

## Search Overview

**Search:** search48  
**Date/Time done:** Thu May 26 11:42:42 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:** 14

*Summary of queries used. Search found structures that:*

match

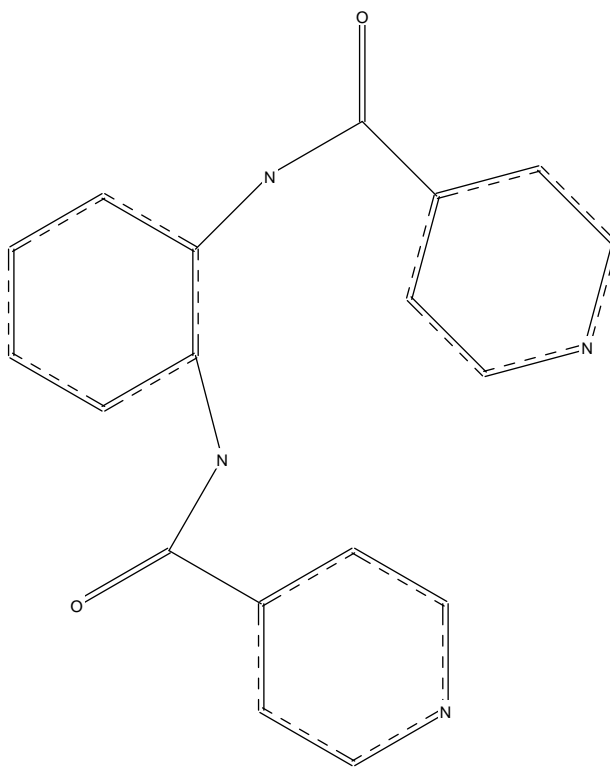
**Query 2**

**Query 3**

**Query 2**

4M

**Query 3**



## Search: search48 (Thu May 26 11:42:42 2011): Hit 1

### BAXNOE

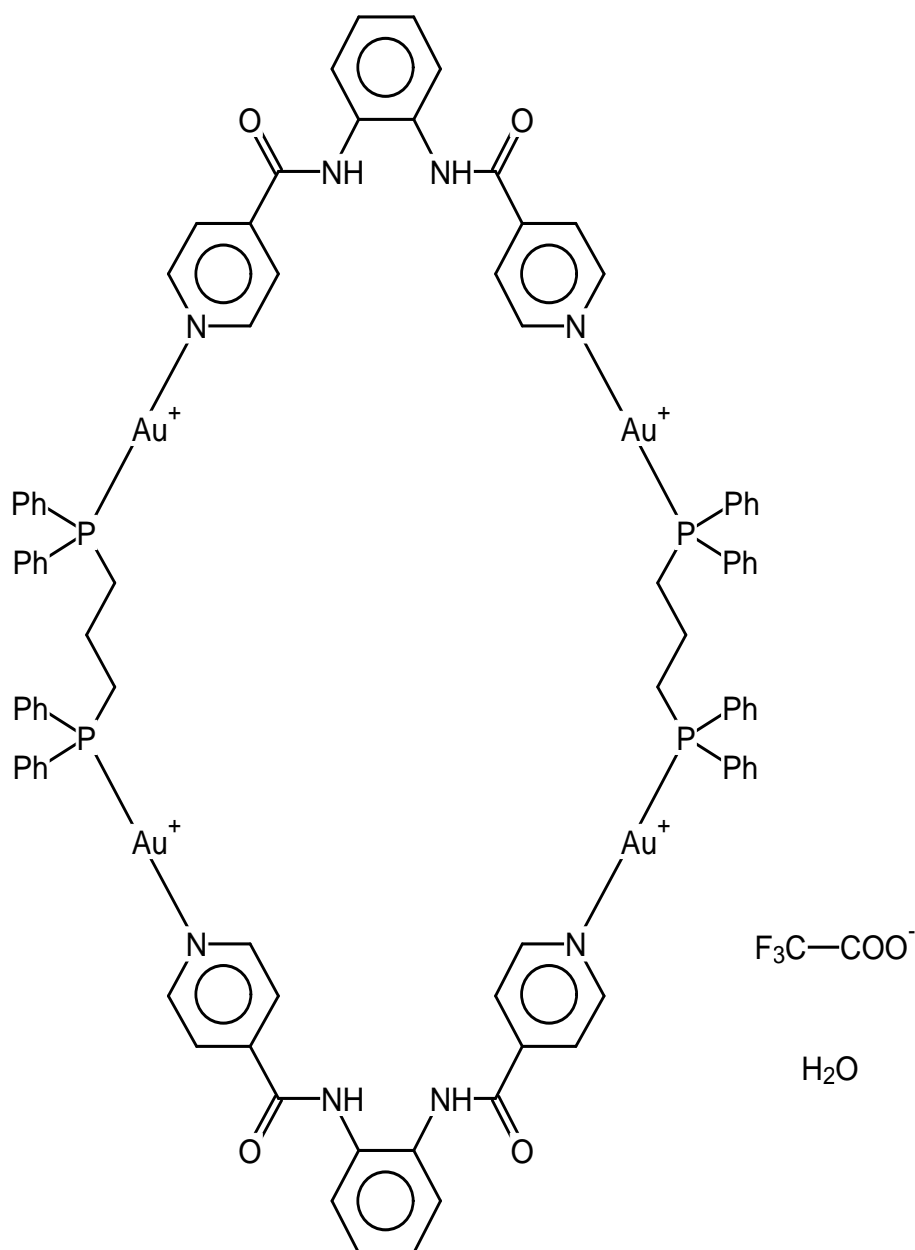
**Reference:** T.J.Burchell, D.J.Eisler, M.C.Jennings, R.J.Puddephatt  
(2003) *Chem.Commun.* ,2228

**Formula:** C<sub>90</sub> H<sub>80</sub> Au<sub>4</sub> N<sub>8</sub> O<sub>4</sub> P<sub>4</sub> 4<sup>+</sup>,4(C<sub>2</sub> F<sub>3</sub> O<sub>2</sub> 1<sup>-</sup>),2(H<sub>2</sub> O<sub>1</sub>)

**Compound Name:** bis(μ<sub>2</sub>-1,2-bis(Isonicotinoylamino)benzene-N,N')-bis(μ<sub>2</sub>-1,3-bis(diphenylphosphino)propane-P,P')-tetra-gold(i) tetrakis(trifluoroacetate) dihydrate

**Space Group:** P-1      **Cell:**      **a** 10.550(30)      **b** 11.730(40)      **c** 19.520(60)  
**Space Group No.:** 2      **(Å, °)**      **α** 98.94(5)      **β** 90.26(5)      **γ** 102.28(5)

