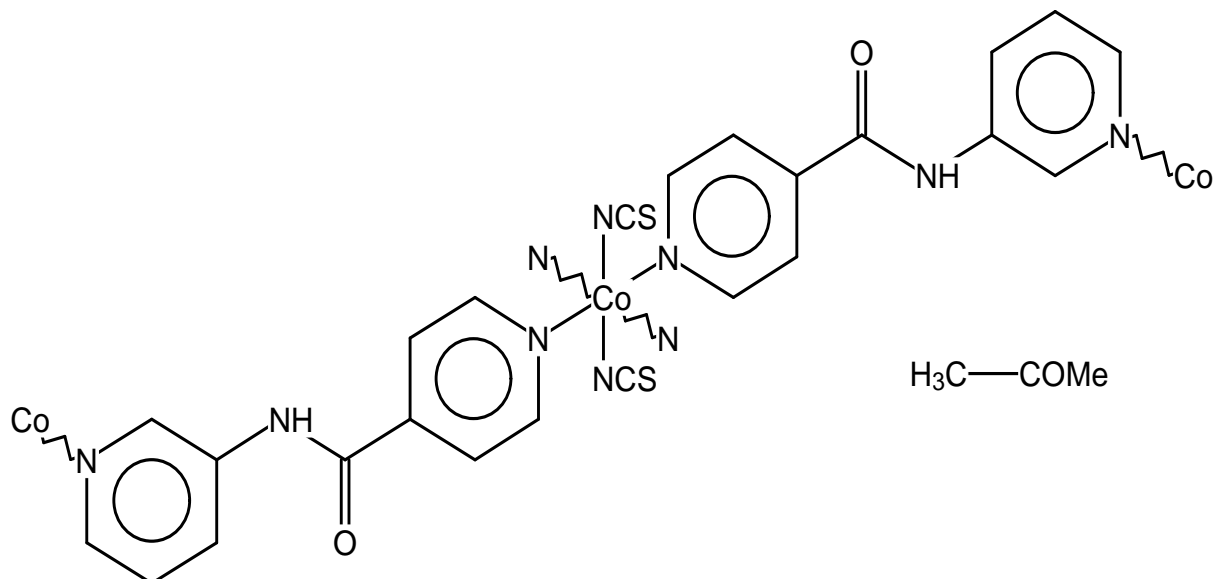
Reference: K.Uemura, S.Kitagawa, M.Kondo, K.Fukui, R.Kitaura,
Ho-Chol Chang, T.Mizutani (2002) *Chem.-Eur.J.* ,**8**,3586

Formula: (C₂₄ H₁₈ Co₁ N₈ O₂ S₂)_n,4n(C₃ H₆ O₁)

Compound Name: catena-(bis(μ₂-N-(3-Pyridyl)isonicotinamide)-bis(isothiocyanato)-cobalt
acetone solvate)

Space Group: P21/n **Cell:** **a** 10.420(0) **b** 14.668(0) **c** 14.253(1)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 97.51(0) **γ** 90.00

R-Factor (%): 6.39 **Temperature(K):** 213 **Density(g/cm³):** 1.239



Search: search5 (Thu May 26 10:17:05 2011): Hit 7

MOVPOC

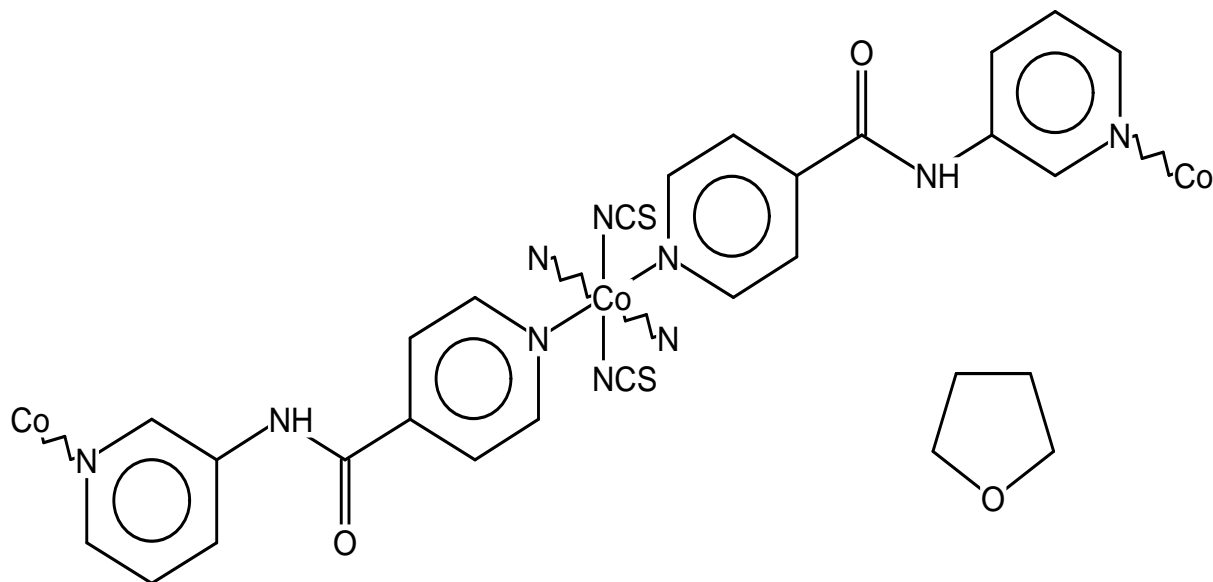
Reference: K.Uemura, S.Kitagawa, M.Kondo, K.Fukui, R.Kitaura,
Ho-Chol Chang, T.Mizutani (2002) *Chem.-Eur.J.* ,**8**,3586

Formula: (C₂₄ H₁₈ Co₁ N₈ O₂ S₂)_n,4n(C₄ H₈ O₁)

Compound Name: catena-(bis(μ₂-N-(3-Pyridyl)isonicotinamido)-bis(isothiocyanato)-cobalt tetrahydrofuran solvate)

Space Group: P21/n **Cell:** **a** 10.460(3) **b** 15.127(8) **c** 14.317(0)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 97.01(0) **γ** 90.00

R-Factor (%): 7.23 **Temperature(K):** 293 **Density(g/cm³):** 1.273



Search: search5 (Thu May 26 10:17:05 2011): Hit 8

PATMON

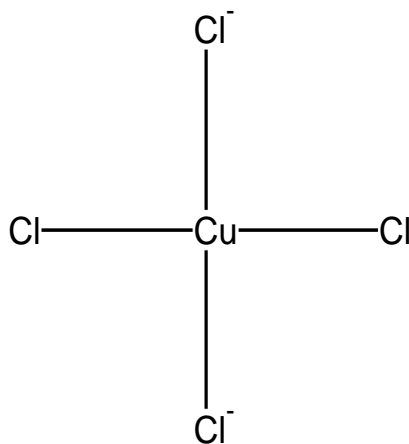
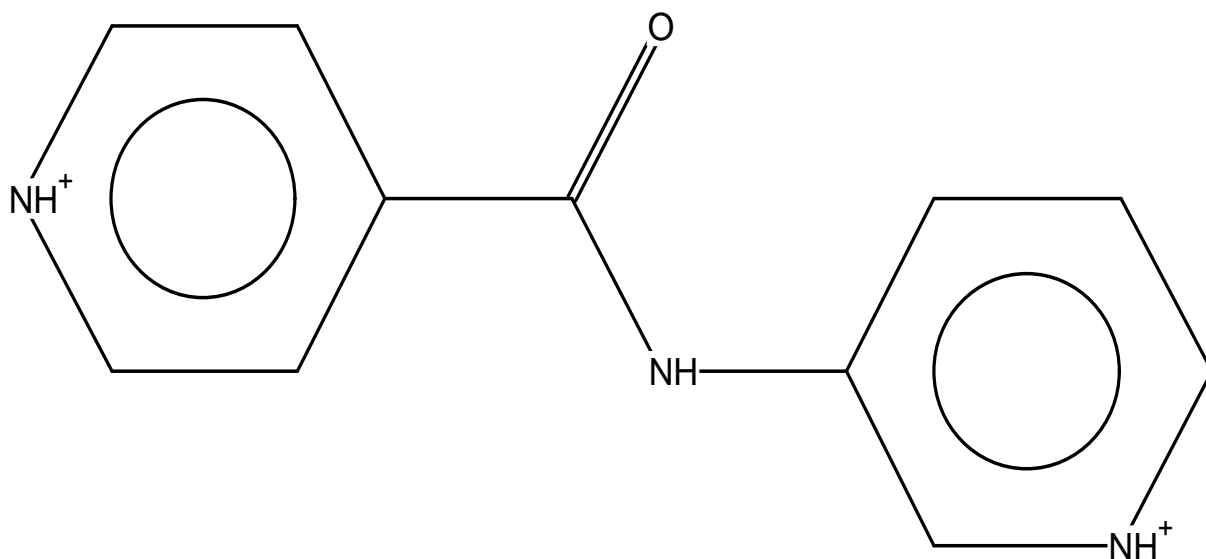
Reference: D.K.Kumar, A.Ballabh, D.A.Jose, P.Dastidar, A.Das
(2005) *Cryst.Growth Des.* ,5,651

Formula: $C_{11} H_{11} N_3 O_1^{2+}, Cl_4 Cu_1^{2-}$

Compound Name: N-(3-Pyridinio)isonicotinamidinium tetrachloro-copper

Space Group: P-1 **Cell:** **a** 7.366(7) **b** 7.380(4) **c** 14.607(8)
Space Group No.: 2 **(Å, °)** α 81.48(4) β 75.94(8) γ 89.73(7)

R-Factor (%): 7.12 **Temperature(K):** 293 **Density(g/cm³):** 1.774



Search: search5 (Thu May 26 10:17:05 2011): Hit 9

SIXVIF

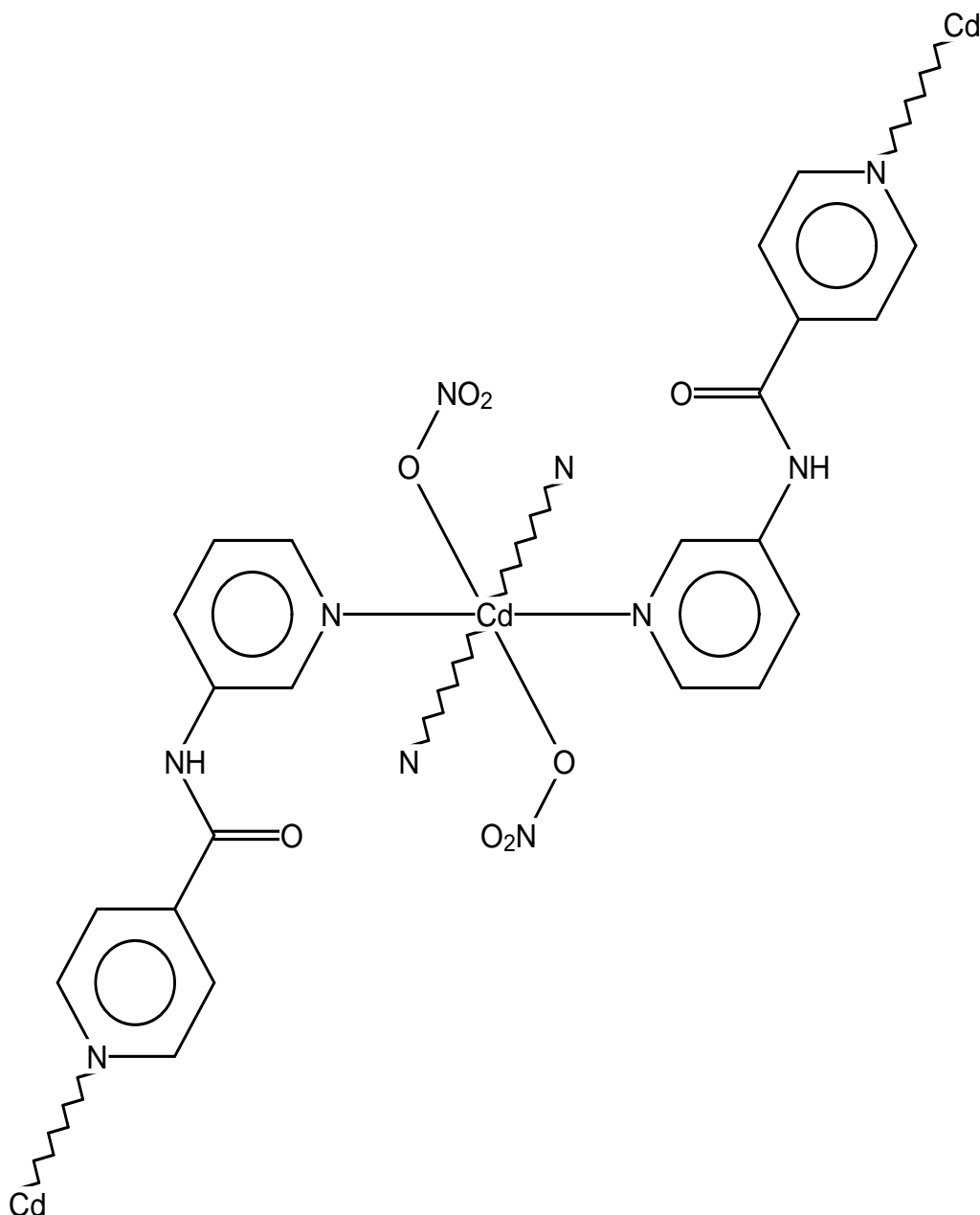
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *CrystEngComm* ,9, 548

Formula: (C₂₂ H₁₈ Cd₁ N₈ O₈)_n

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

Space Group: P-1 **Cell:** **a** 7.878(1) **b** 8.234(1) **c** 9.895(1)
Space Group No.: 2 **(Å, °)** **α** 93.22(0) **β** 98.04(0) **γ** 112.54(0)

R-Factor (%): 3.04 **Temperature(K):** 100 **Density(g/cm³):** 1.809



Search: search5 (Thu May 26 10:17:05 2011): Hit 10

SIXVUR

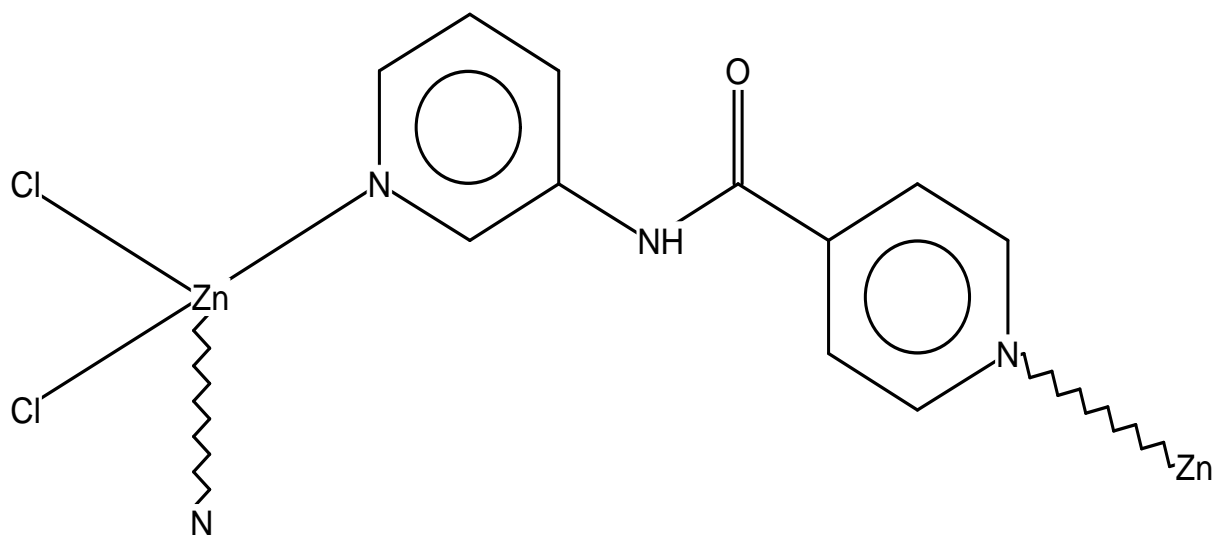
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *CrystEngComm* ,9, 548

Formula: (C₁₁ H₉ Cl₂ N₃ O₁ Zn₁)_n

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

Space Group: P21/n **Cell:** **a** 8.738(4) **b** 9.491(4) **c** 15.969(7)
Space Group No.: 14 **(Å, °)** α 90.00 β 92.92(0) γ 90.00

R-Factor (%): 3.41 **Temperature(K):** 100 **Density(g/cm³):** 1.685



Search: search5 (Thu May 26 10:17:05 2011): Hit 11

VODCUN

Reference: K.Uemura (2008) *Inorg.Chem.Commun.* ,11,741

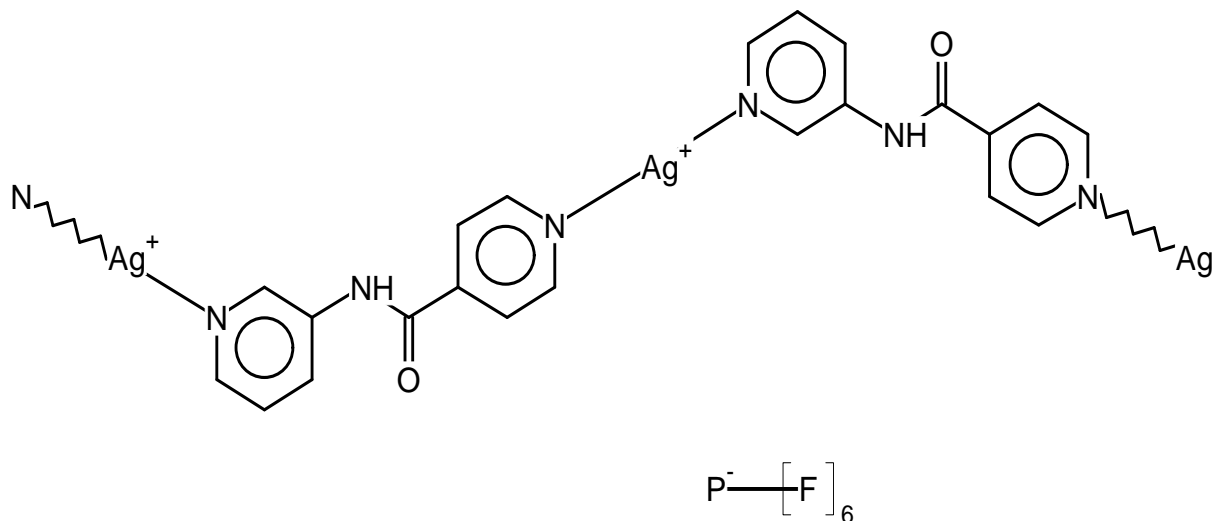
Formula: $(C_{22} H_{18} Ag_2 N_6 O_2^{2+})_n, 2n(F_6 P_1^{1-})$