**R-Factor (%):** 4.08      **Temperature(K):** 100      **Density(g/cm<sup>3</sup>):** 1.951



## Search: search48 (Thu May 26 11:42:42 2011): Hit 2

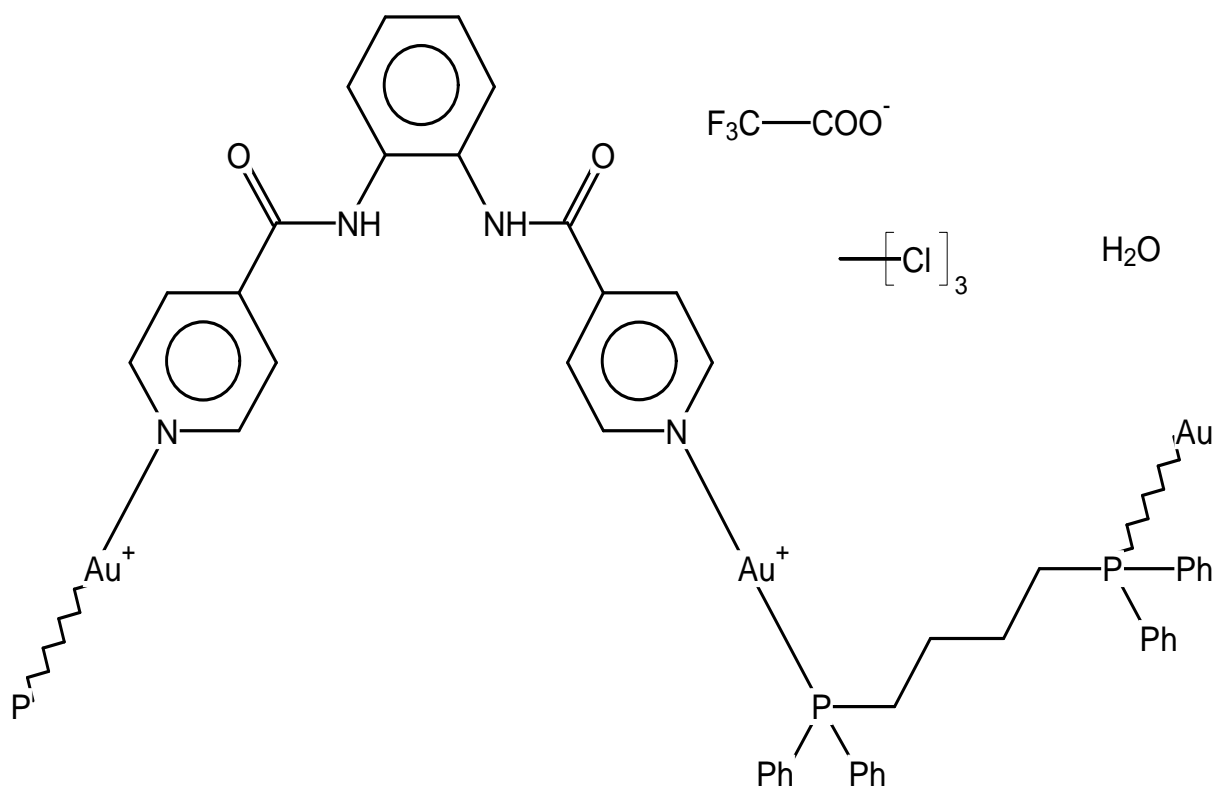
### BAXNUK

**Reference:** T.J.Burchell, D.J.Eisler, M.C.Jennings, R.J.Puddephatt  
(2003) *Chem. Commun.* ,2228

**Formula:**  $(C_{46}H_{42}Au_2N_4O_2P_2^{2+})_n, 2n(C_2F_3O_2^{1-}), 0.5n(C_1H_1Cl_3), 0.5n(H_2O_1)$

**Compound Name:** catena-(( $\mu_2$ -1,2-bis(Isonicotinoylamino)benzene-N,N')-( $\mu_2$ -1,4-bis(diphenylphosphino)butane-P,P')-di-gold(i) bis(trifluoroacetate) chloroform solvate hemihydrate)

<b>Space Group:</b>	C2/c	<b>Cell:</b>	<b>a</b> 34.465(7)	<b>b</b> 21.644(4)	<b>c</b> 9.319(1)
<b>Space Group No.:</b>	15	<b>(Å, °)</b>	$\alpha$ 90.00	$\beta$ 100.01(3)	$\gamma$ 90.00
<b>R-Factor (%):</b>	7.89	<b>Temperature(K):</b>	200	<b>Density(g/cm<sup>3</sup>):</b>	1.391



## Search: search48 (Thu May 26 11:42:42 2011): Hit 3

### COJLET

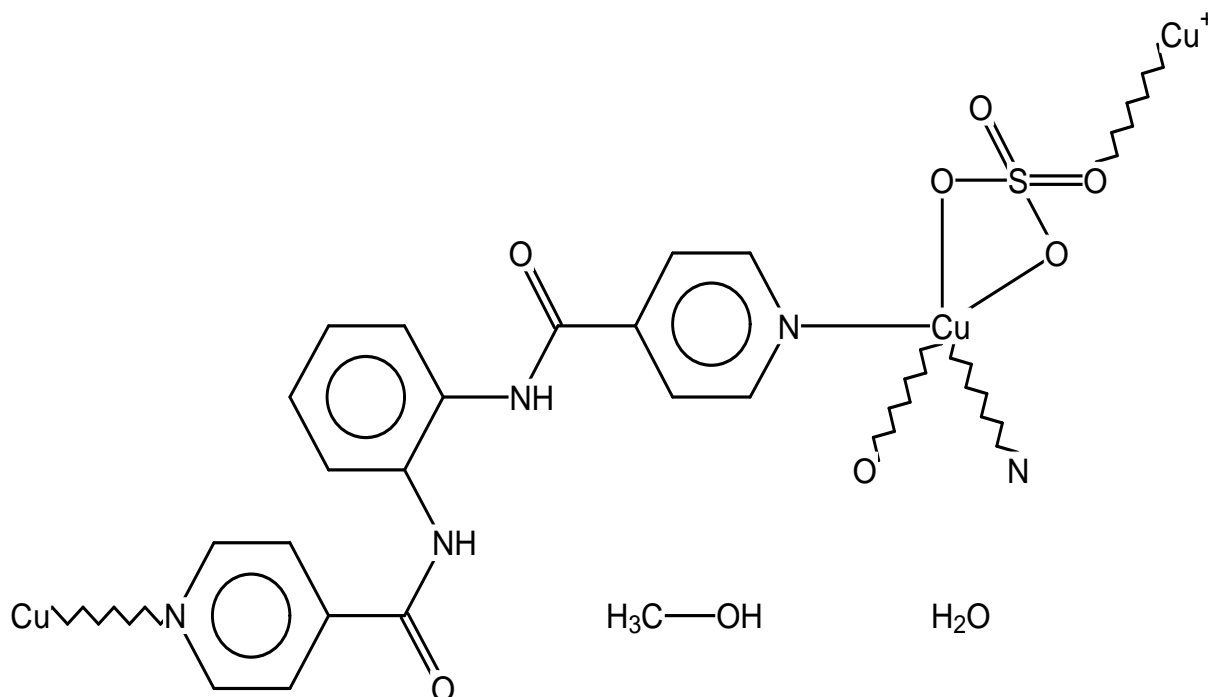
**Reference:** Ping Zhang, Yun-Yin Niu, Ben-Lai Wu, Hong-Yun Zhang, Cao-Yuan Niu, Hong-Wei Hou (2008) *Inorg.Chim.Acta* ,**361**,2609

**Formula:** (C<sub>18</sub> H<sub>14</sub> Cu<sub>1</sub> N<sub>4</sub> O<sub>6</sub> S<sub>1</sub>)<sub>n</sub>,2n(C<sub>1</sub> H<sub>4</sub> O<sub>1</sub>),n(H<sub>2</sub> O<sub>1</sub>)

**Compound Name:** catena-((μ<sub>2</sub>-N,N'-(1,2-Phenylene)-diisonicotinamide-N'',N''')-(μ<sub>2</sub>-sulfato-O,O',O'')-copper(ii) bis(methanol) clathrate monohydrate)

**Space Group:** P21/c      **Cell:**      **a** 11.203(1)      **b** 12.026(2)      **c** 18.078(3)  
**Space Group No.:** 14      **(Å, °)**      **α** 90.00      **β** 101.87(0)      **γ** 90.00

**R-Factor (%):** 3.88      **Temperature(K):** 291      **Density(g/cm<sup>3</sup>):** 1.561



## Search: search48 (Thu May 26 11:42:42 2011): Hit 4

### COJLIX

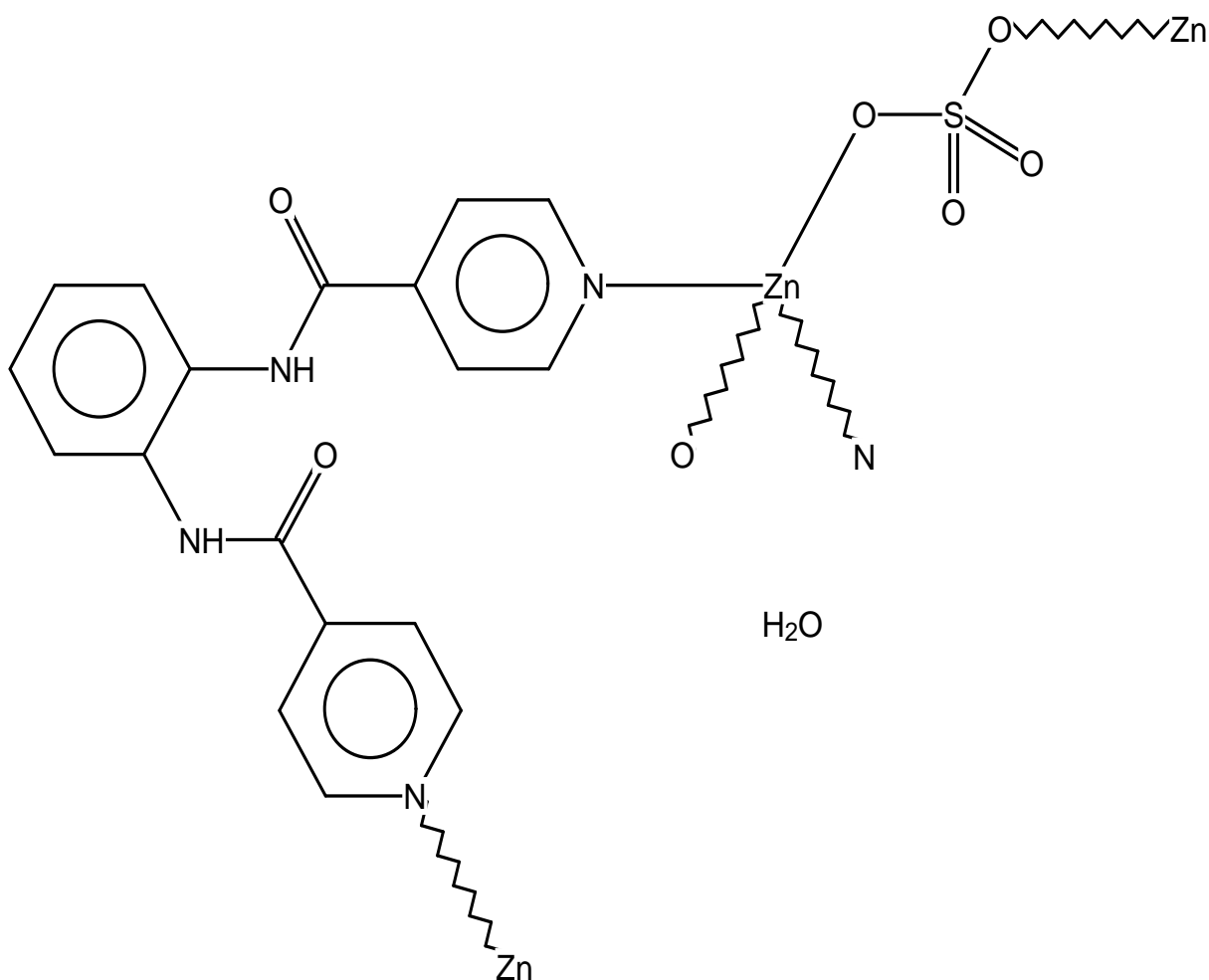
**Reference:** Ping Zhang, Yun-Yin Niu, Ben-Lai Wu, Hong-Yun Zhang, Cao-Yuan Niu, Hong-Wei Hou (2008) *Inorg.Chim.Acta* ,**361**,2609

**Formula:** (C<sub>18</sub> H<sub>14</sub> N<sub>4</sub> O<sub>6</sub> S<sub>1</sub> Zn<sub>1</sub>)<sub>n</sub>,2n(H<sub>2</sub> O<sub>1</sub>)

**Compound Name:** catena-((μ<sub>2</sub>-N,N'-(1,2-Phenylene)-diisonicotinamide-N'',N''')-(μ<sub>2</sub>-sulfato-O,O')-zinc(ii) dihydrate)

**Space Group:** Pccn      **Cell:**      **a** 22.667(4)      **b** 23.716(4)      **c** 9.245(1)  
**Space Group No.:** 56      **(Å, °)**      **α** 90.00      **β** 90.00      **γ** 90.00

**R-Factor (%):** 6.67      **Temperature(K):** 291      **Density(g/cm<sup>3</sup>):** 1.379



## Search: search48 (Thu May 26 11:42:42 2011): Hit 5

### EXEHOE

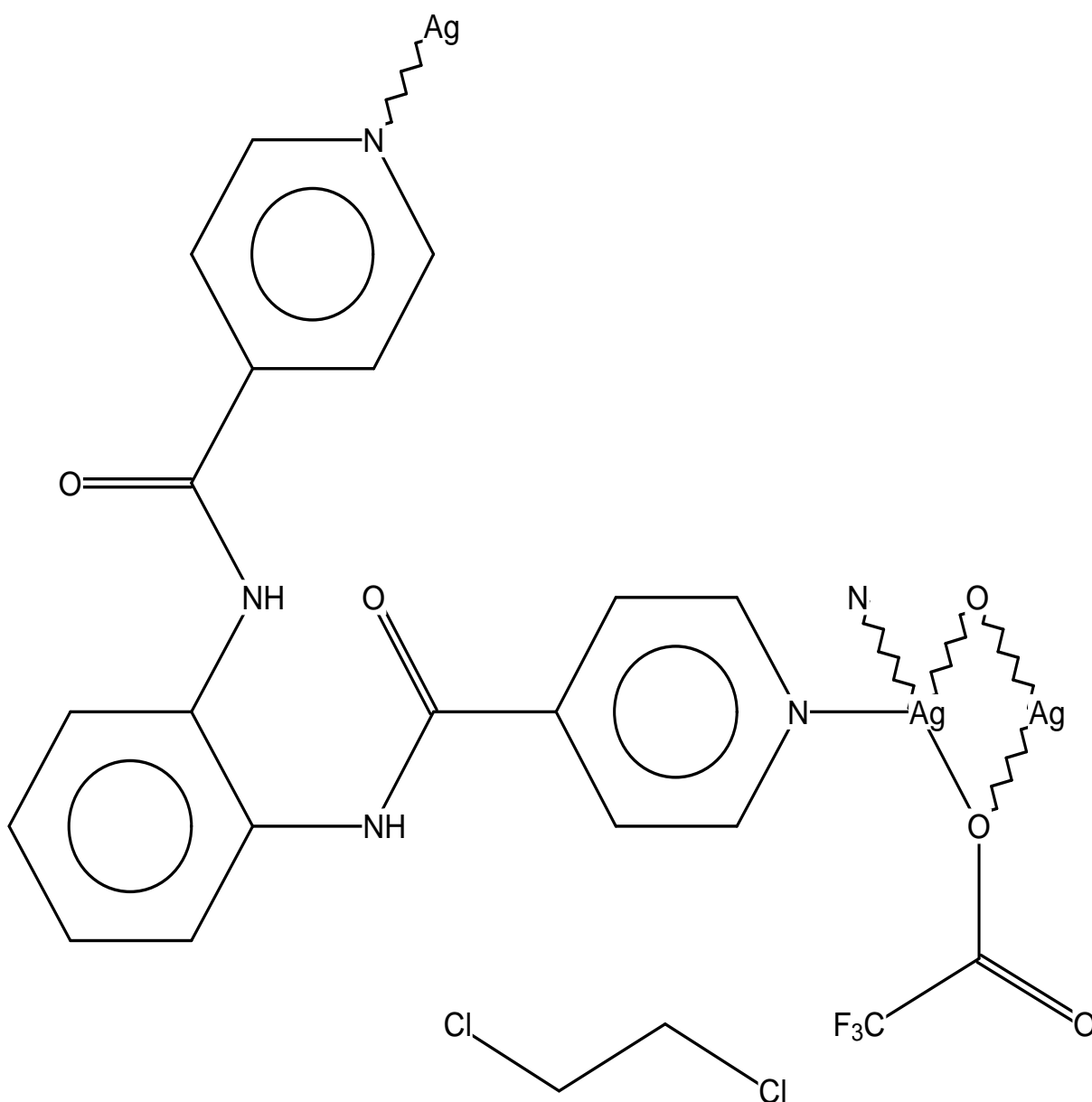
**Reference:** T.J.Burchell, D.J.Eisler, R.J.Puddephatt (2004)  
*Chem. Commun.* ,944