Compound Name: catena-[bis(μ_2 -N-Pyridin-3-ylisonicotinamido)-di-silver(i) bis(hexafluorophosphate)]

Space Group: P21/a **Cell:** **a** 17.896(2) **b** 7.728(1) **c** 21.378(0)

Space Group No.: 14 **(Å, °)** α 90.00 β 92.31(0) γ 90.00

R-Factor (%): 5.91 **Temperature(K):** 293 **Density(g/cm³):** 2.033



Search: search5 (Thu May 26 10:17:05 2011): Hit 12

VODDAU

Reference: K.Uemura (2008) *Inorg.Chem.Commun.* ,11,741

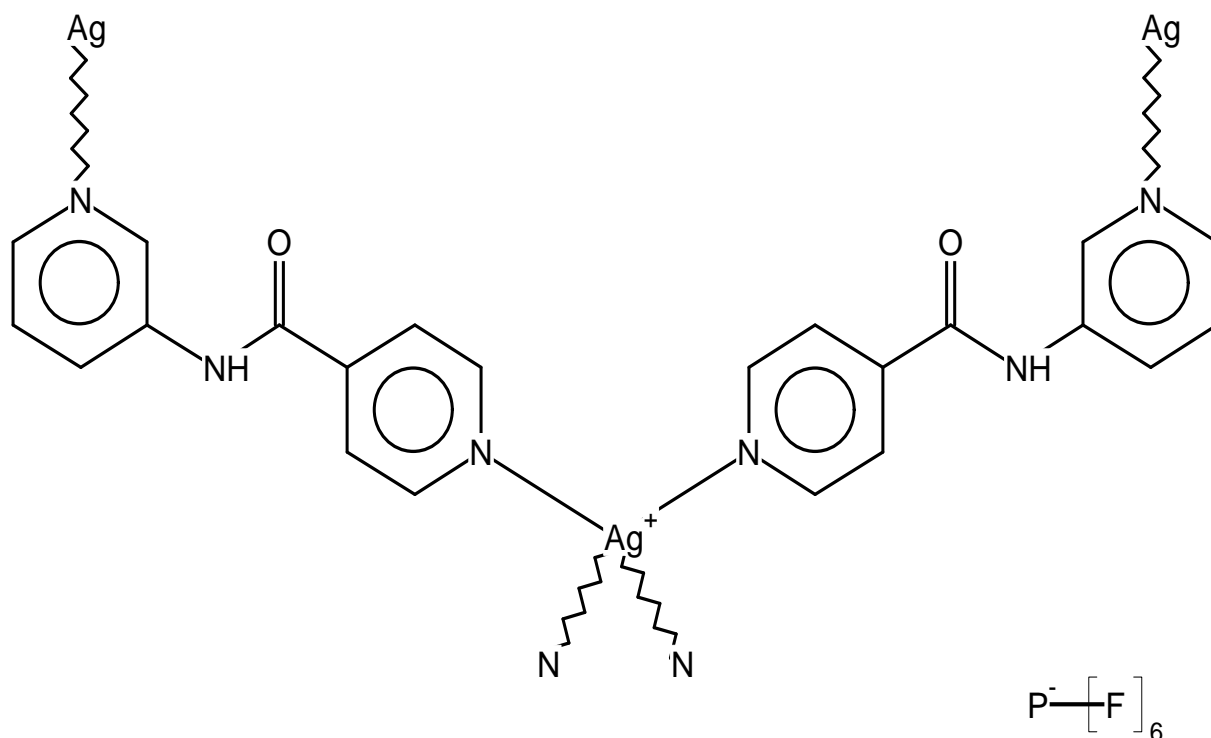
Formula: (C₂₂ H₁₈ Ag₁ N₆ O₂ 1⁺)_n,n(F₆ P₁ 1⁻)

Compound Name: catena-[bis(μ₂-N-Pyridin-3-ylisonicotinamido)-silver(i) hexafluorophosphate]

Space Group: P21/n **Cell:** **a** 11.522(2) **b** 11.955(2) **c** 18.206(0)

Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 100.72(0) **γ** 90.00

R-Factor (%): 5.31 **Temperature(K):** 293 **Density(g/cm³):** 1.756



Search: search5 (Thu May 26 10:17:05 2011): Hit 13

YEPDON

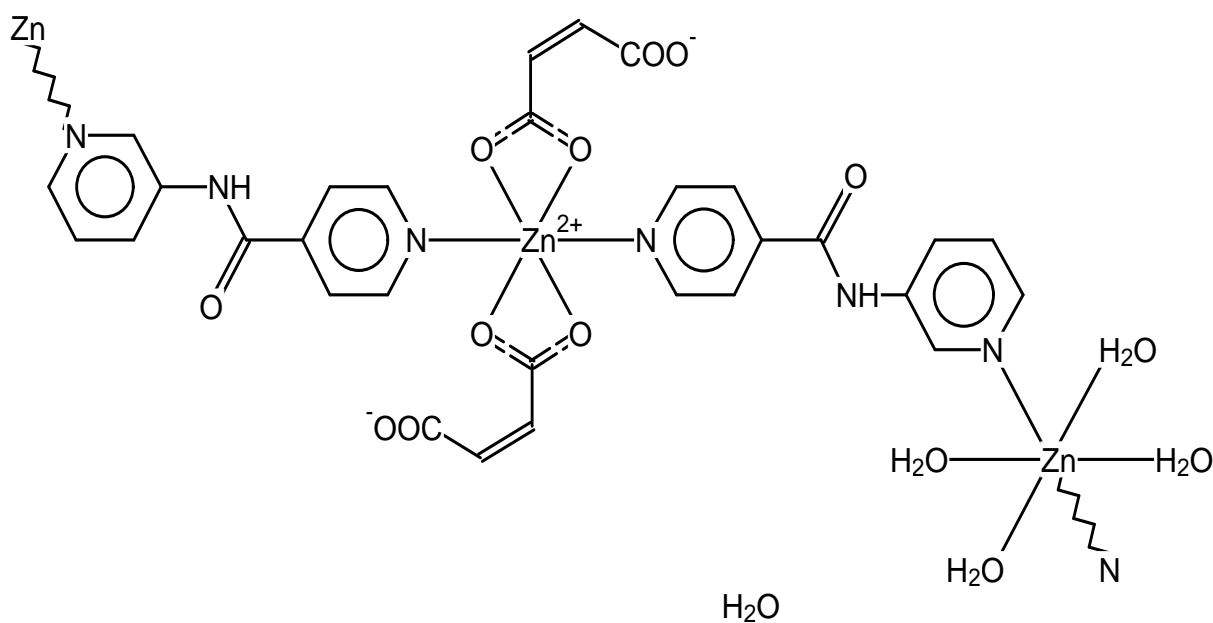
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *Cryst.Growth Des.* ,
6,1903

Formula: $(C_{30} H_{30} N_6 O_{14} Zn_2)_n \cdot 2n(H_2 O)_1$

Compound Name: catena-(bis(μ_2 -N-(3-Pyridyl)isonicotinamide-N,N')-tetra-aqua-
bis(maleato-O,O')-di-zinc(ii) dihydrate)

Space Group: C2/c **Cell:** **a** 28.415(1) **b** 7.348(0) **c** 17.094(1)
Space Group No.: 15 (**Å, °**) α 90.00 β 108.47(0) γ 90.00

R-Factor (%): 2.40 **Temperature(K):** 100 **Density(g/cm³):** 1.698



Search Overview

Search: search6
Date/Time done: Thu May 26 10:18:38 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

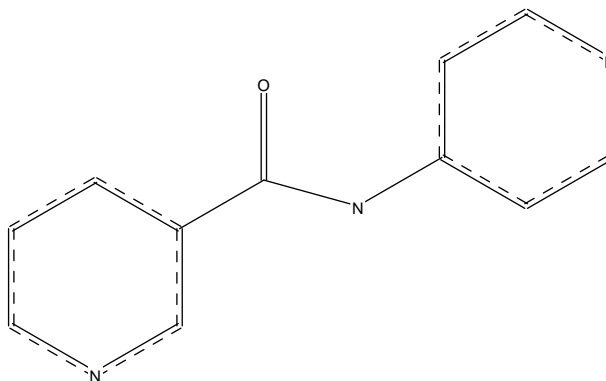
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

4M

Search: search6 (Thu May 26 10:18:38 2011): Hit 1

DEPTAU

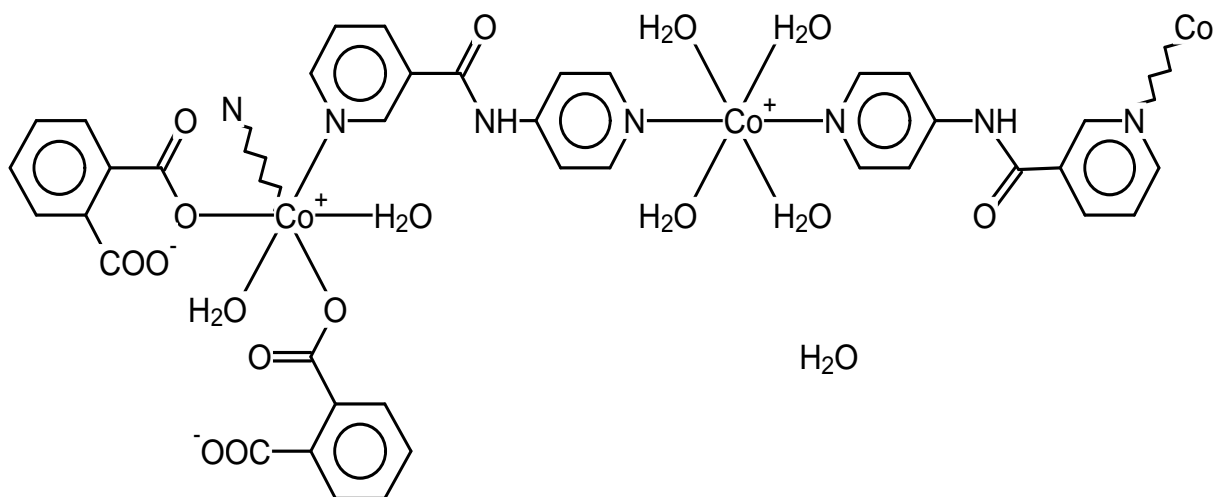
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *J.Mol.Struct.* ,**796**, 139

Formula: (C₃₈ H₃₈ Co₂ N₆ O₁₆)_n.2.26n(H₂ O₁)

Compound Name: catena-(bis(N-(4-Pyridyl)nicotinamide)-bis(phthalato)-hexaaqua-di-cobalt(ii) hydrate)

Space Group: P21/c **Cell:** **a** 11.656(0) **b** 8.036(0) **c** 23.634(1)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 103.40(0) **γ** 90.00

R-Factor (%): 4.11 **Temperature(K):** 100 **Density(g/cm³):** 1.532



Search: search6 (Thu May 26 10:18:38 2011): Hit 2

KAZVUD

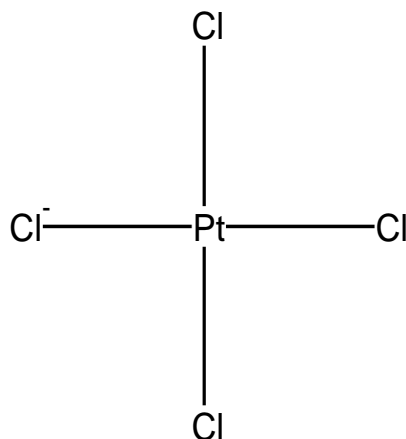
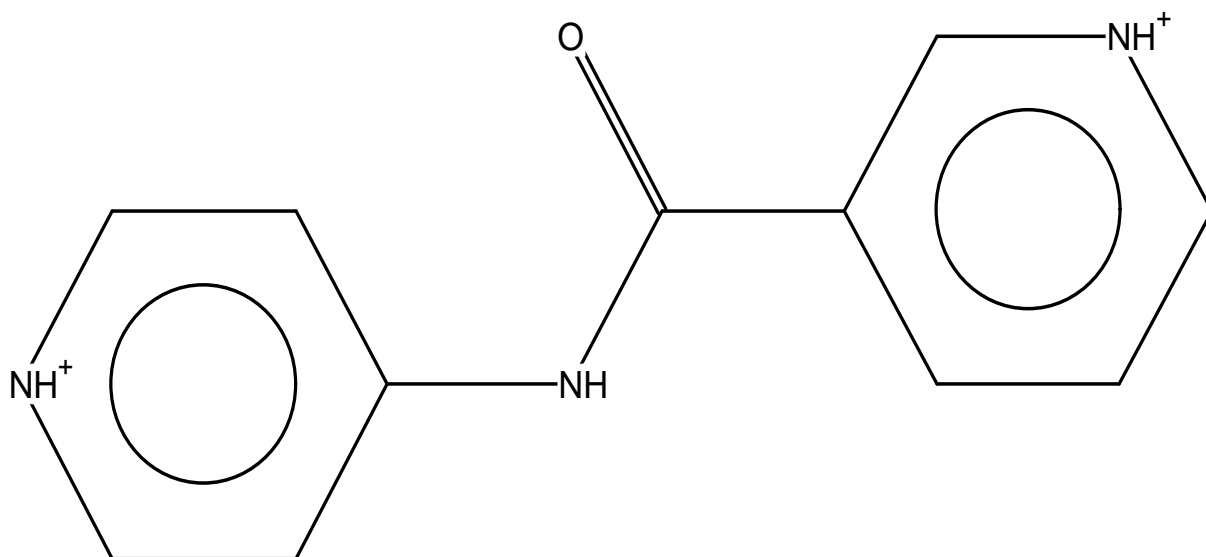
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *Cryst.Growth Des.* ,
6,216

Formula: $C_{11} H_{11} N_3 O_1^{2+}, Cl_4 Pt_1^{2-}$

Compound Name: N-(4-Pyridinio)nicotinamidinium tetrachloro-platinum

Space Group: Pbcu **Cell:** **a** 27.370(9) **b** 6.884(2) **c** 15.483(5)
Space Group No.: 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.17 **Temperature(K):** 298 **Density(g/cm³):** 2.450



Search: search6 (Thu May 26 10:18:38 2011): Hit 3

MOYXOO

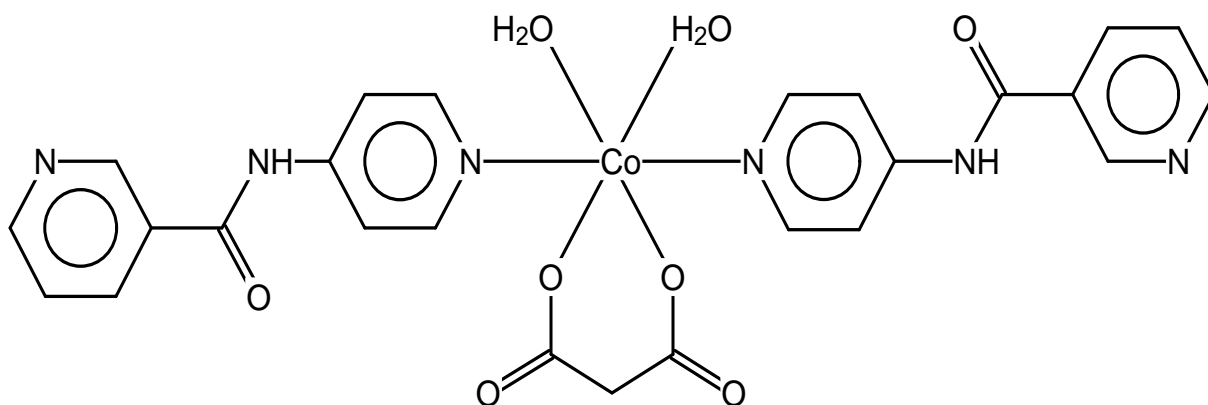
Reference: D.K.Kumar (2009) *Inorg.Chim.Acta* ,**362**,1767

Formula: C₂₅ H₂₄ Co₁ N₆ O₈

Compound Name: (malonato)-bis(N-(4-pyridinyl)nicotinamide)-diaqua-cobalt(ii)

Space Group: C2/c **Cell:** **a** 22.092(4) **b** 7.532(1) **c** 17.168(3)
Space Group No.: 15 **(Å, °)** α 90.00 β 119.02(0) γ 90.00

R-Factor (%): 6.81 **Temperature(K):** 100 **Density(g/cm³):** 1.583



Search: search6 (Thu May 26 10:18:38 2011): Hit 4

MOYXUU

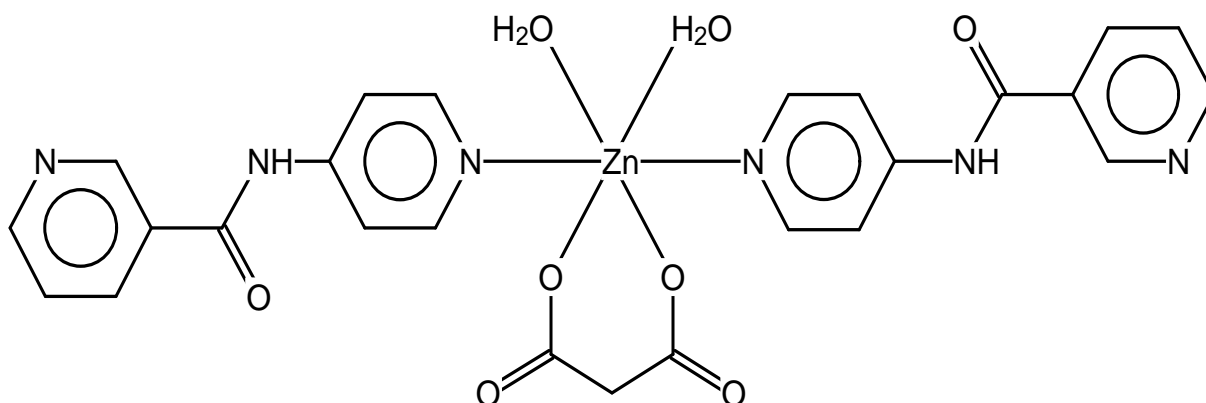
Reference: D.K.Kumar (2009) *Inorg.Chim.Acta* ,**362**,1767

Formula: C₂₅ H₂₄ N₆ O₈ Zn₁

Compound Name: (malonato)-bis(N-(4-pyridinyl)nicotinamide)-diaqua-zinc(ii)