**Formula:**  $(C_{20}H_{14}Ag_1F_3N_4O_4)_n \cdot 1.25n(C_2H_4Cl_2)$

**Compound Name:** catena-(( $\mu_2$ -Trifluoroacetato)-( $\mu_2$ -1,2-bis(pyridine-4-carboxamido)benzene)-silver(i) 1,2-dichloroethane solvate)

**Space Group:** C2/m      **Cell:**    **a** 9.407(1)    **b** 24.330(5)    **c** 11.965(2)  
**Space Group No.:** 12      **(Å, °)**     $\alpha$  90.00       $\beta$  98.98(3)     $\gamma$  90.00

**R-Factor (%):** 5.52      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.628



## Search: search48 (Thu May 26 11:42:42 2011): Hit 6

EXEHOE01

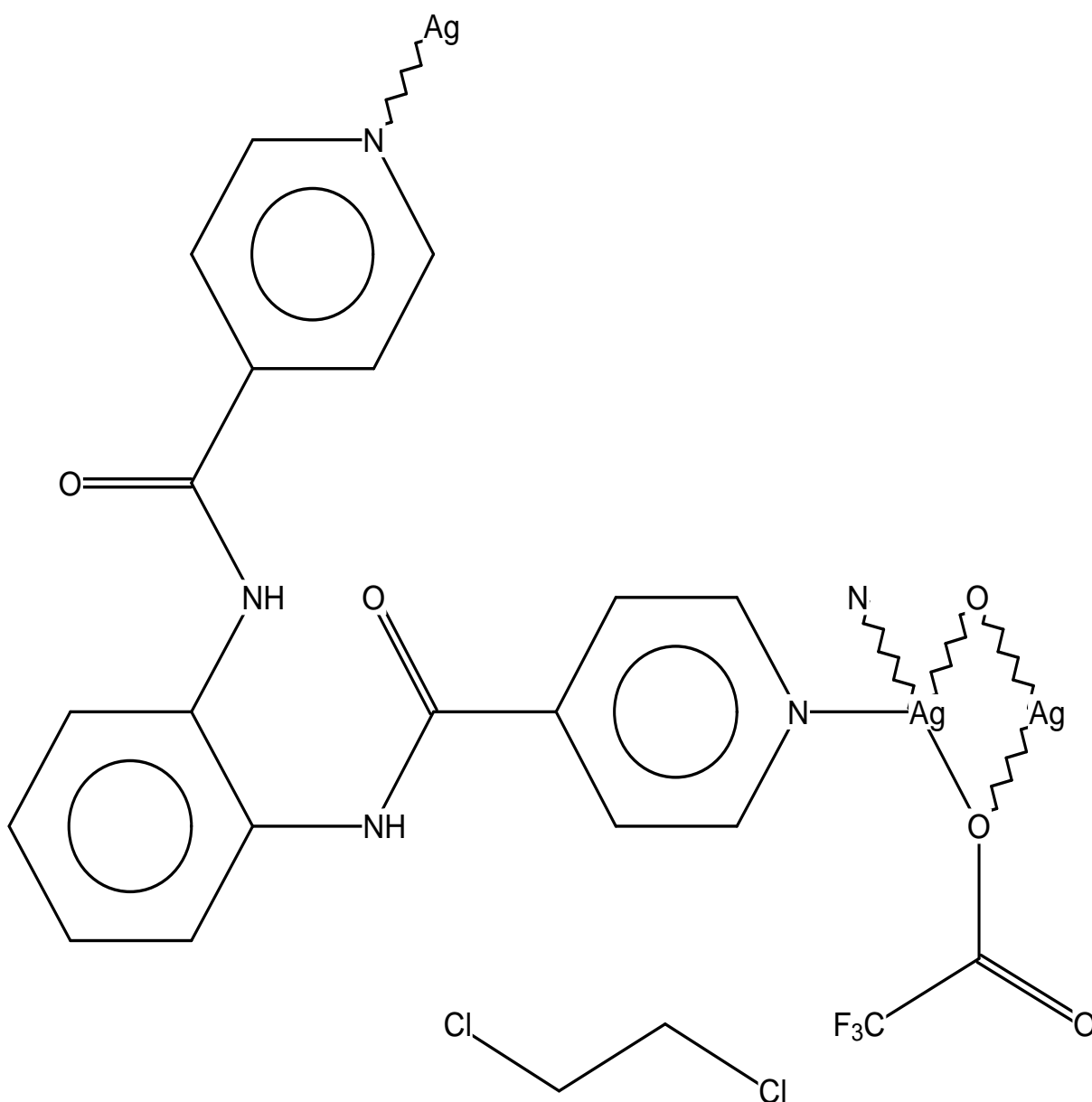
**Reference:** T.J.Burchell, D.J.Eisler, R.J.Puddephatt (2006)  
*Cryst. Growth Des.*, **6**,974

**Formula:**  $(C_{20} H_{14} Ag_1 F_3 N_4 O_4)_n \cdot 1.25n(C_2 H_4 Cl_2)$

**Compound Name:** catena-(tetrakis(( $\mu_2$ -Trifluoroacetato-O,O)-( $\mu_2$ -1,2-bis(pyridine-4-carboxamido)benzene)-silver(i)) pentakis(1,2-dichloroethane) clathrate)

**Space Group:** C2/m      **Cell:**    **a** 9.407(1)    **b** 24.330(5)    **c** 11.965(2)  
**Space Group No.:** 12      **(Å, °)**     $\alpha$  90.00       $\beta$  98.98(3)     $\gamma$  90.00