Space Group: C2/c **Cell:** **a** 22.069(2) **b** 7.548(0) **c** 17.153(1)
Space Group No.: 15 **(Å, °)** α 90.00 β 118.95(0) γ 90.00

R-Factor (%): 5.92 **Temperature(K):** 100 **Density(g/cm³):** 1.599



Search: search6 (Thu May 26 10:18:38 2011): Hit 5

MOYYAB

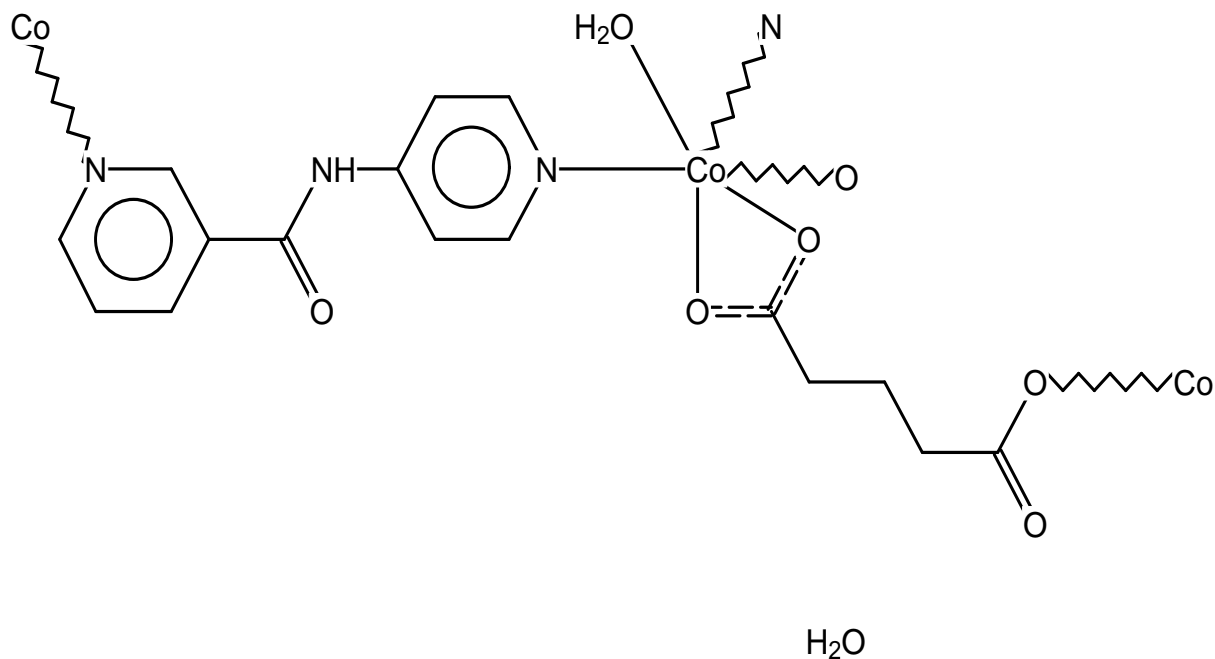
Reference: D.K.Kumar (2009) *Inorg.Chim.Acta* ,**362**,1767

Formula: (C₁₆ H₁₇ Co₁ N₃ O₆)_n,n(H₂ O₁)

Compound Name: catena-((μ₂-N-(4-Pyridinyl)nicotinamide)-(μ₂-glutarato)-aqua-cobalt(ii) monohydrate)

Space Group: C2/c **Cell:** **a** 23.462(2) **b** 8.957(0) **c** 17.297(1)
Space Group No.: 15 **(Å, °)** **α** 90.00 **β** 108.77(0) **γ** 90.00

R-Factor (%): 5.52 **Temperature(K):** 100 **Density(g/cm³):** 1.638



Search: search6 (Thu May 26 10:18:38 2011): Hit 6

PAQLEZ

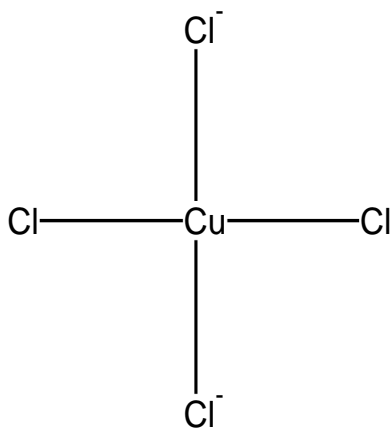
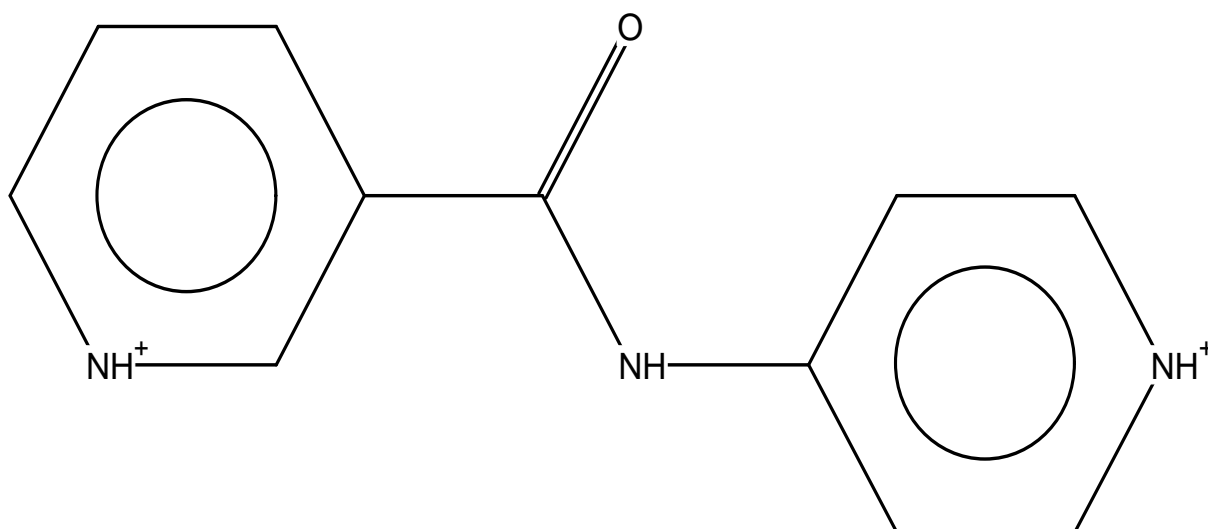
Reference: D.K.Kumar, A.Ballabh, D.A.Jose, P.Dastidar, A.Das
(2005) *Cryst.Growth Des.* ,5,651

Formula: C₁₁ H₁₁ N₃ O₁²⁺, Cl₄ Cu₁²⁻

Compound Name: N-(4-Pyridinio)nicotinamidinium tetrachloro-copper

Space Group: P-1 **Cell:** **a** 8.276(0) **b** 8.820(0) **c** 11.713(1)
Space Group No.: 2 **(Å, °)** α 99.67(0) β 94.10(0) γ 112.41(0)

R-Factor (%): 4.13 **Temperature(K):** 273 **Density(g/cm³):** 1.752



Search: search6 (Thu May 26 10:18:38 2011): Hit 7

YEPDUT

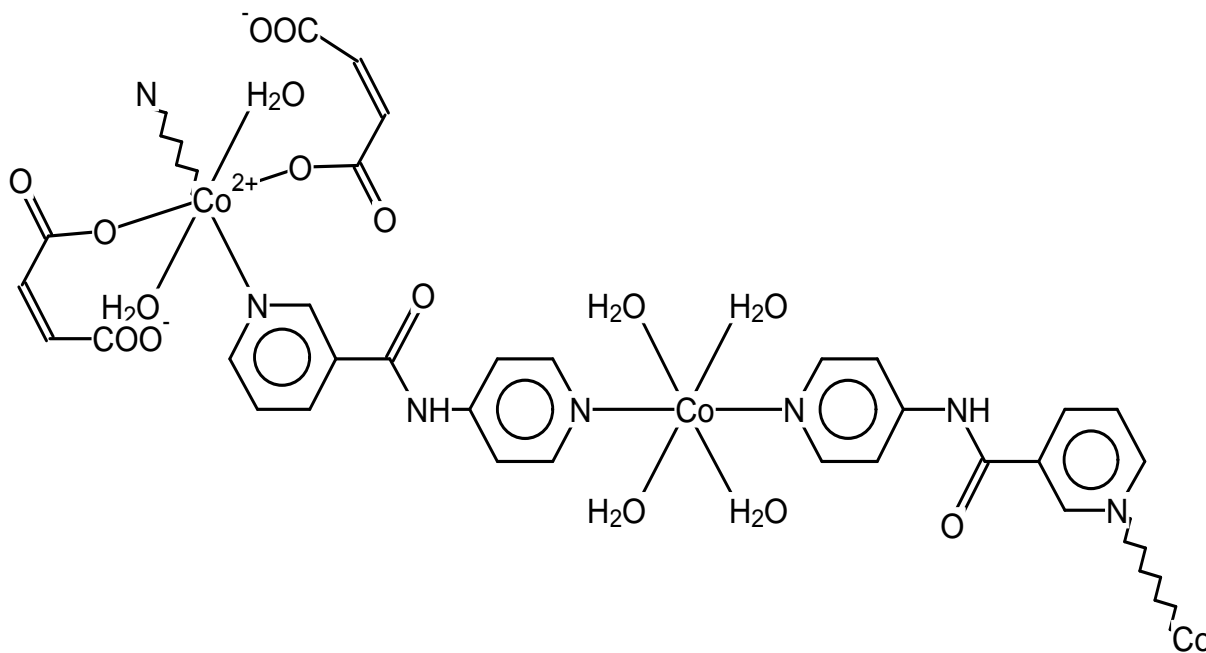
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *Cryst.Growth Des.* ,
6,1903

Formula: $(C_{30} H_{34} Co_2 N_6 O_{16})n, 2n(H_2 O_1)$

Compound Name: catena-(bis(μ_2 -N-(4-Pyridyl)nicotinamide-N,N')-hexa-aqua-bis(maleato-O)-di-cobalt dihydrate)

Space Group: P-1 **Cell:** **a** 7.892(1) **b** 10.213(1) **c** 11.673(1)
Space Group No.: 2 (**Å, °**) α 104.83(0) β 95.28(0) γ 90.16(0)

R-Factor (%): 7.10 **Temperature(K):** 100 **Density(g/cm³):** 1.630



Search: search6 (Thu May 26 10:18:38 2011): Hit 8

YEPFAB

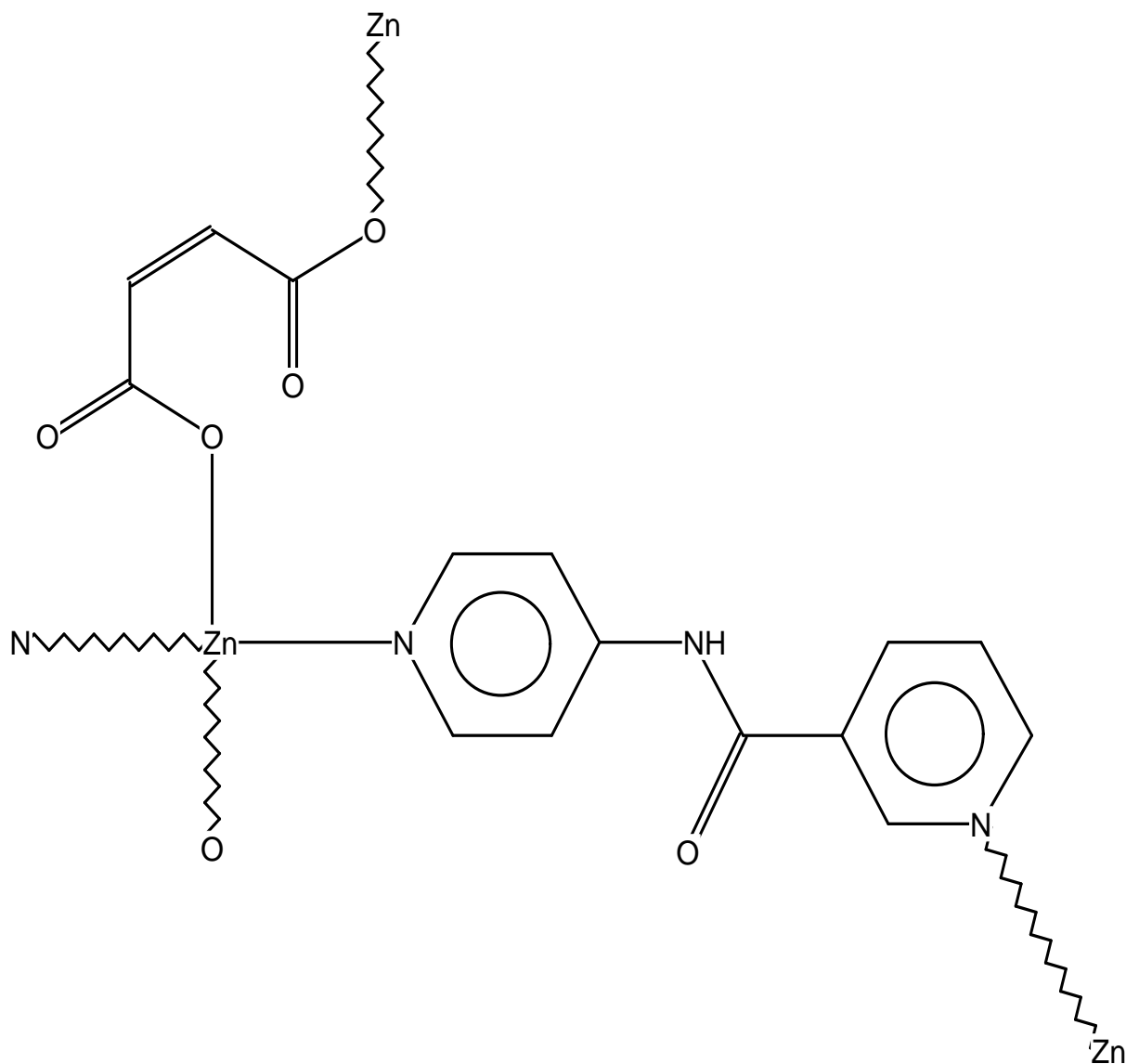
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *Cryst.Growth Des.* ,
6,1903

Formula: (C₁₅ H₁₁ N₃ O₅ Zn₁)_n

Compound Name: catena-((μ₂-Maleato-O,O')-(μ₂-N-(4-pyridyl)nicotinamide-N,N')-zinc)

Space Group: P21/n **Cell:** **a** 7.236(0) **b** 19.159(1) **c** 10.721(0)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 104.73(0) **γ** 90.00

R-Factor (%): 2.72 **Temperature(K):** 100 **Density(g/cm³):** 1.750



Search: search6 (Thu May 26 10:18:38 2011): Hit 9

YEPFEF

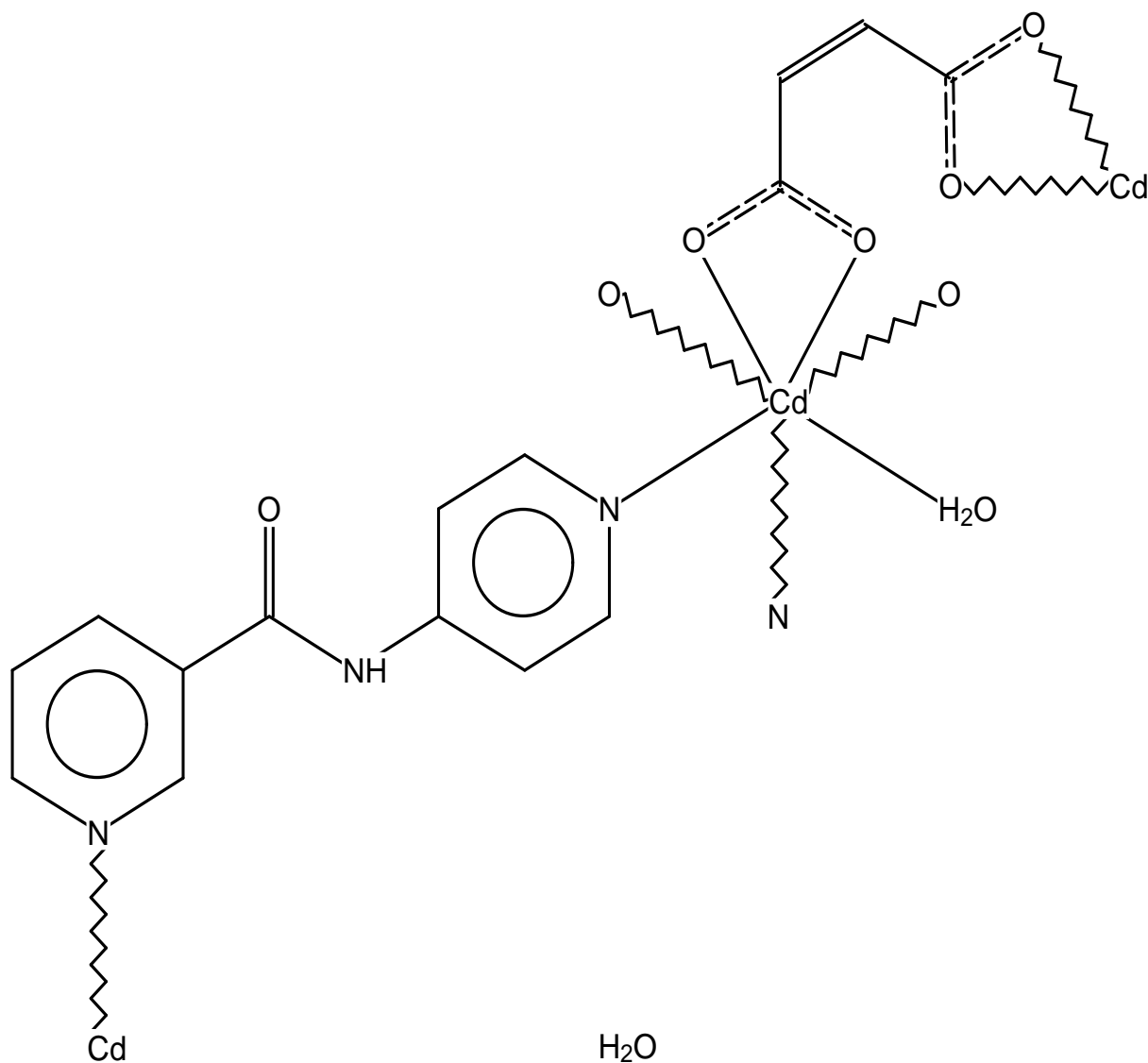
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *Cryst.Growth Des.* ,
6,1903

Formula: $(C_{15} H_{13} Cd_1 N_3 O_6)_n \cdot 2n(H_2 O_1)$

Compound Name: catena-((μ_2 -Maleato-O,O',O'',O''')-(μ_2 -N-(4-pyridyl)nicotinamide-N,N')-
aqua-cadmium dihydrate)

Space Group: C2 **Cell:** **a** 24.139(2) **b** 9.138(0) **c** 8.270(0)
Space Group No.: 5 (**Å, °**) α 90.00 β 107.59(0) γ 90.00

R-Factor (%): 4.61 **Temperature(K):** 100 **Density(g/cm³):** 1.832



Search: search6 (Thu May 26 10:18:38 2011): Hit 10

YEPFIJ

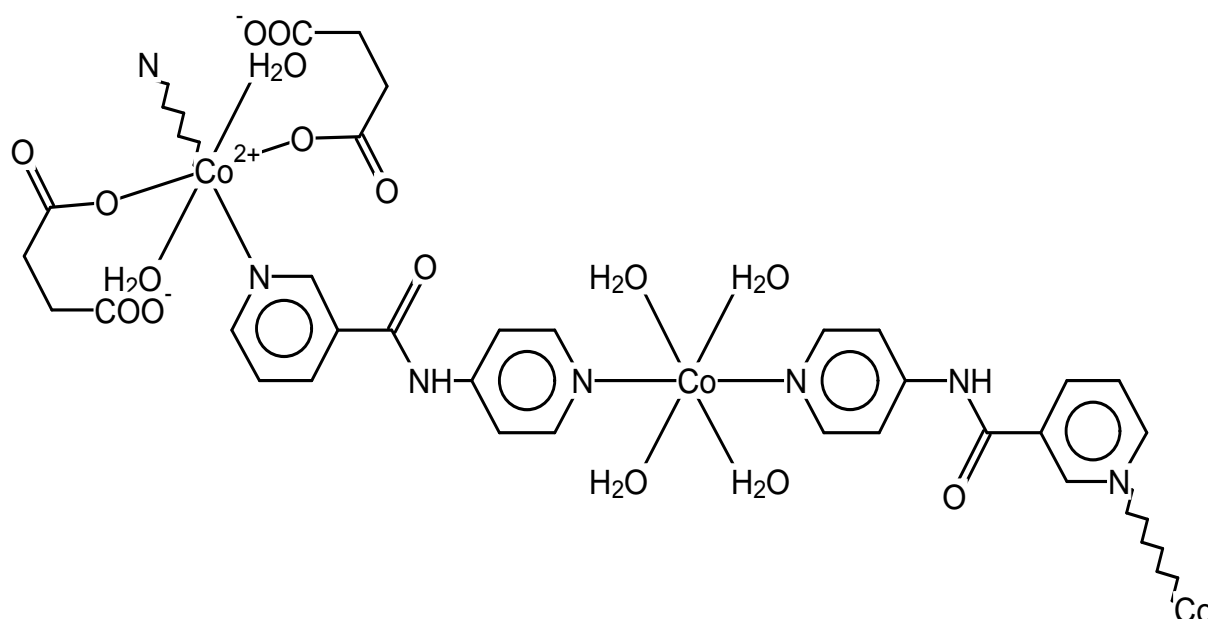
Reference: D.K.Kumar, A.Das, P.Dastidar (2006) *Cryst.Growth Des.* ,
6,1903

Formula: $(C_{30} H_{38} Co_2 N_6 O_{16})_n \cdot 2.56n(H_2 O)_1$

Compound Name: catena-(bis(μ_2 -N-(4-Pyridyl)nicotinamide-N,N')-hexa-aqua-bis(succinato-O)-di-cobalt hydrate)

Space Group: P-1 **Cell:** **a** 8.004(0) **b** 10.729(0) **c** 11.336(0)
Space Group No.: 2 (**Å, °**) α 78.36(0) β 87.12(0) γ 79.89(0)

R-Factor (%): 2.82 **Temperature(K):** 100 **Density(g/cm³):** 1.597



H₂O

Search Overview

Search: search7
Date/Time done: Thu May 26 10:20:13 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: 9

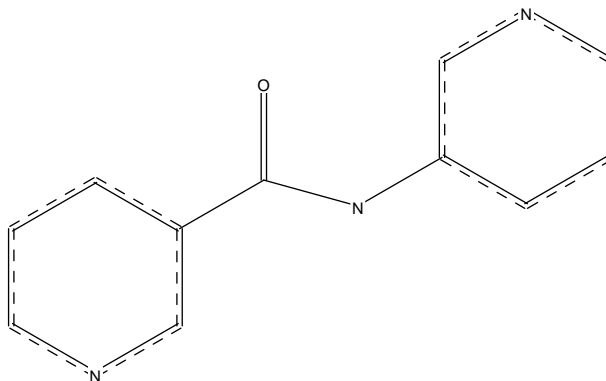
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

4M

Search: search7 (Thu May 26 10:20:13 2011): Hit 1

AVUBAU

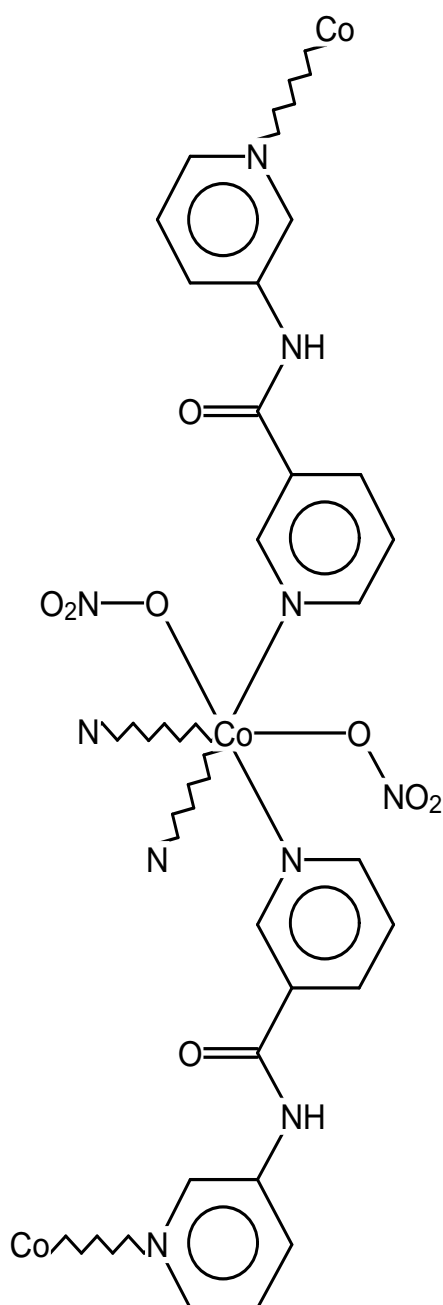
Reference: K.Uemura, S.Kitagawa, K.Fukui, K.Saito (2004)
J.Am.Chem.Soc. ,**126**,3817

Formula: (C₂₂ H₁₈ Co₁ N₈ O₈)_n

Compound Name: catena-(bis(μ₂-N-(3-Pyridyl)nicotinamide-N,N')-bis(nitrato-O)-cobalt(ii))

Space Group: Pbcn **Cell:** **a** 18.300(0) **b** 10.759(3) **c** 11.458(2)
Space Group No.: 60 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 6.63 **Temperature(K):** 223 **Density(g/cm³):** 1.712



Search: search7 (Thu May 26 10:20:13 2011): Hit 2

AVUBEY

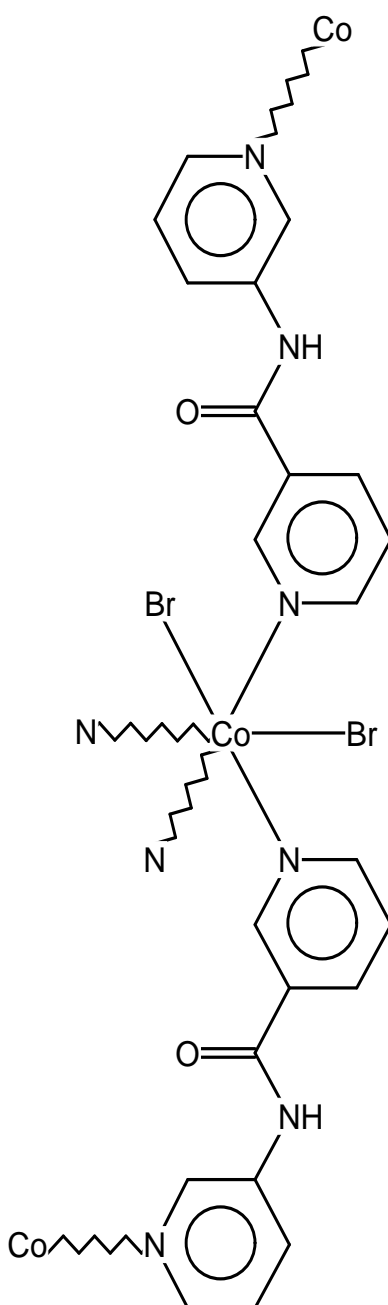
Reference: K.Uemura, S.Kitagawa, K.Fukui, K.Saito (2004)
J.Am.Chem.Soc. ,**126**,3817

Formula: (C₂₂ H₁₈ Br₂ Co₁ N₆ O₂)_n

Compound Name: catena-(bis(μ_2 -N-(3-Pyridyl)nicotinamide-N,N')-dibromo-cobalt(ii))

Space Group: Ccca **Cell:** **a** 10.481(7) **b** 19.030(10) **c** 10.894(8)
Space Group No.: 68 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.32 **Temperature(K):** 293 **Density(g/cm³):** 1.887



Search: search7 (Thu May 26 10:20:13 2011): Hit 3

MOVPU1

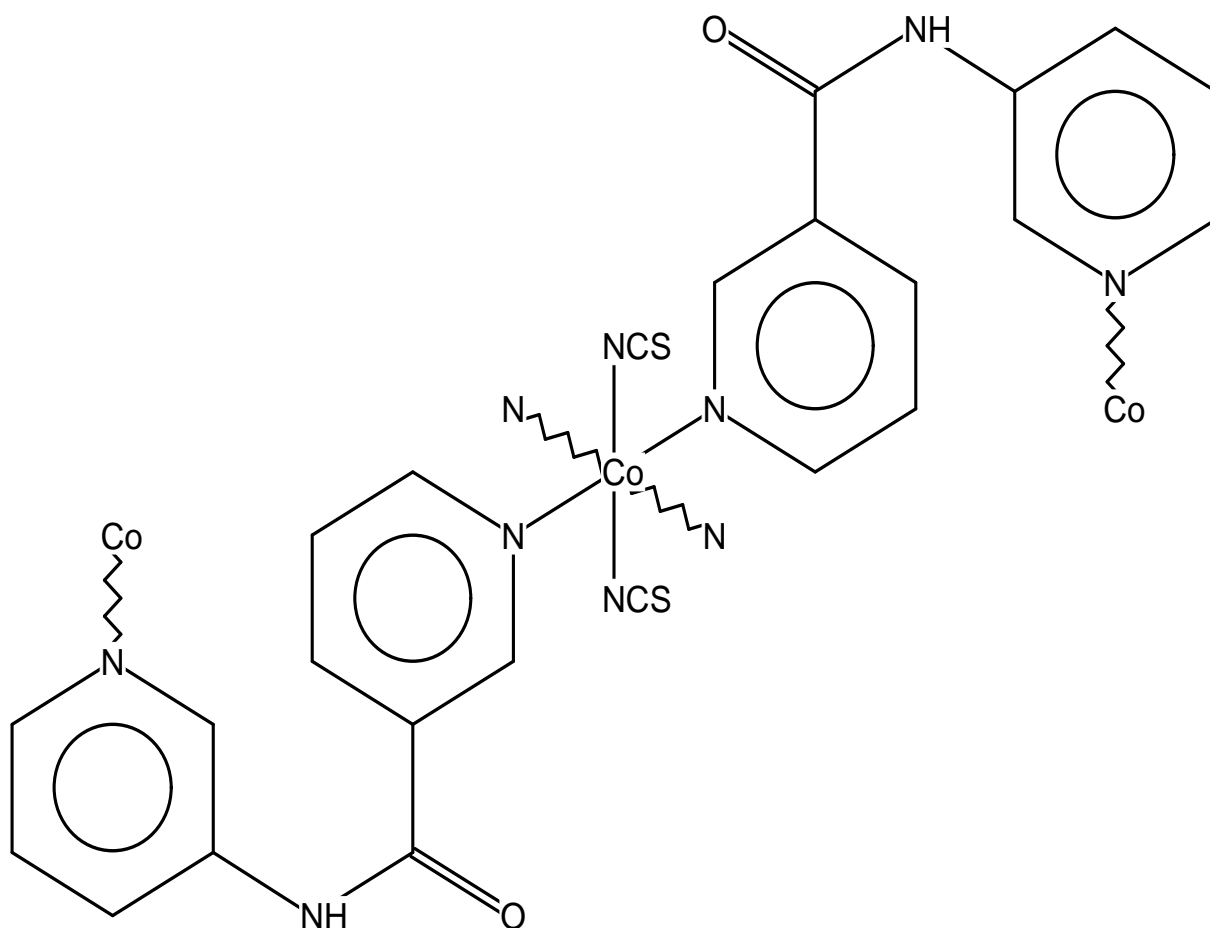
Reference: K.Uemura, S.Kitagawa, M.Kondo, K.Fukui, R.Kitaura,
Ho-Chol Chang, T.Mizutani (2002) *Chem.-Eur.J.* ,**8**,3586

Formula: (C₂₄ H₁₈ Co₁ N₈ O₂ S₂)_n

Compound Name: catena-(bis(μ₂-N-(3-Pyridyl)nicotinamido)-bis(isothiocyanato)-cobalt)

Space Group: P21/c **Cell:** **a** 8.805(3) **b** 15.585(7) **c** 9.521(0)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 98.73(0) **γ** 90.00

R-Factor (%): 5.76 **Temperature(K):** 293 **Density(g/cm³):** 1.475



Search: search7 (Thu May 26 10:20:13 2011): Hit 4

SIXTUP

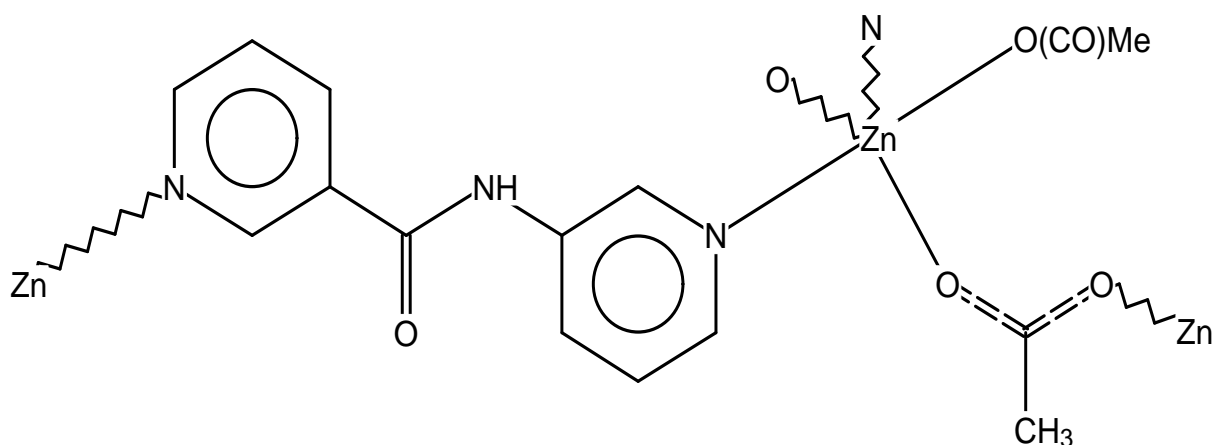
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *CrystEngComm*, **9**, 548

Formula: (C₁₅ H₁₅ N₃ O₅ Zn₁)_n

Compound Name: catena-((μ₂-N-(3-Pyridyl)nicotinamide-N',N'')-(μ₂-acetato-O,O')-(acetato-O)-zinc(ii))

Space Group: P-1 **Cell:** **a** 7.964(1) **b** 9.153(1) **c** 10.963(1)
Space Group No.: 2 **(Å, °)** **α** 84.75(0) **β** 79.25(0) **γ** 79.58(0)

R-Factor (%): 4.71 **Temperature(K):** 298 **Density(g/cm³):** 1.649



Search: search7 (Thu May 26 10:20:13 2011): Hit 5

SIXVAX

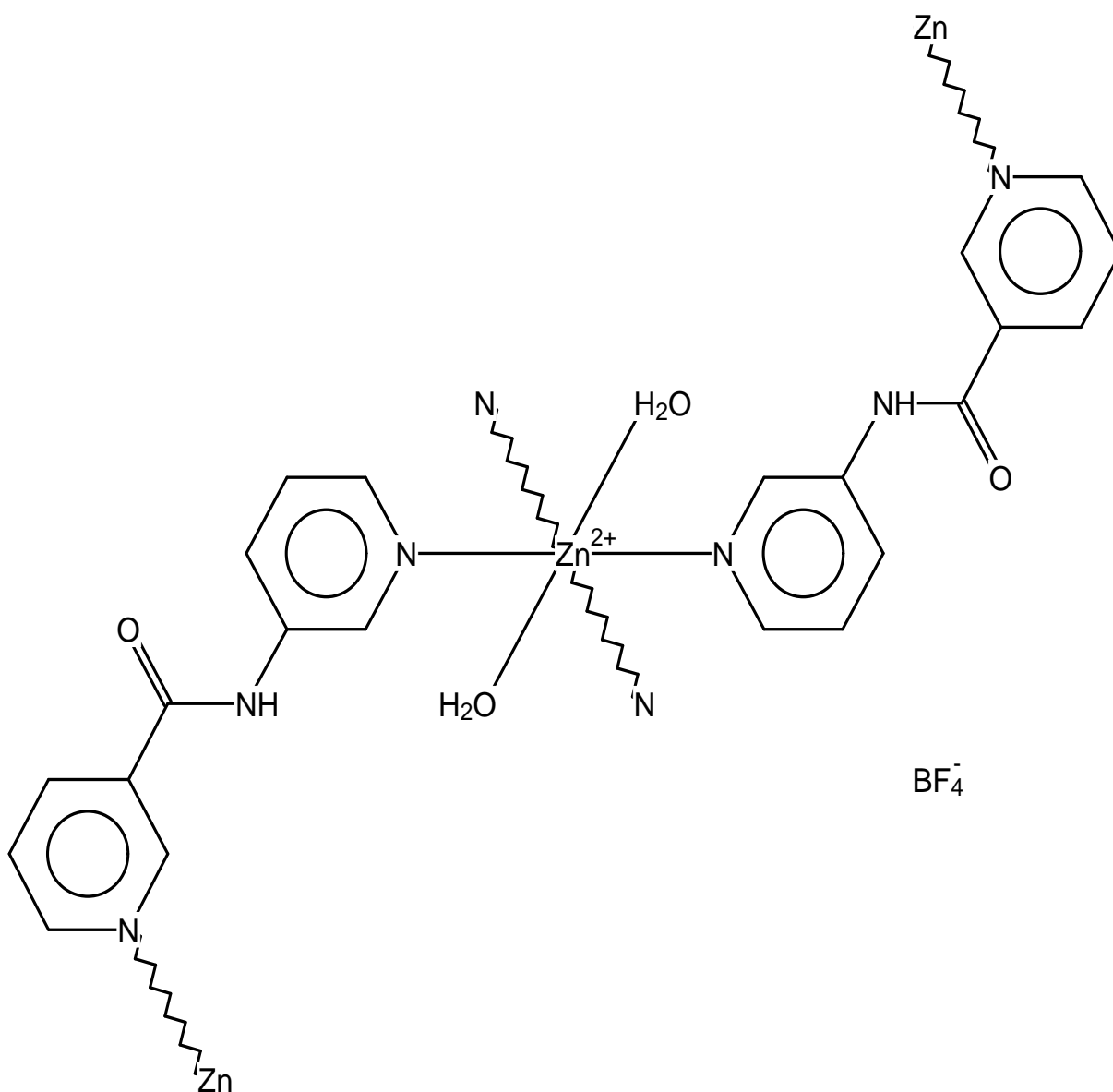
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *CrystEngComm* ,9, 548