**R-Factor (%):** 5.52      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.628



## Search: search48 (Thu May 26 11:42:42 2011): Hit 7

KEHGK

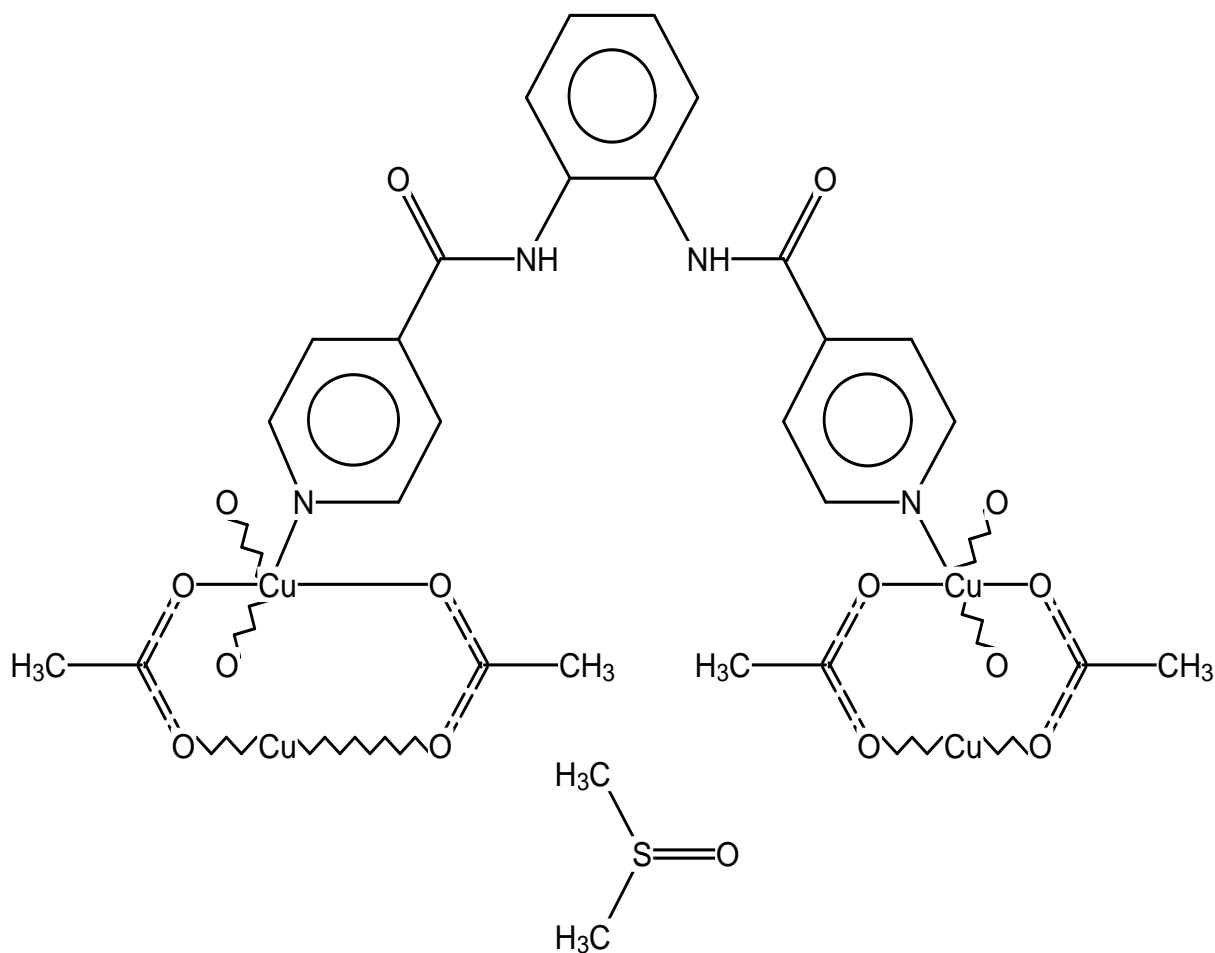
**Reference:** J.Pansanel, A.Jouaiti, S.Ferlay, M.W.Hosseini,  
J.-M.Planeix, N.Kyritsakas (2006) *New J.Chem.* ,**30**,683

**Formula:** (C<sub>26</sub> H<sub>26</sub> Cu<sub>2</sub> N<sub>4</sub> O<sub>10</sub>)<sub>n</sub>,2n(C<sub>2</sub> H<sub>6</sub> O<sub>1</sub> S<sub>1</sub>)

**Compound Name:** catena-(tetrakis(μ<sub>2</sub>-Acetato)-(μ<sub>2</sub>-1,2-bis(isonicotinoylamino)benzene)-  
di-copper dimethylsulfoxide solvate)

**Space Group:** P-1      **Cell:**      **a** 8.227(0)      **b** 14.322(0)      **c** 15.703(0)  
**Space Group No.:** 2      **(Å, °)**      **α** 76.88(0)      **β** 89.00(0)      **γ** 82.82(0)

**R-Factor (%):** 7.60      **Temperature(K):** 173      **Density(g/cm<sup>3</sup>):** 1.557





## Search: search48 (Thu May 26 11:42:42 2011): Hit 8

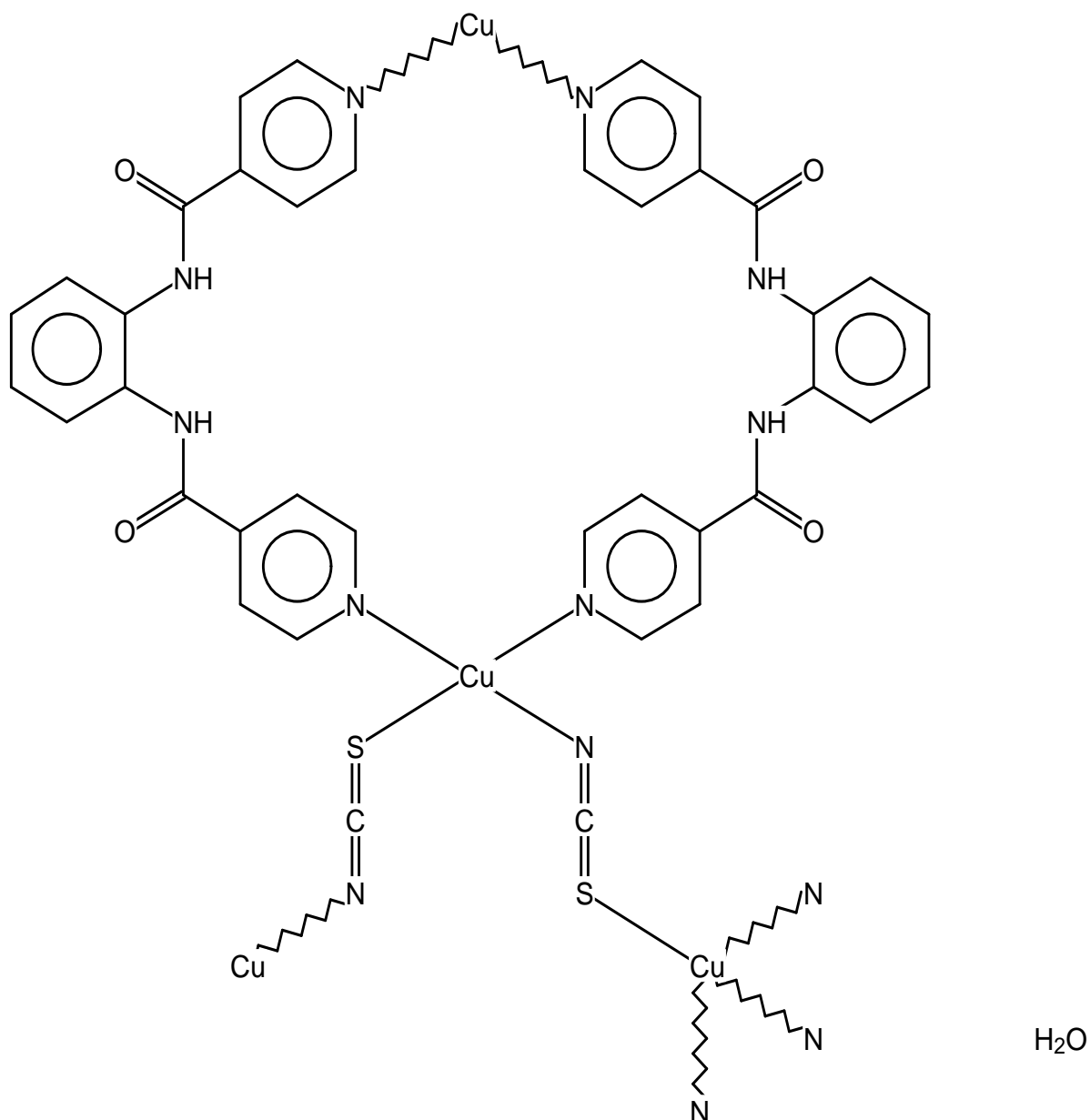
### SOTREZ

**Reference:** Yun-Yin Niu, Ben-Lai Wu, Qing-Li Wang, Xiao-Ling Guo, Hong-Yun Zhang, Hong-Wei Hou, Yi Han, Ling-Fang Wang (2009) *Inorg.Chim.Acta* ,**362**,556

**Formula:** (C<sub>38</sub> H<sub>28</sub> Cu<sub>2</sub> N<sub>10</sub> O<sub>4</sub> S<sub>2</sub>)<sub>n</sub>,2n(H<sub>2</sub> O<sub>1</sub>)

**Compound Name:** catena-(bis(μ<sub>2</sub>-N,N'-(1,2-Phenylene)di-isonicotinamide-N,N')-bis(μ<sub>2</sub>-thiocyanato-N,S)-di-copper(i) dihydrate)