Formula: $(C_{22}H_{22}N_6O_4Zn_1^{2+})_n, 2n(B_1F_4^{-1})$

Compound Name: catena-(bis(μ_2 -N-(3-Pyridyl)nicotinamide-N',N'')-diaqua-zinc(ii) bis(tetrafluoroborate))

Space Group: P21/c **Cell:** **a** 8.486(4) **b** 9.551(4) **c** 16.351(6)
Space Group No.: 14 **(Å, °)** α 90.00 β 97.79(2) γ 90.00

R-Factor (%): 6.67 **Temperature(K):** 298 **Density(g/cm³):** 1.703



Search: search7 (Thu May 26 10:20:13 2011): Hit 6

SIXVEB

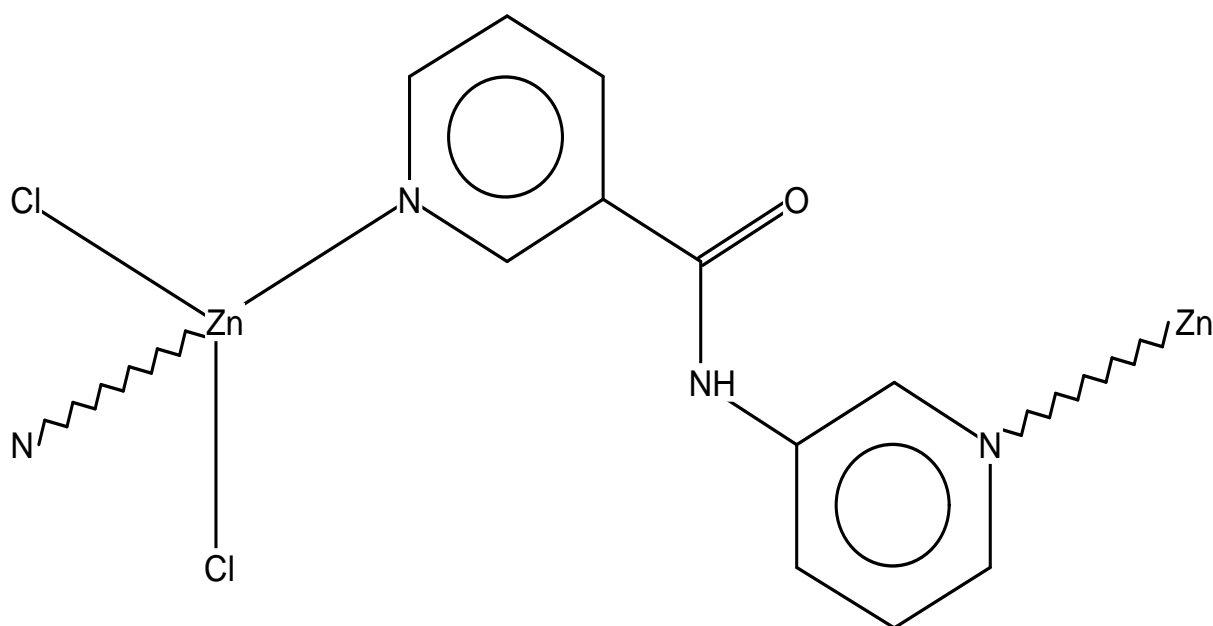
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *CrystEngComm*, **9**, 548

Formula: (C₁₁ H₉ Cl₂ N₃ O₁ Zn₁)_n

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

Space Group: P21/c **Cell:** **a** 7.805(3) **b** 13.773(6) **c** 13.362(4)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 119.81(1) **γ** 90.00

R-Factor (%): 10.14 **Temperature(K):** 298 **Density(g/cm³):** 1.788



Search: search7 (Thu May 26 10:20:13 2011): Hit 7

SIXVOL

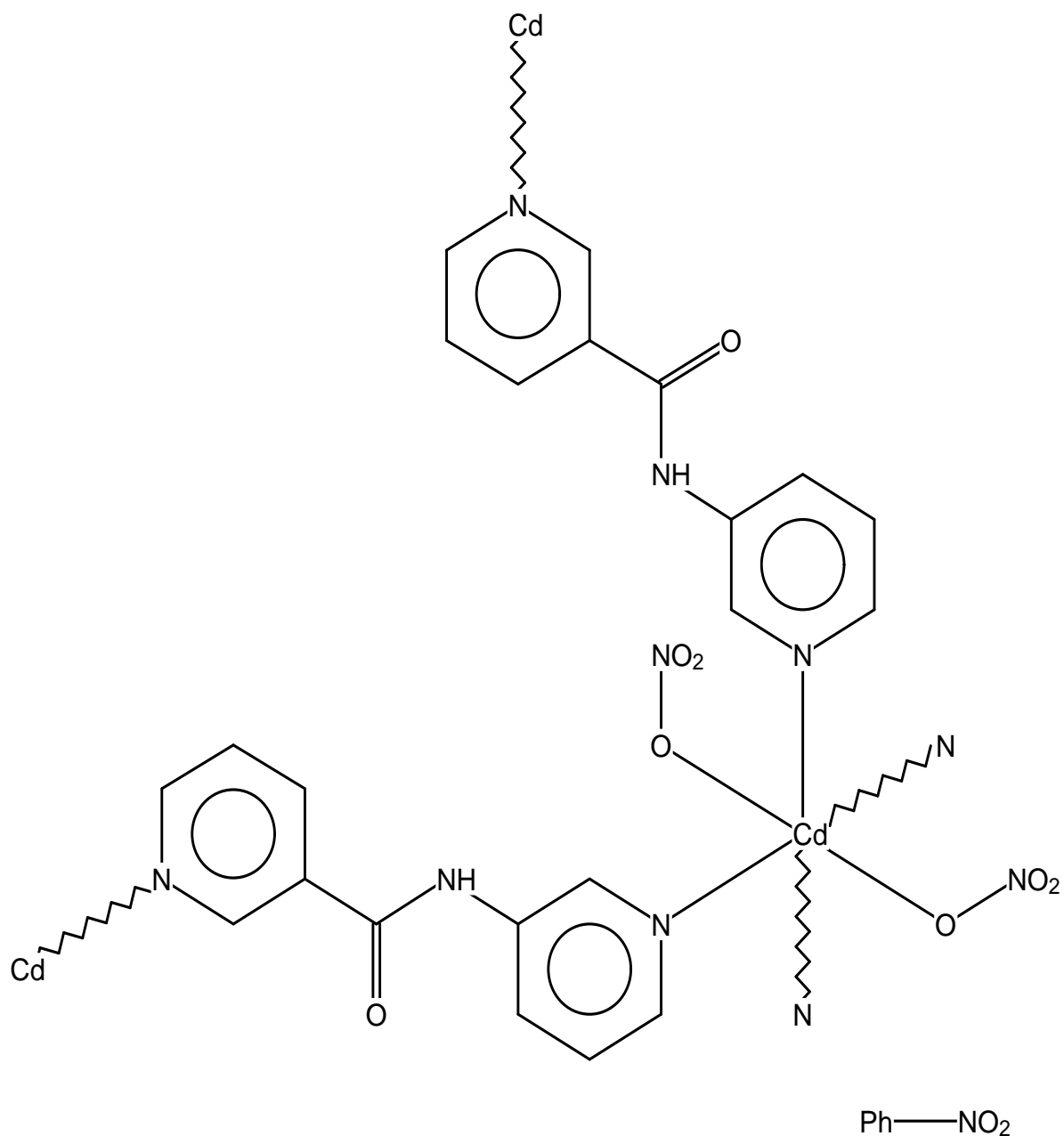
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *CrystEngComm* ,9, 548

Formula: (C₂₂ H₁₈ Cd₁ N₈ O₈)_n,n(C₆ H₅ N₁ O₂)

Compound Name: catena-(bis(μ₂-N-(3-Pyridyl)nicotinamide-N',N'')-bis(nitrato-O)-cadmium(ii) nitrobenzene clathrate)

Space Group: P21/c **Cell:** **a** 10.281(1) **b** 22.399(2) **c** 15.244(1)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 124.86(0) **γ** 90.00

R-Factor (%): 8.71 **Temperature(K):** 100 **Density(g/cm³):** 1.748



Search: search7 (Thu May 26 10:20:13 2011): Hit 8

VIPTIY

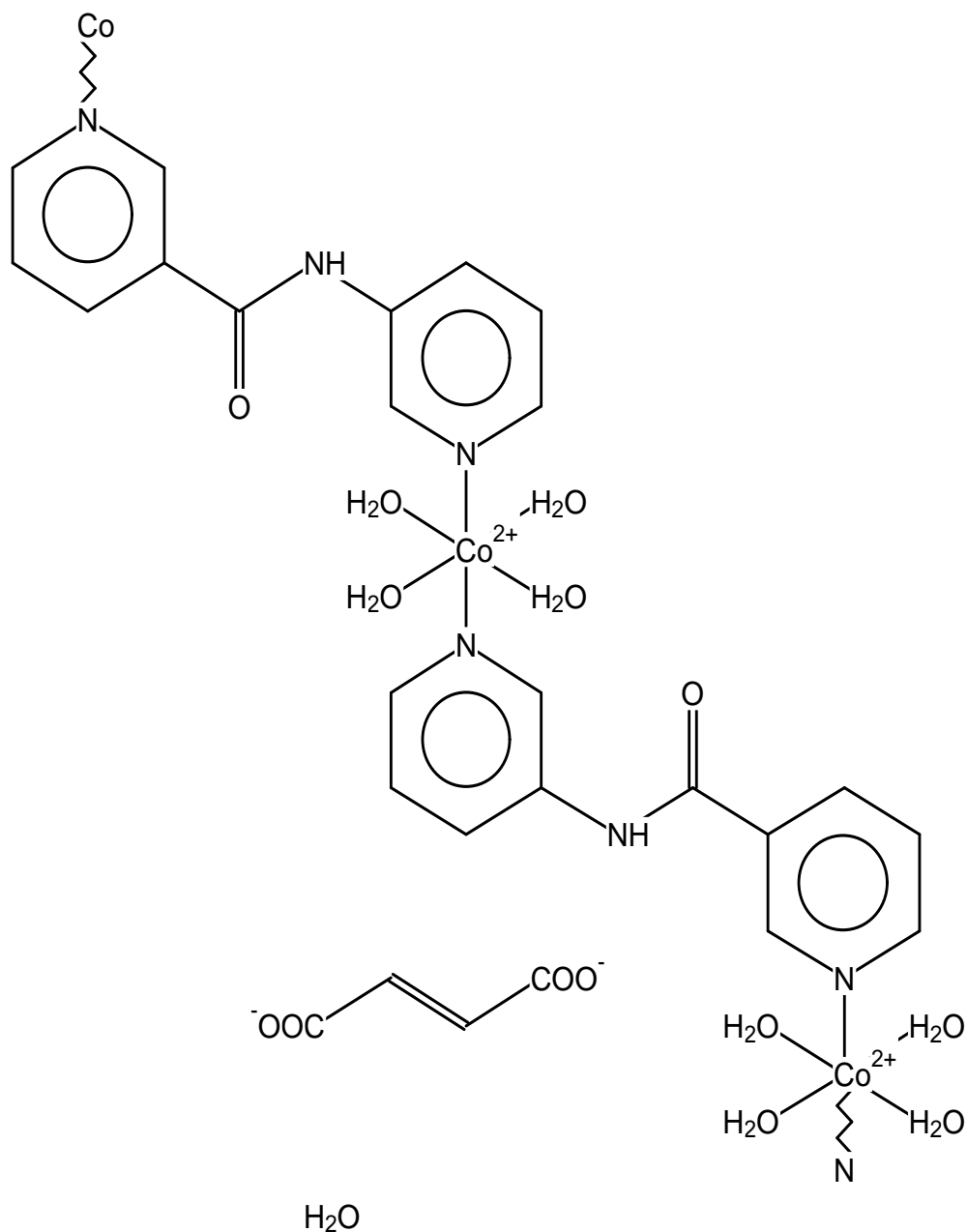
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *CrystEngComm* ,9, 895

Formula: $(C_{22} H_{34} Co_2 N_6 O_{10}^{4+})_n, 2n(C_4 H_2 O_4^{2-}), 4n(H_2 O_1)$

Compound Name: catena-(bis(μ_2 -N-(3-Pyridyl)nicotinamide)-octaaqua-di-cobalt(ii) bis(fumarate) tetrahydrate)

Space Group: P21/c **Cell:** **a** 8.395(0) **b** 15.806(1) **c** 14.883(1)
Space Group No.: 14 (**Å, °**) α 90.00 β 100.33(0) γ 90.00

R-Factor (%): 5.31 **Temperature(K):** 100 **Density(g/cm³):** 1.642



Search: search7 (Thu May 26 10:20:13 2011): Hit 9

VIPTOE

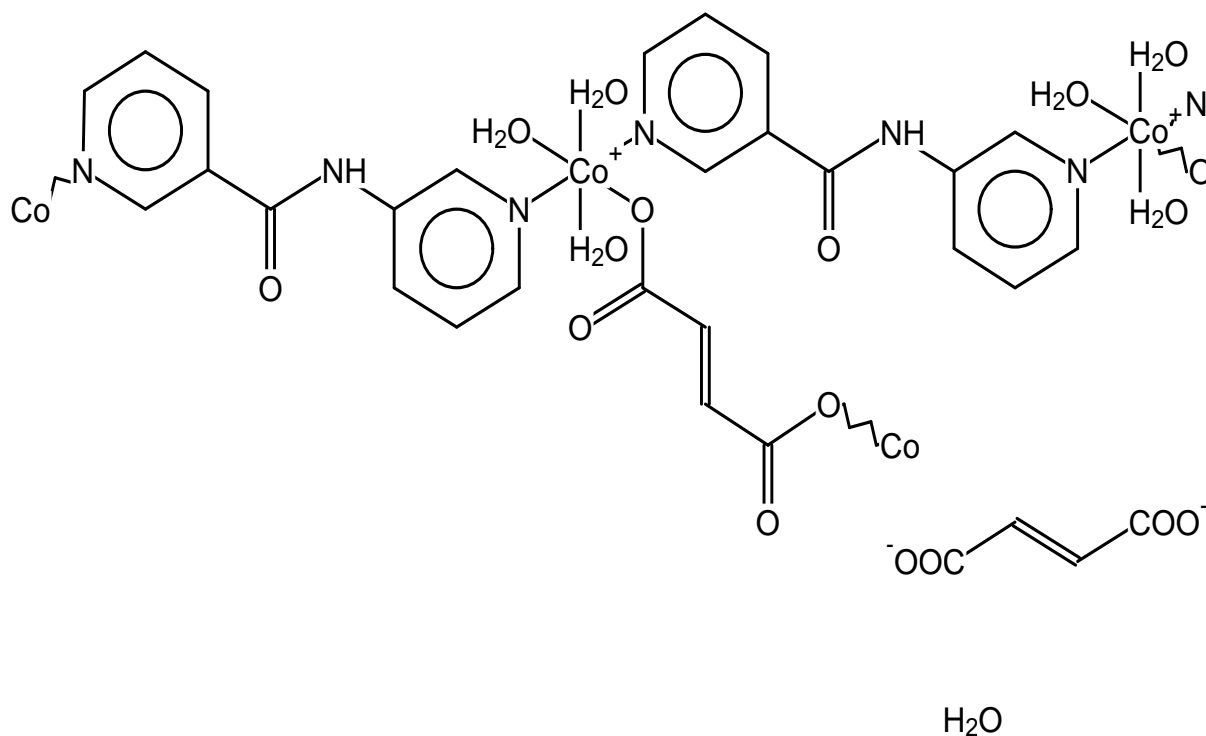
Reference: D.K.Kumar, A.Das, P.Dastidar (2007) *CrystEngComm*, **9**, 895

Formula: $(C_{26} H_{32} Co_2 N_6 O_{12}^{2+})_n, n(C_4 H_2 O_4^{2-}), 4n(H_2 O_1)$

Compound Name: catena-(bis(μ_2 -N-(3-Pyridyl)nicotinamide)-(μ_2 -fumarato)-hexaaqua-dicobalt(ii) fumarate tetrahydrate)

Space Group: P-1 **Cell:** **a** 8.836(1) **b** 10.421(1) **c** 10.856(1)
Space Group No.: 2 (**Å, °**) α 78.77(0) β 75.25(0) γ 68.71(0)

R-Factor (%): 6.50 **Temperature(K):** 100 **Density(g/cm³):** 1.716



Search Overview

Search: search10
Date/Time done: Thu May 26 10:24:54 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: 5

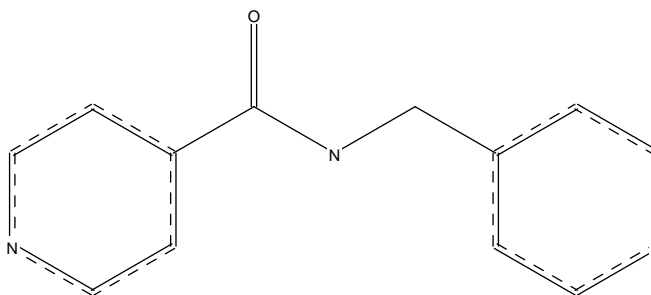
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