**Space Group:** Pccn      **Cell:**      **a** 18.866(2)      **b** 24.059(3)      **c** 9.961(1)  
**Space Group No.:** 56      **(Å, °)**      **α** 90.00      **β** 90.00      **γ** 90.00  
**R-Factor (%):** 6.96      **Temperature(K):** 291      **Density(g/cm<sup>3</sup>):** 1.346



## Search: search48 (Thu May 26 11:42:42 2011): Hit 9

### TEHLUO

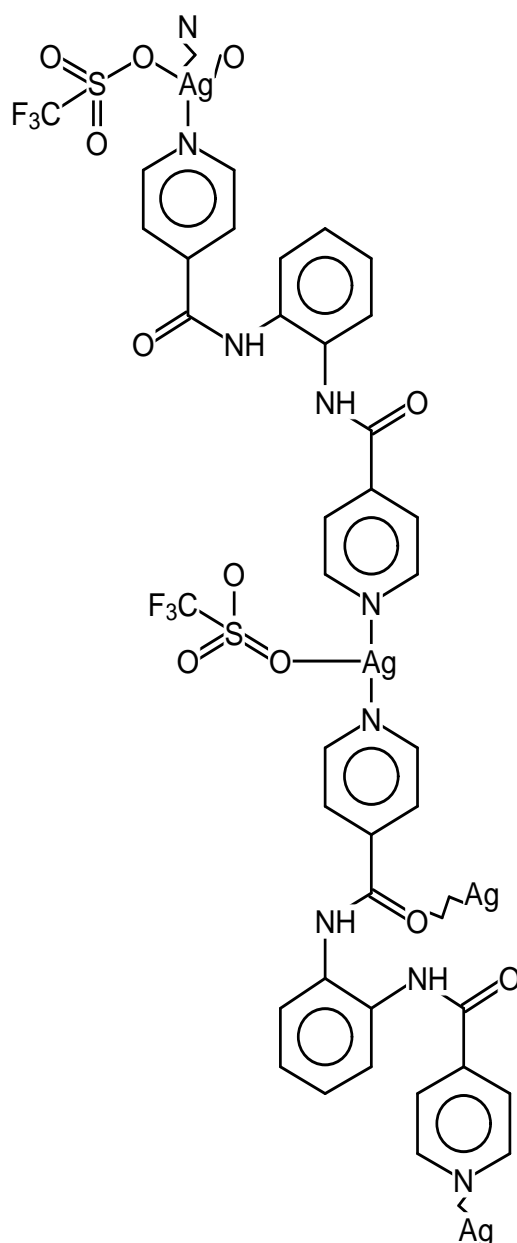
**Reference:** T.J.Burchell, D.J.Eisler, R.J.Puddephatt (2006)  
*Cryst.Growth Des.* ,**6**,974

**Formula:** (C<sub>38</sub> H<sub>28</sub> Ag<sub>2</sub> F<sub>6</sub> N<sub>8</sub> O<sub>10</sub> S<sub>2</sub>)<sub>n</sub>

**Compound Name:** catena-((μ<sub>3</sub>-1,2-bis(Pyridine-4-carboxamido)benzene)-(μ<sub>2</sub>-1,2-bis(pyridine-4-carboxamido)benzene)-bis(trifluoromethanesulfonato)-di-silver(i))

**Space Group:** P-1      **Cell:**      **a** 10.719(2)      **b** 10.728(2)      **c** 18.594(4)  
**Space Group No.:** 2      **(Å, °)**      **α** 84.66(3)      **β** 84.95(3)      **γ** 79.61(3)

**R-Factor (%):** 5.66      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.830



## Search: search48 (Thu May 26 11:42:42 2011): Hit 10

### TEHMAV

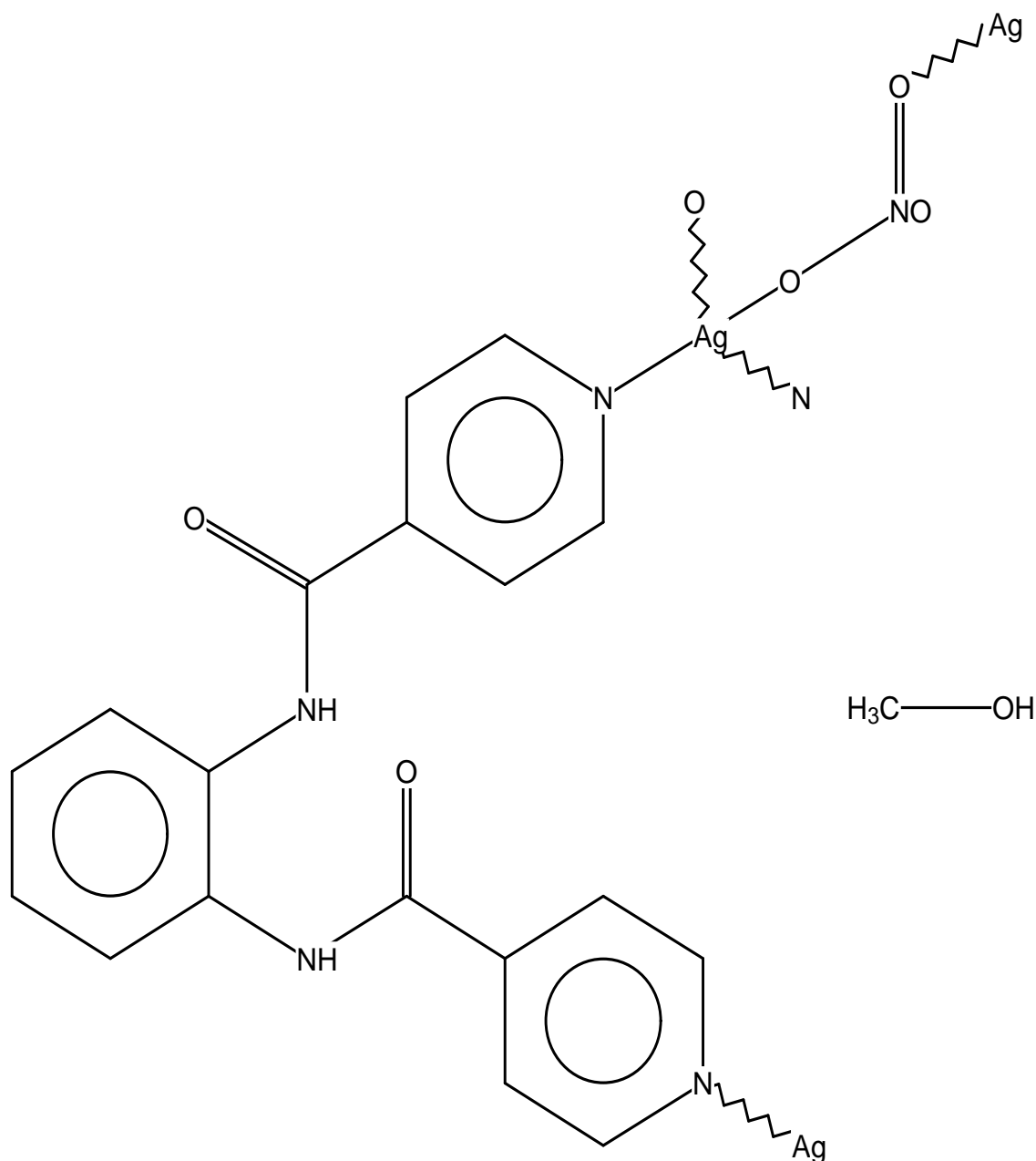
**Reference:** T.J.Burchell, D.J.Eisler, R.J.Puddephatt (2006)  
*Cryst.Growth Des.* ,6,974

**Formula:** (C<sub>18</sub> H<sub>14</sub> Ag<sub>1</sub> N<sub>5</sub> O<sub>5</sub>)<sub>n</sub>,2n(C<sub>1</sub> H<sub>4</sub> O<sub>1</sub>)

**Compound Name:** catena-((μ<sub>2</sub>-Nitrato-O,O')-(μ<sub>2</sub>-1,2-bis(pyridine-4-carboxamido)benzene)-silver(i) bis(methanol) clathrate)