4M

Search: search10 (Thu May 26 10:24:54 2011): Hit 1

KIWPUC

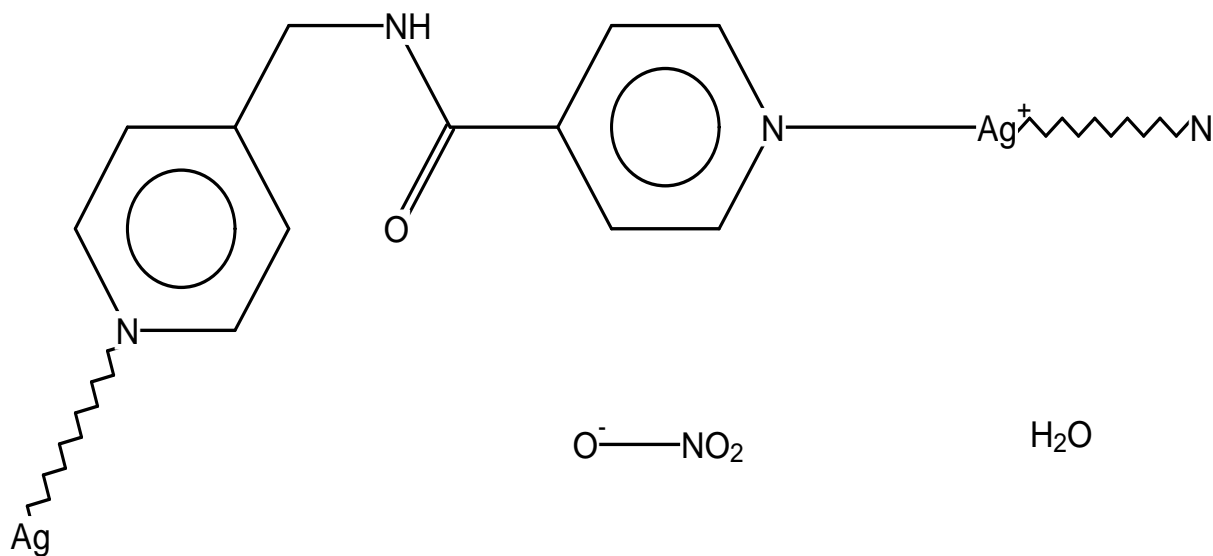
Reference: Yu-Tao Ma, Bai-Wang Sun, S.W.Ng (2008)
Acta Crystallogr., Sect. E: Struct. Rep. Online ,**64**,m470

Formula: (C₁₂ H₁₁ Ag₁ N₃ O₁¹⁺)_n,n(N₁ O₃¹⁻),n(H₂ O₁)

Compound Name: catena-((μ₂-N-(4-Pyridylmethyl)pyridine-4-carboxamide-κ²N:N')-silver(i) nitrate monohydrate)

Space Group: Pbc_a **Cell:** **a** 12.912(7) **b** 9.021(5) **c** 24.520(10)
Space Group No.: 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.26 **Temperature(K):** 295 **Density(g/cm³):** 1.866



Search: search10 (Thu May 26 10:24:54 2011): Hit 2

KIWPUC01

Reference: K.Uemura, Y.Kumamoto, S.Kitagawa (2008)
Chem.-Eur.J. ,**14**,9565

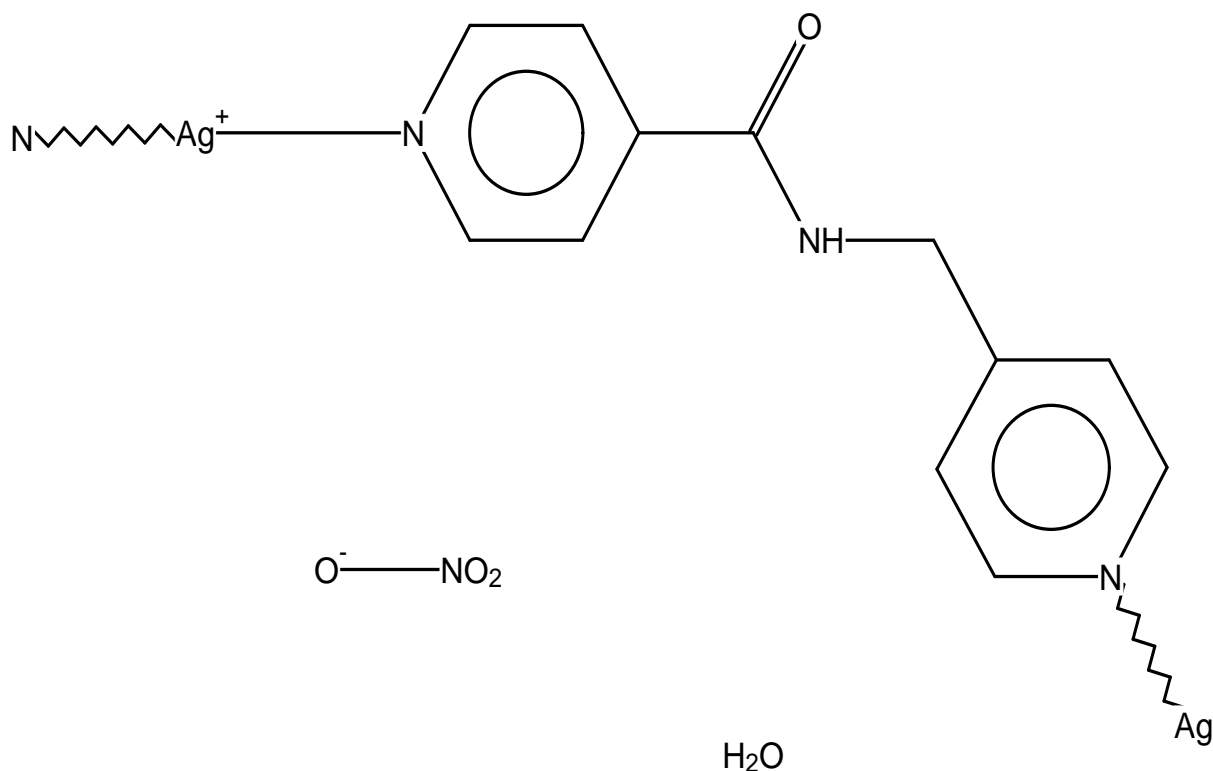
Formula: (C₁₂ H₁₁ Ag₁ N₃ O₁¹⁺)_n,n(N₁ O₃¹⁻),n(H₂ O₁)

Compound Name: catena-((μ₂-N-((Pyridin-4-yl)methyl)pyridine-4-carboxamide-N,N')-silver(i) nitrate monohydrate)

Synonym: catena-((μ₂-N-((Pyridin-4-yl)methyl)isonicotinamide-N,N')-silver(i) nitrate monohydrate)

Space Group: Pbc_a **Cell:** **a** 12.903(5) **b** 9.022(4) **c** 24.540(10)
Space Group No.: 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.77 **Temperature(K):** 293 **Density(g/cm³):** 1.865



Search: search10 (Thu May 26 10:24:54 2011): Hit 3

POJZOE

Reference: K.Uemura, Y.Kumamoto, S.Kitagawa (2008)
Chem.-Eur.J. ,**14**,9565

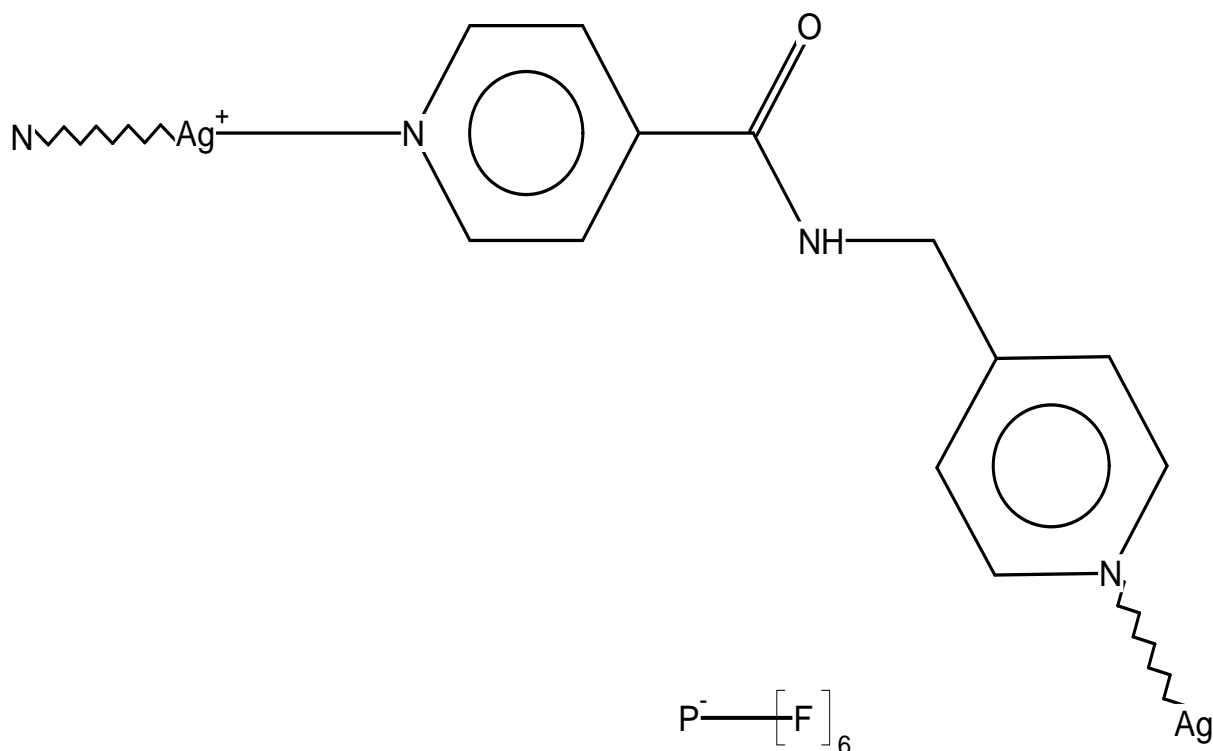
Formula: (C₁₂ H₁₁ Ag₁ N₃ O₁ 1⁺)_n,n(F₆ P₁ 1⁻)

Compound Name: catena-((μ₂-N-((Pyridin-4-yl)methyl)pyridine-4-carboxamide-N,N')-silver(i) hexafluorophosphate)

Synonym: catena-((μ₂-N-((Pyridin-4-yl)methyl)isonicotinamide-N,N')-silver(i) hexafluorophosphate)

Space Group: P21/n **Cell:** **a** 9.704(4) **b** 25.400(10) **c** 12.458(5)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 94.89(0) **γ** 90.00

R-Factor (%): 7.08 **Temperature(K):** 293 **Density(g/cm³):** 2.024



Search: search10 (Thu May 26 10:24:54 2011): Hit 4

POJZUK

Reference: K.Uemura, Y.Kumamoto, S.Kitagawa (2008)
Chem.-Eur.J. ,**14**,9565

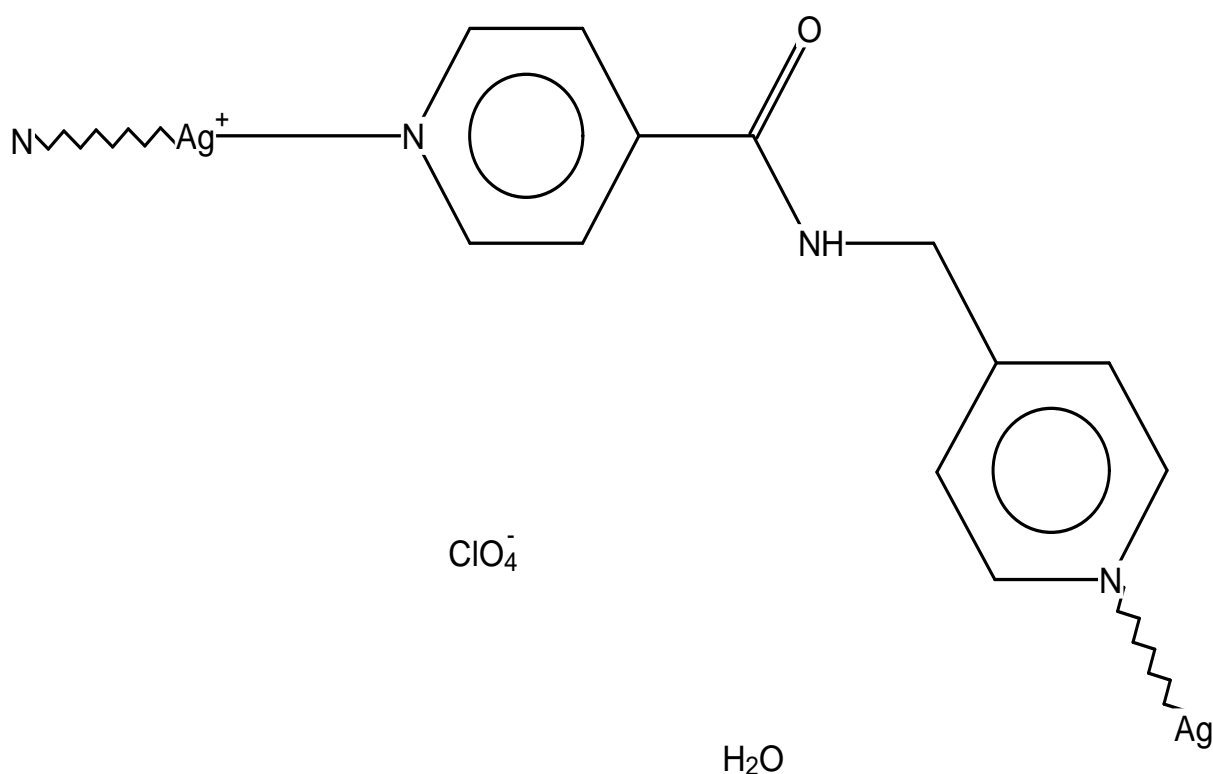
Formula: (C₁₂ H₁₁ Ag₁ N₃ O₁¹⁺)_n,n(Cl₁ O₄¹⁻)_n(H₂ O₁)

Compound Name: catena-((μ₂-N-((Pyridin-4-yl)methyl)pyridine-4-carboxamide-N,N')-silver(i) perchlorate monohydrate)

Synonym: catena-((μ₂-N-((Pyridin-4-yl)methyl)isonicotinamide-N,N')-silver(i) perchlorate monohydrate)

Space Group: Pbc_a **Cell:** **a** 13.409(0) **b** 9.383(0) **c** 25.048(1)
Space Group No.: 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 6.87 **Temperature(K):** 293 **Density(g/cm³):** 1.849



Search: search10 (Thu May 26 10:24:54 2011): Hit 5

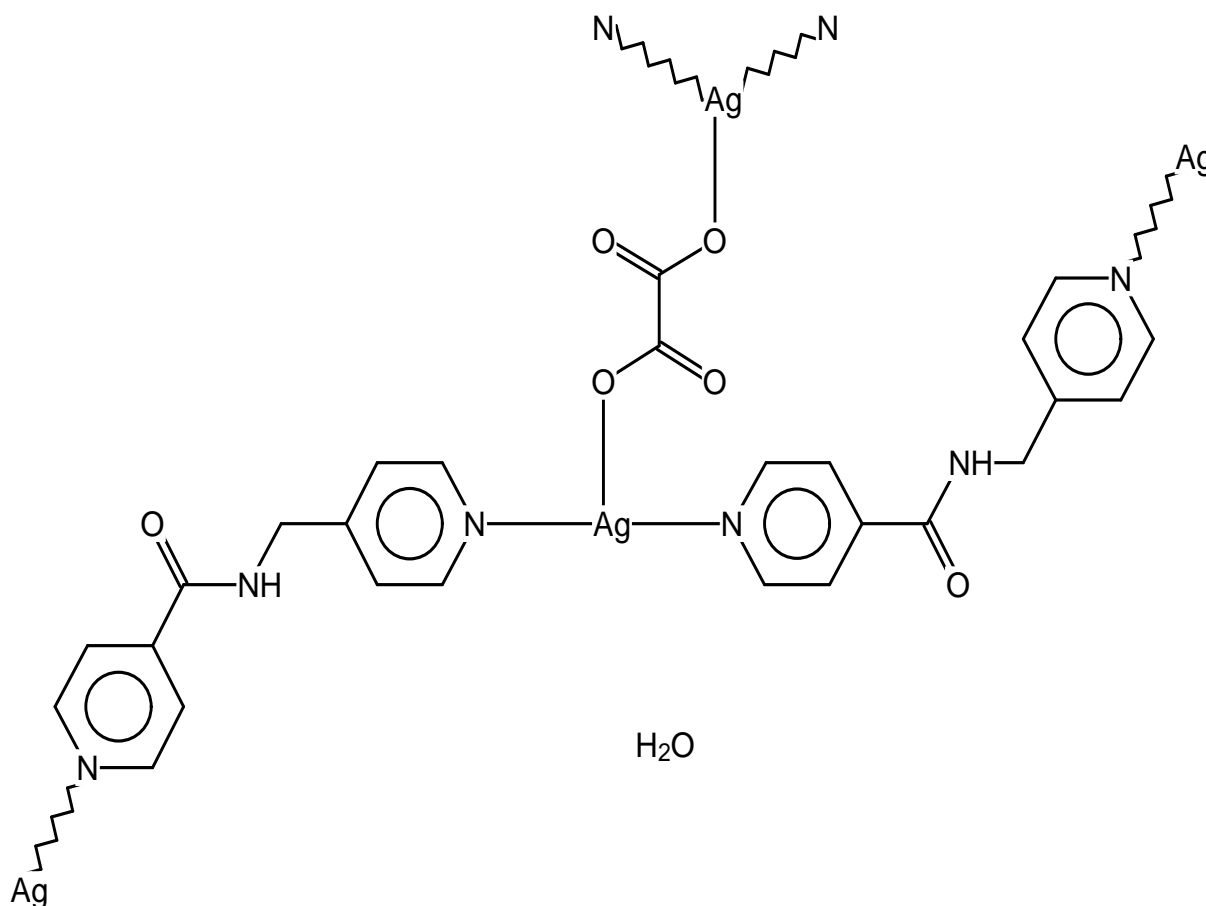
UGOREN

Reference: Ming-Liang Tong, Yin-Miao Wu, Jie Ru, Xiao-Ming Chen, Ho-Chol Chang, S.Kitagawa (2002) *Inorg.Chem.* ,**41**,4846