**Space Group:** Pccn      **Cell:**    **a** 19.253(4)    **b** 24.785(5)    **c** 9.678(1)  
**Space Group No.:** 56      **(Å, °)**    **α** 90.00      **β** 90.00      **γ** 90.00

**R-Factor (%):** 4.92      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.589



## Search: search48 (Thu May 26 11:42:42 2011): Hit 11

### XAHROO

**Reference:** T.J.Burchell, D.J.Eisler, R.J.Puddephatt (2004)  
*Inorg.Chem.* ,**43**,5550

**Formula:** C<sub>36</sub> H<sub>28</sub> Cl<sub>4</sub> Hg<sub>2</sub> N<sub>8</sub> O<sub>4</sub>,2(C<sub>4</sub> H<sub>8</sub> O<sub>1</sub>)

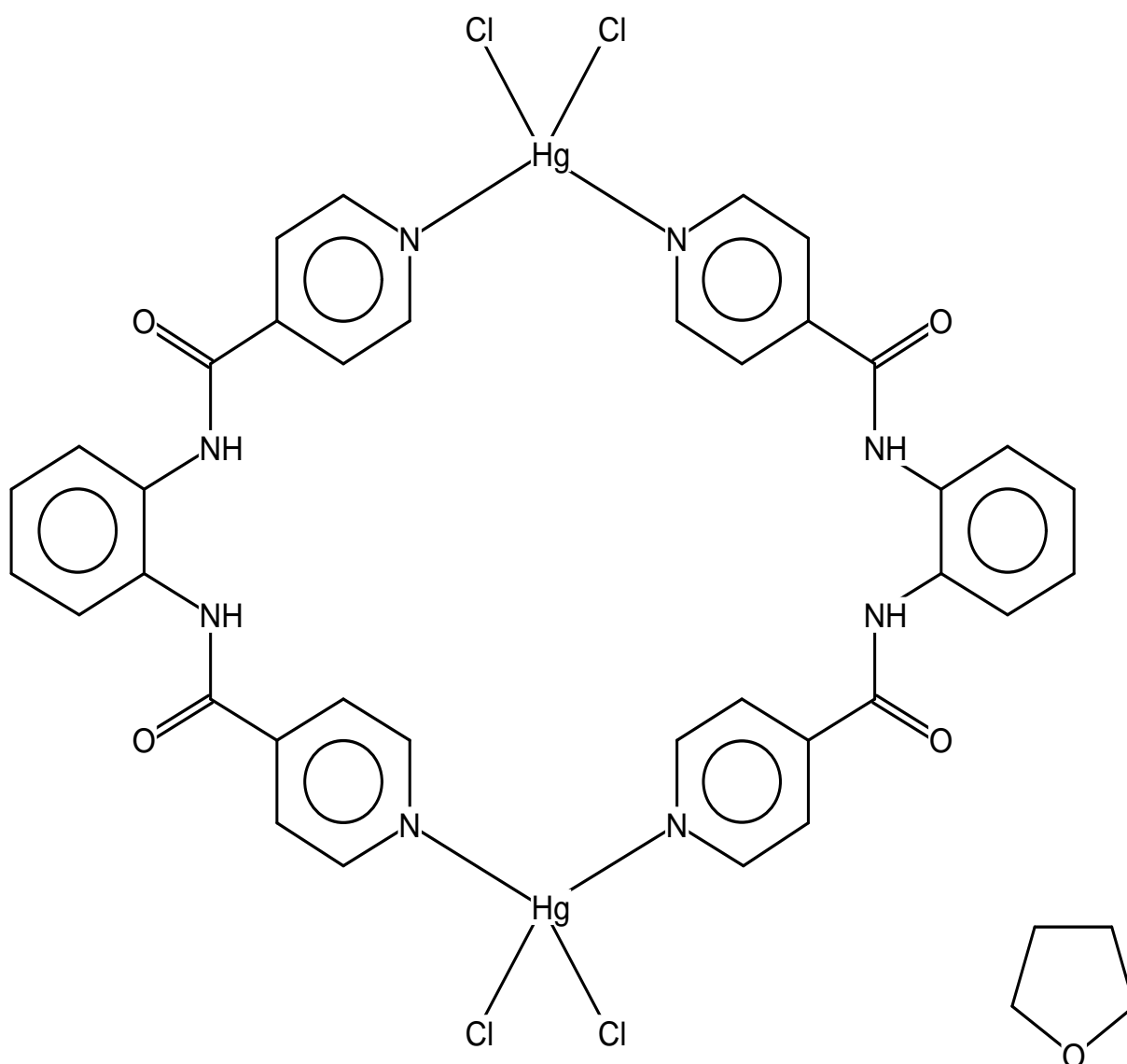
**Compound Name:** bis( $\mu_2$ -1,2-bis(4-Pyridylcarbonylamino)benzene)-tetrachloro-di-mercury(ii) tetrahydrofuran clathrate tetrahydrofuran solvate

**Synonym:** bis( $\mu_2$ -1,2-bis(Isonicotinamido)benzene)-tetrachloro-di-mercury(ii) tetrahydrofuran clathrate tetrahydrofuran solvate

**Space Group:** P-1      **Cell:**      **a** 9.833(0)      **b** 10.915(0)      **c** 12.241(0)

**Space Group No.:** 2      **(Å, °)**       $\alpha$  82.83(0)       $\beta$  74.78(0)       $\gamma$  81.50(0)

**R-Factor (%):** 6.10      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.760



## Search: search48 (Thu May 26 11:42:42 2011): Hit 12

XAHRUU

**Reference:** T.J.Burchell, D.J.Eisler, R.J.Puddephatt (2004)  
*Inorg.Chem.* ,**43**,5550

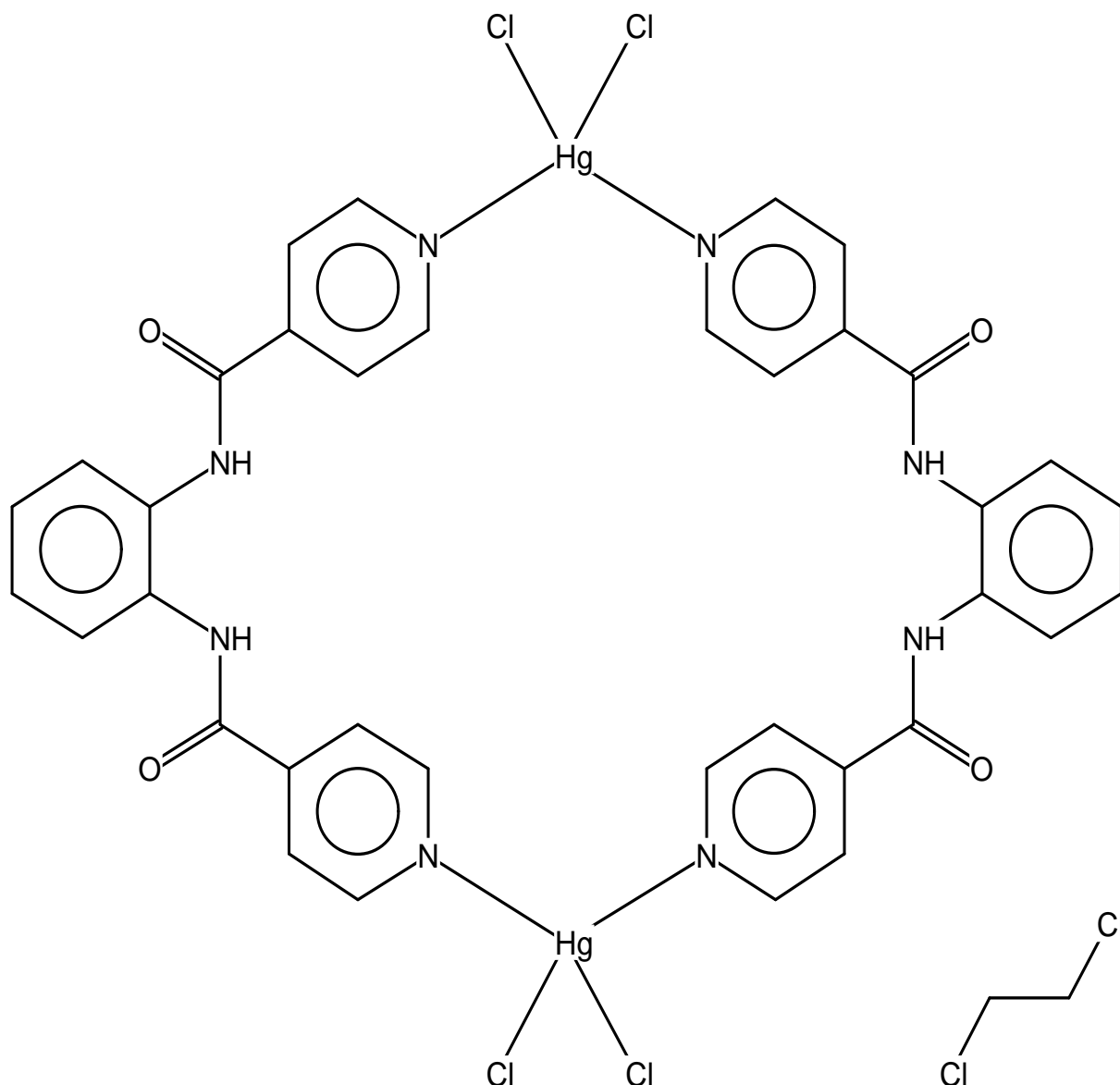
**Formula:** C<sub>36</sub> H<sub>28</sub> Cl<sub>4</sub> Hg<sub>2</sub> N<sub>8</sub> O<sub>4</sub>, C<sub>2</sub> H<sub>4</sub> Cl<sub>2</sub>