Formula: (C₂₆ H₂₂ Ag₂ N₆ O₆)_n,9n(H₂ O₁)

Compound Name: catena-((μ₂-Oxalato)-bis(μ₂-N-((pyrid-4-yl)methyl)pyridine-4-carboxamide-N',N''))-di-silver(i) nonahydrate

Space Group:	C2/c	Cell:	a 28.947(8)	b 8.617(3)	c 16.307(6)
Space Group No.:	15	(Å, °)	α 90.00	β 121.07(1)	γ 90.00
R-Factor (%):	5.13	Temperature(K):	293	Density(g/cm³):	1.701



Search Overview

Search: search11
Date/Time done: Thu May 26 10:26:24 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: 5

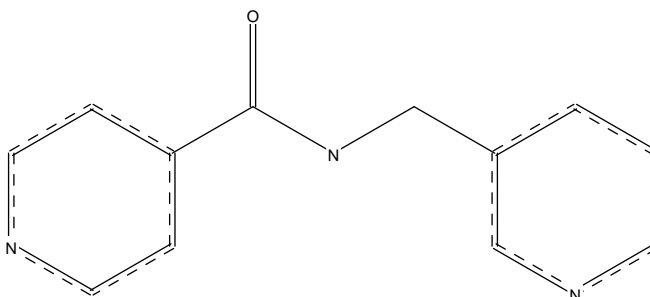
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

4M

Search: search11 (Thu May 26 10:26:24 2011): Hit 1

POKBAT

Reference: K.Uemura, Y.Kumamoto, S.Kitagawa (2008)
Chem.-Eur.J. ,**14**,9565

Formula: (C₁₂ H₁₁ Ag₁ N₃ O₁ 1⁺)_n,n(F₆ P₁ 1⁻)

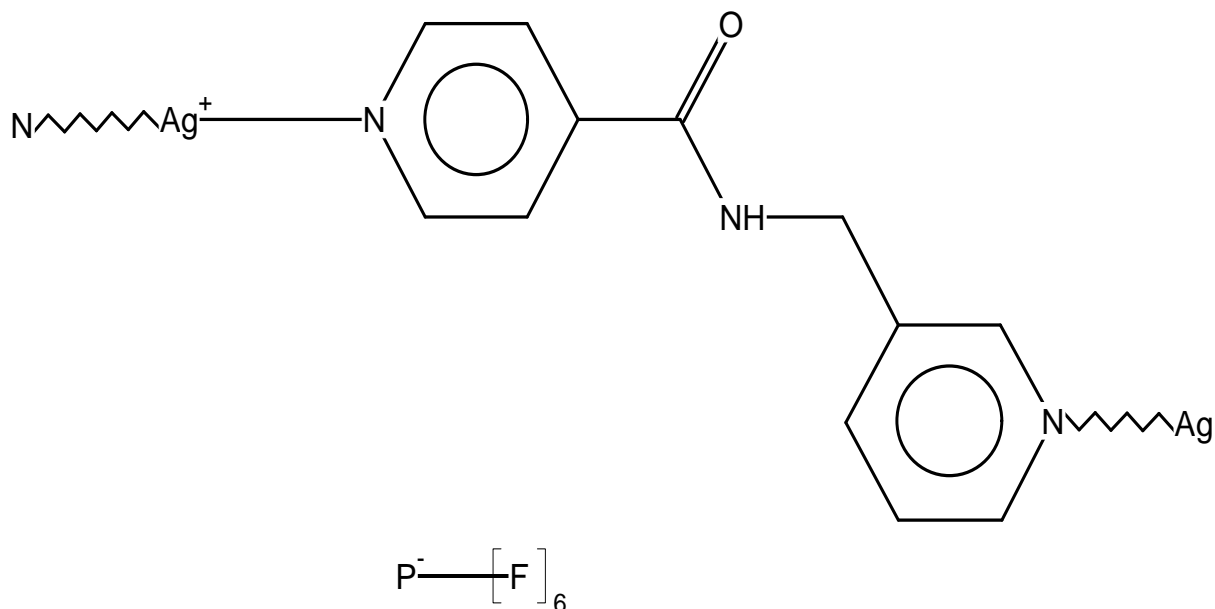
Compound Name: catena-((μ₂-N-((Pyridin-3-yl)methyl)pyridine-4-carboxamide-N,N')-silver(i) hexafluorophosphate)

Synonym: catena-((μ₂-N-((Pyridin-3-yl)methyl)isonicotinamide-N,N')-silver(i) hexafluorophosphate)

Space Group: P21/c **Cell:** **a** 8.501(1) **b** 19.951(3) **c** 9.622(0)

Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 108.43(0) **γ** 90.00

R-Factor (%): 5.28 **Temperature(K):** 293 **Density(g/cm³):** 2.000



Search: search11 (Thu May 26 10:26:24 2011): Hit 2

POKBEX

Reference: K.Uemura, Y.Kumamoto, S.Kitagawa (2008)
Chem.-Eur.J. ,**14**,9565

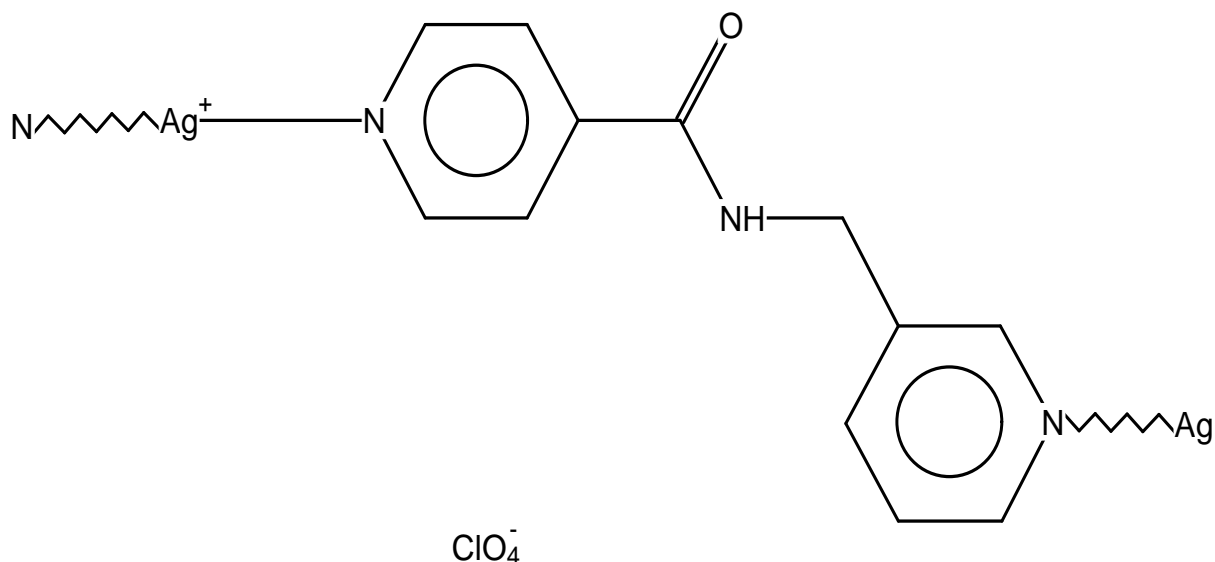
Formula: (C₁₂ H₁₁ Ag₁ N₃ O₁¹⁺)_n,n(Cl₁ O₄¹⁻)

Compound Name: catena-((μ₂-N-((Pyridin-3-yl)methyl)pyridine-4-carboxamide-N,N')-silver(i) perchlorate)

Synonym: catena-((μ₂-N-((Pyridin-3-yl)methyl)isonicotinamide-N,N')-silver(i) perchlorate)

Space Group: P21/c **Cell:** **a** 8.489(0) **b** 18.888(7) **c** 9.227(2)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 105.09(0) **γ** 90.00

R-Factor (%): 3.88 **Temperature(K):** 293 **Density(g/cm³):** 1.955



Search: search11 (Thu May 26 10:26:24 2011): Hit 3

POKBIB

Reference: K.Uemura, Y.Kumamoto, S.Kitagawa (2008)
Chem.-Eur.J. ,**14**,9565

Formula: (C₁₂ H₁₁ Ag₁ N₃ O₁ 1⁺)_n,n(B₁ F₄ 1⁻)

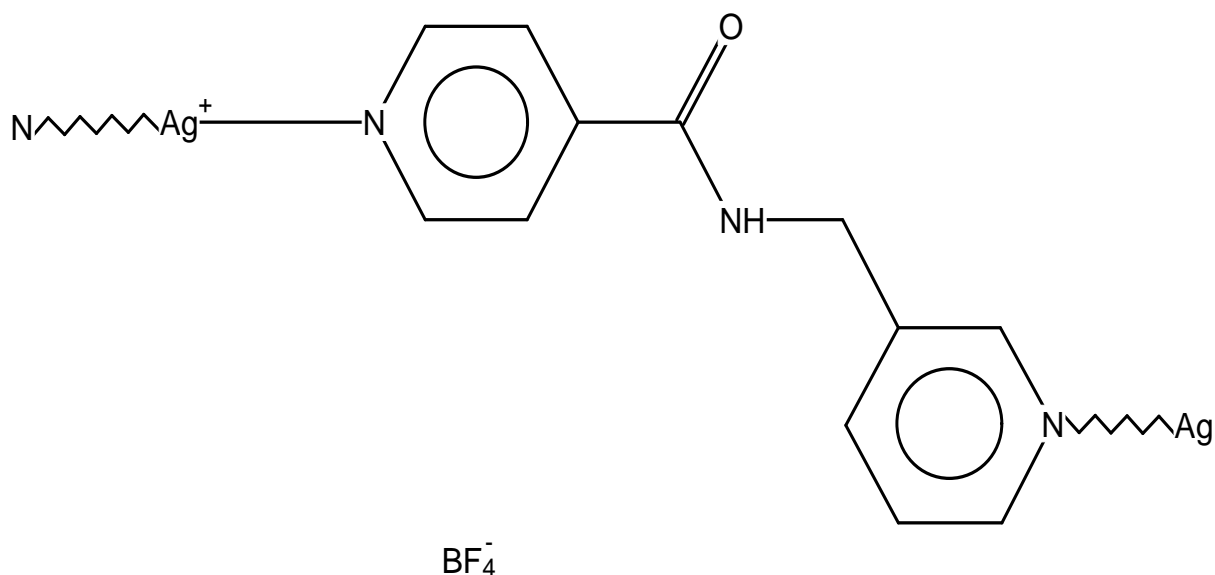
Compound Name: catena-((μ₂-N-((Pyridin-3-yl)methyl)pyridine-4-carboxamide-N,N')-silver(i) tetrafluoroborate)

Synonym: catena-((μ₂-N-((Pyridin-3-yl)methyl)isonicotinamide-N,N')-silver(i) tetrafluoroborate)

Space Group: P21/c **Cell:** **a** 8.514(4) **b** 18.763(9) **c** 9.071(4)

Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 104.63(0) **γ** 90.00

R-Factor (%): 4.35 **Temperature(K):** 293 **Density(g/cm³):** 1.932



Search: search11 (Thu May 26 10:26:24 2011): Hit 4

RISNOX

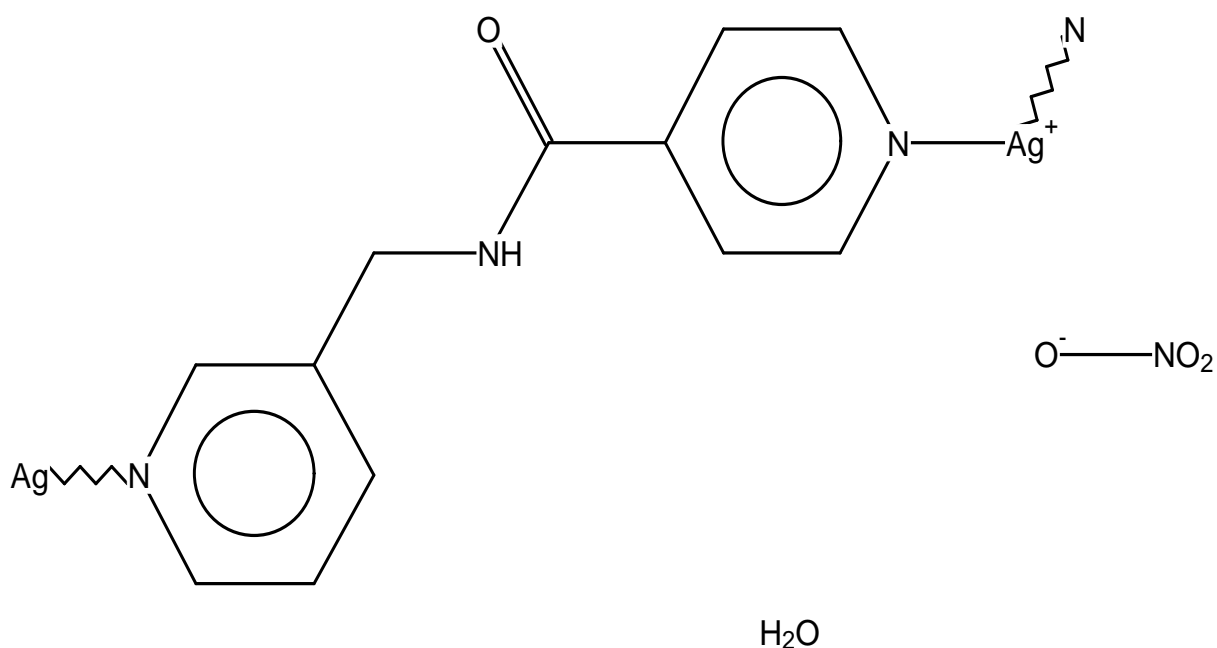
Reference: Yu-Tao Ma, Qi-Hua Zhao (2008)
Acta Crystallogr., Sect. E: Struct. Rep. Online, **64**, m110

Formula: (C₁₂ H₁₁ Ag₁ N₃ O₁¹⁺)_n, n(N₁ O₃¹⁻), n(H₂ O₁)

Compound Name: catena-((μ₂-N-(3-Pyridylmethyl)pyridine-4-carboxamide)-silver(i) nitrate monohydrate)

Space Group: P21/c **Cell:** **a** 12.177(2) **b** 13.022(3) **c** 8.911(1)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 94.21(3) **γ** 90.00

R-Factor (%): 4.24 **Temperature(K):** 293 **Density(g/cm³):** 1.891



Search: search11 (Thu May 26 10:26:24 2011): Hit 5

RISNOX01

Reference: K.Uemura, Y.Kumamoto, S.Kitagawa (2008)
Chem.-Eur.J. ,**14**,9565

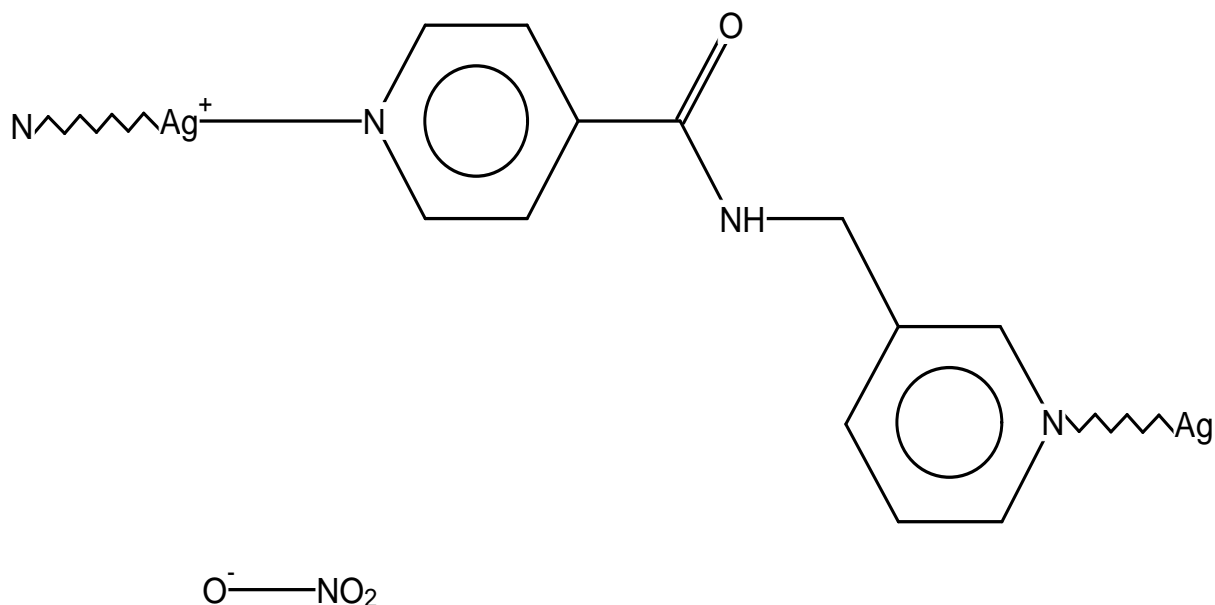
Formula: (C₁₂ H₁₁ Ag₁ N₃ O₁¹⁺),n,n(N₁ O₃¹⁻),n(H₂ O₁)

Compound Name: catena-((μ₂-N-((Pyridin-3-yl)methyl)pyridine-4-carboxamide-N,N')-silver(i) nitrate monohydrate)

Synonym: catena-((μ₂-N-((Pyridin-3-yl)methyl)isonicotinamide-N,N')-silver(i) nitrate monohydrate)

Space Group: P21/a **Cell:** **a** 8.951(5) **b** 13.049(7) **c** 12.215(7)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 94.21(0) **γ** 90.00

R-Factor (%): 3.25 **Temperature(K):** 293 **Density(g/cm³):** 1.873



Search Overview

Search: search12
Date/Time done: Thu May 26 10:27:57 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: 5

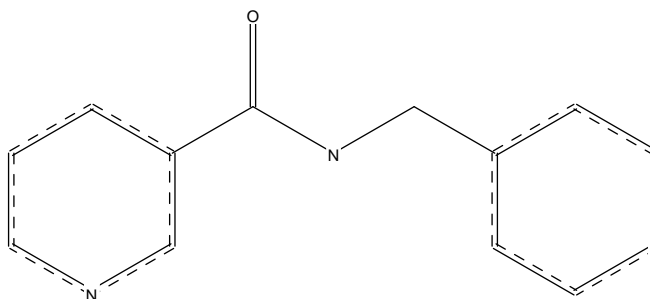
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

4M

Search: search12 (Thu May 26 10:27:57 2011): Hit 1

HEVGEV

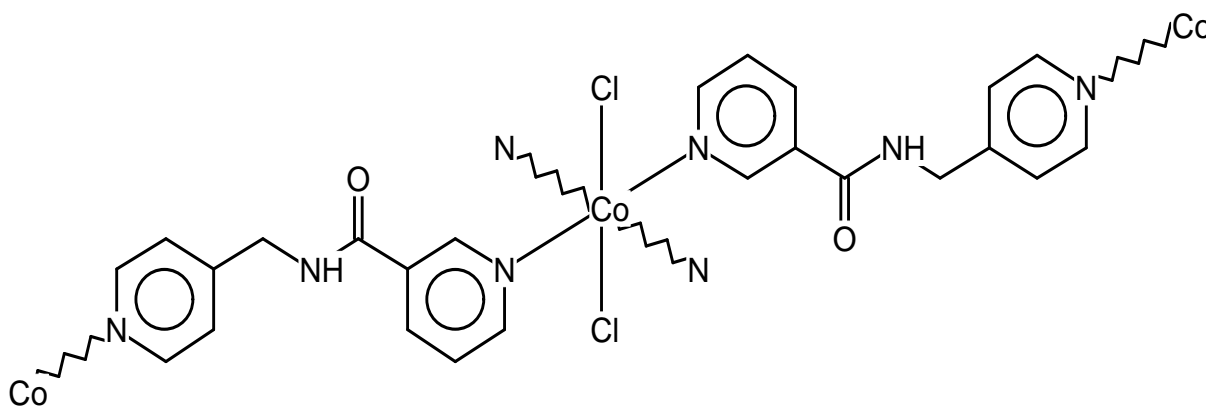
Reference: K.Uemura, K.Saito, S.Kitagawa, H.Kita (2006)
J.Am.Chem.Soc. ,**128**,16122

Formula: (C₂₄ H₂₂ Cl₂ Co₁ N₆ O₂)_n

Compound Name: catena-(bis(μ₂-N-(Pyrid-4-ylmethyl)nicotinamide-N',N'')-dichloro-cobalt(ii))

Space Group: P-1 **Cell:** **a** 7.899(7) **b** 8.782(7) **c** 8.980(8)
Space Group No.: 2 **(Å, °)** **α** 84.70(2) **β** 81.32(2) **γ** 82.50(2)

R-Factor (%): 4.10 **Temperature(K):** 293 **Density(g/cm³):** 1.517



Search: search12 (Thu May 26 10:27:57 2011): Hit 2

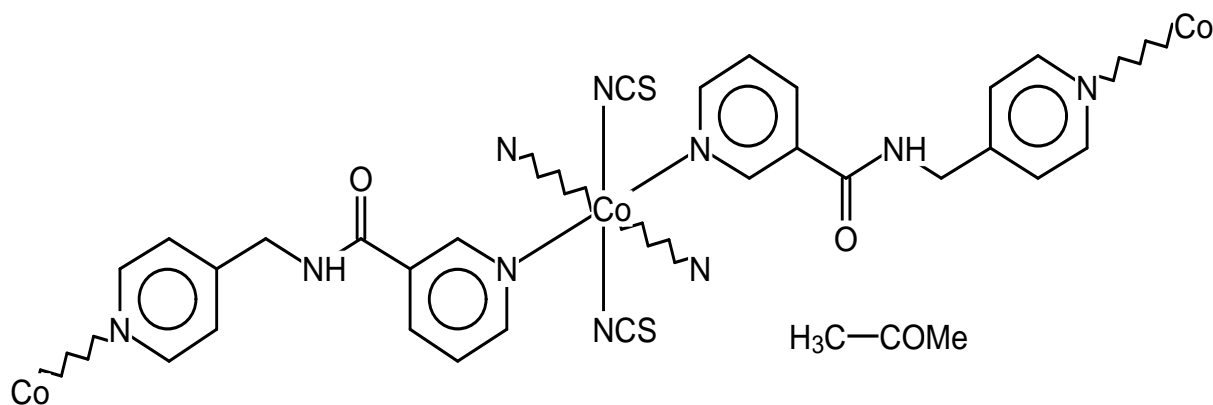
HEVGIZ

Reference: K.Uemura, K.Saito, S.Kitagawa, H.Kita (2006)
J.Am.Chem.Soc. ,**128**,16122

Formula: (C₂₆ H₂₂ Co₁ N₈ O₂ S₂)_n,2n(C₃ H₆ O₁)

Compound Name: catena-(bis(μ₂-N-(Pyrid-4-ylmethyl)nicotinamide-N',N'')-bis(isothiocyanato-N)-cobalt(ii) bis(acetone) clathrate)

Space Group:	P21/n	Cell:	a 11.371(2)	b 10.063(1)	c 15.536(0)
Space Group No.:	14	(Å, °)	α 90.00	β 104.64(0)	γ 90.00
R-Factor (%):	6.52	Temperature(K):	293	Density(g/cm³):	1.386



Search: search12 (Thu May 26 10:27:57 2011): Hit 3

HEVGOF

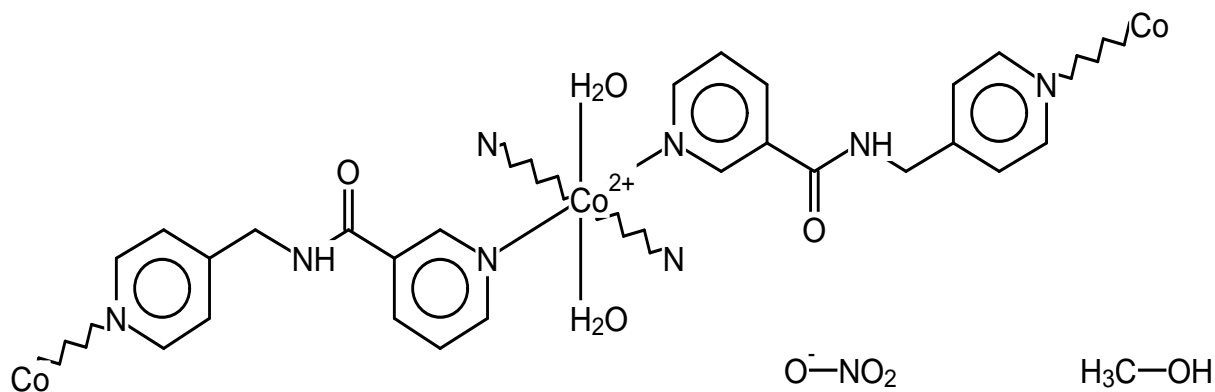
Reference: K.Uemura, K.Saito, S.Kitagawa, H.Kita (2006)
J.Am.Chem.Soc. ,**128**,16122

Formula: $(C_{24} H_{26} Co_1 N_6 O_4^{2+})_n, 2n(N_1 O_3^{1-}), 2n(C_1 H_4 O_1)$

Compound Name: catena-(bis(μ_2 -N-(Pyrid-4-ylmethyl)nicotinamide-N',N'')-diaqua-cobalt(ii) dinitrate bis(methanol) clathrate)

Space Group: P-1 **Cell:** **a** 8.072(0) **b** 9.760(1) **c** 11.260(1)
Space Group No.: 2 (**Å, °**) α 107.24(0) β 104.60(0) γ 101.29(0)

R-Factor (%): 5.05 **Temperature(K):** 213 **Density(g/cm³):** 1.503



Search: search12 (Thu May 26 10:27:57 2011): Hit 4

POKBOH

Reference: K.Uemura, Y.Kumamoto, S.Kitagawa (2008)
Chem.-Eur.J. ,**14**,9565

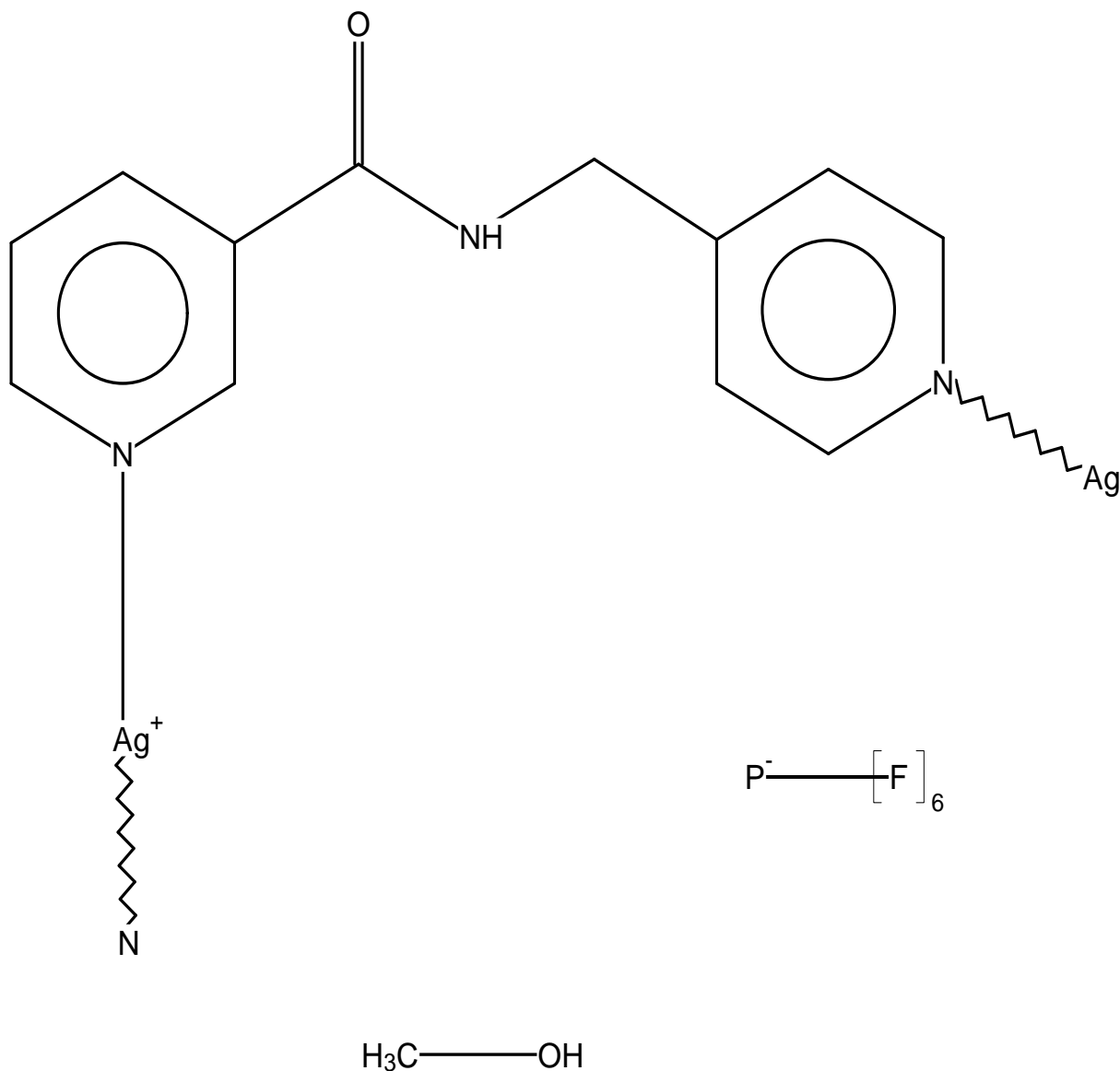
Formula: (C₁₂ H₁₁ Ag₁ N₃ O₁¹⁺),n,n(F₆ P₁¹⁻),n(C₁ H₄ O₁)

Compound Name: catena-((μ₂-N-((Pyridin-4-yl)methyl)pyridine-3-carboxamide-N,N')-silver hexafluorophosphate methanol solvate)

Synonym: catena-((μ₂-N-((Pyridin-4-yl)methyl)nicotinamide-N,N')-silver(i) hexafluorophosphate methanol solvate)

Space Group: P43 **Cell:** **a** 7.936(0) **b** 7.936(0) **c** 28.283(3)
Space Group No.: 78 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 7.32 **Temperature(K):** 223 **Density(g/cm³):** 1.858



Search: search12 (Thu May 26 10:27:57 2011): Hit 5

POKBOH01

Reference: K.Uemura, Y.Kumamoto, S.Kitagawa (2008)
Chem.-Eur.J. ,**14**,9565

Formula: (C₁₂ H₁₁ Ag₁ N₃ O₁¹⁺),n,n(F₆ P₁¹⁻),n(C₁ H₄ O₁)

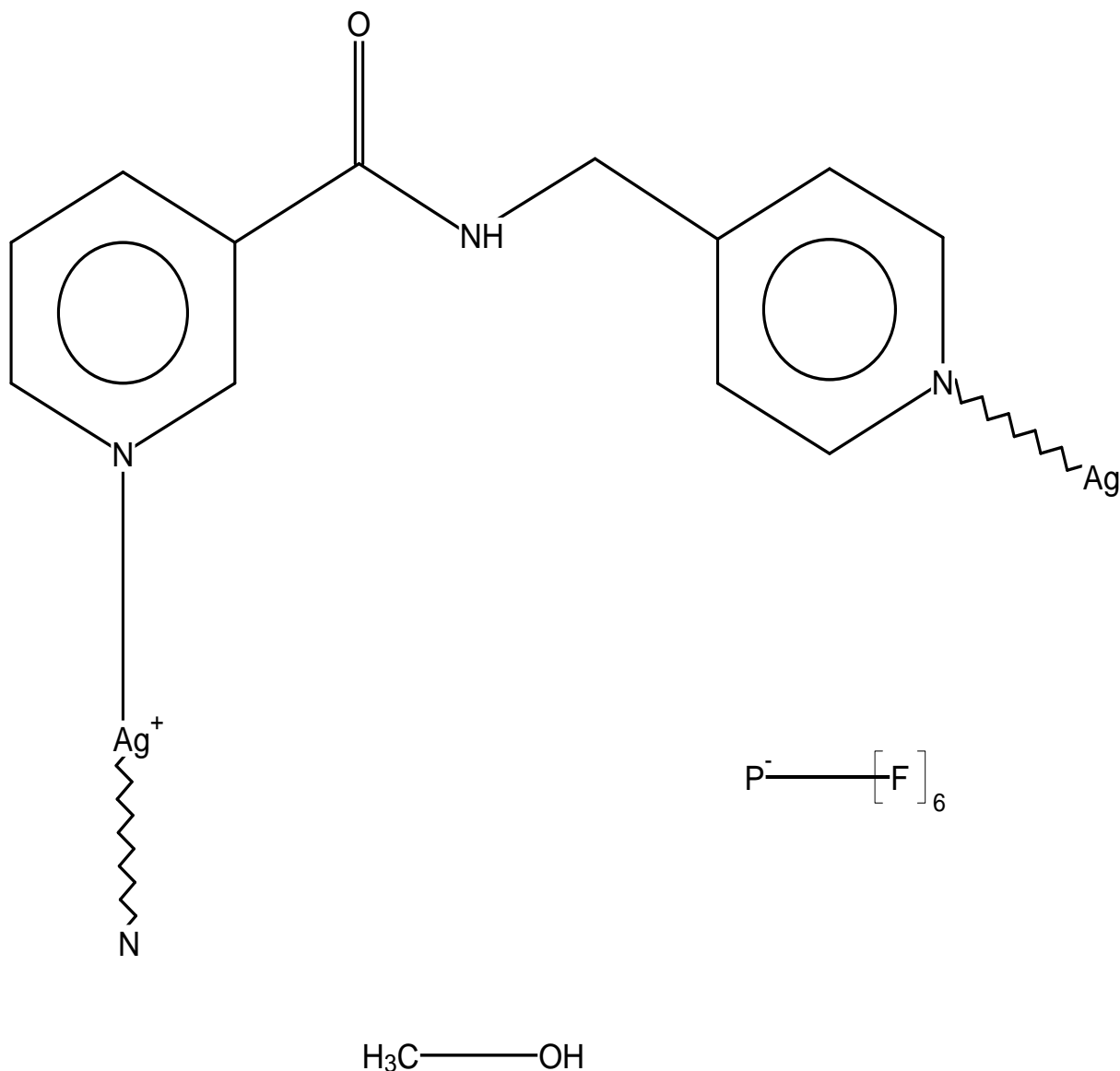
Compound Name: catena-((μ₂-N-((Pyridin-4-yl)methyl)pyridine-3-carboxamide-N,N')-silver hexafluorophosphate methanol solvate)

Synonym: catena-((μ₂-N-((Pyridin-4-yl)methyl)nicotinamide-N,N')-silver(i) hexafluorophosphate methanol solvate)

Space Group: P41 **Cell:** **a** 7.939(0) **b** 7.939(0) **c** 28.250(3)

Space Group No.: 76 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 8.02 **Temperature(K)**: 223 **Density(g/cm³)**: 1.858



Search Overview

Search: search21
Date/Time done: Thu May 26 10:38:10 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: 1

Summary of queries used. Search found structures that:

match

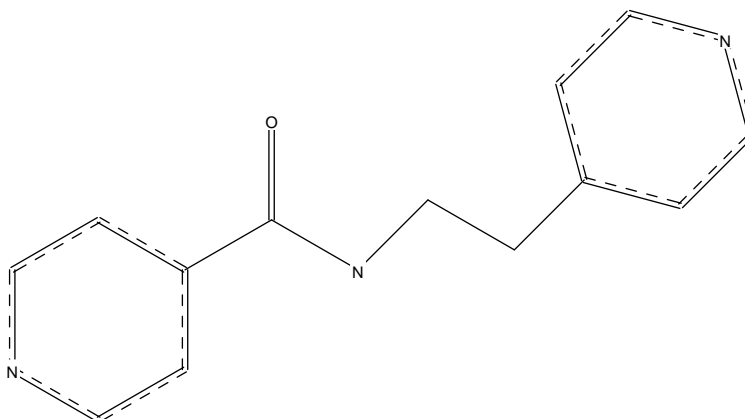
Query 2

Query 3

Query 2

4M

Query 3



Search: search21 (Thu May 26 10:38:10 2011): Hit 1

AVUBIC

Reference: K.Uemura, S.Kitagawa, K.Fukui, K.Saito (2004)
J.Am.Chem.Soc. ,**126**,3817

Formula: (C₂₈ H₂₆ Co₁ N₈ O₂ S₂)_n,4n(C₃ H₆ O₁)

Compound Name: catena-(bis(μ₂-N-(2-(Pyridin-4-yl)ethyl)isonicotinamide-N,N')-bis(isothiocyanato)-cobalt(ii) acetone solvate)

Space Group: P21/c **Cell:** **a** 11.115(3) **b** 22.046(7) **c** 9.717(3)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 100.83(0) **γ** 90.00

R-Factor (%): 8.32 **Temperature(K):** 293 **Density(g/cm³):** 1.224