**Compound Name:** bis( $\mu_2$ -1,2-bis(4-Pyridylcarbonylamino)benzene)-tetrachloro-di-mercury(ii) 1,2-dichloroethane clathrate

**Synonym:** bis( $\mu_2$ -1,2-bis(Isonicotinamido)benzene)-tetrachloro-di-mercury(ii) 1,2-dichloroethane clathrate

**Space Group:** P-1      **Cell:**      **a** 9.071(0)      **b** 10.401(0)      **c** 11.575(0)  
**Space Group No.:** 2      **(Å, °)**       $\alpha$  81.21(0)       $\beta$  77.65(0)       $\gamma$  86.29(0)

**R-Factor (%):** 3.92      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 2.015



## Search: search48 (Thu May 26 11:42:42 2011): Hit 13

XAHSAB

**Reference:** T.J.Burchell, D.J.Eisler, R.J.Puddephatt (2004)  
*Inorg.Chem.* ,**43**,5550

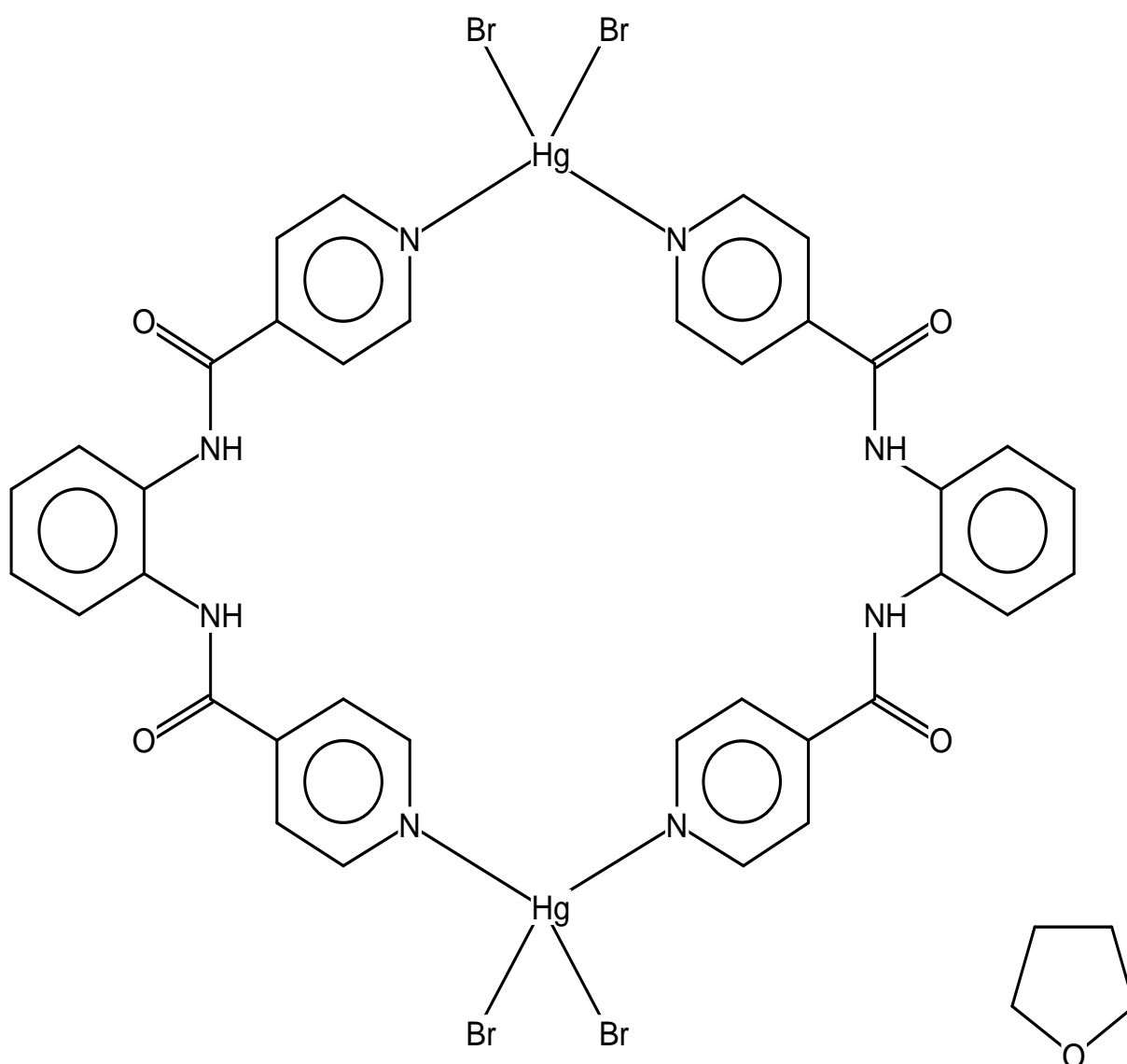
**Formula:** C<sub>36</sub> H<sub>28</sub> Br<sub>4</sub> Hg<sub>2</sub> N<sub>8</sub> O<sub>4</sub>,2(C<sub>4</sub> H<sub>8</sub> O<sub>1</sub>)

**Compound Name:** bis( $\mu_2$ -1,2-bis(4-Pyridylcarbonylamino)benzene)-tetrabromo-di-mercury(ii) tetrahydrofuran clathrate tetrahydrofuran solvate

**Synonym:** bis( $\mu_2$ -1,2-bis(Isonicotinamido)benzene)-tetrabromo-di-mercury(ii) tetrahydrofuran clathrate tetrahydrofuran solvate

**Space Group:** P-1      **Cell:**      **a** 9.385(0)      **b** 12.242(0)      **c** 12.987(0)  
**Space Group No.:** 2      **(Å, °)**       $\alpha$  104.57(0)       $\beta$  103.51(0)       $\gamma$  111.30(0)

**R-Factor (%):** 4.61      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.987



## Search: search48 (Thu May 26 11:42:42 2011): Hit 14

XAHSEF

**Reference:** T.J.Burchell, D.J.Eisler, R.J.Puddephatt (2004)  
*Inorg.Chem.* ,**43**,5550

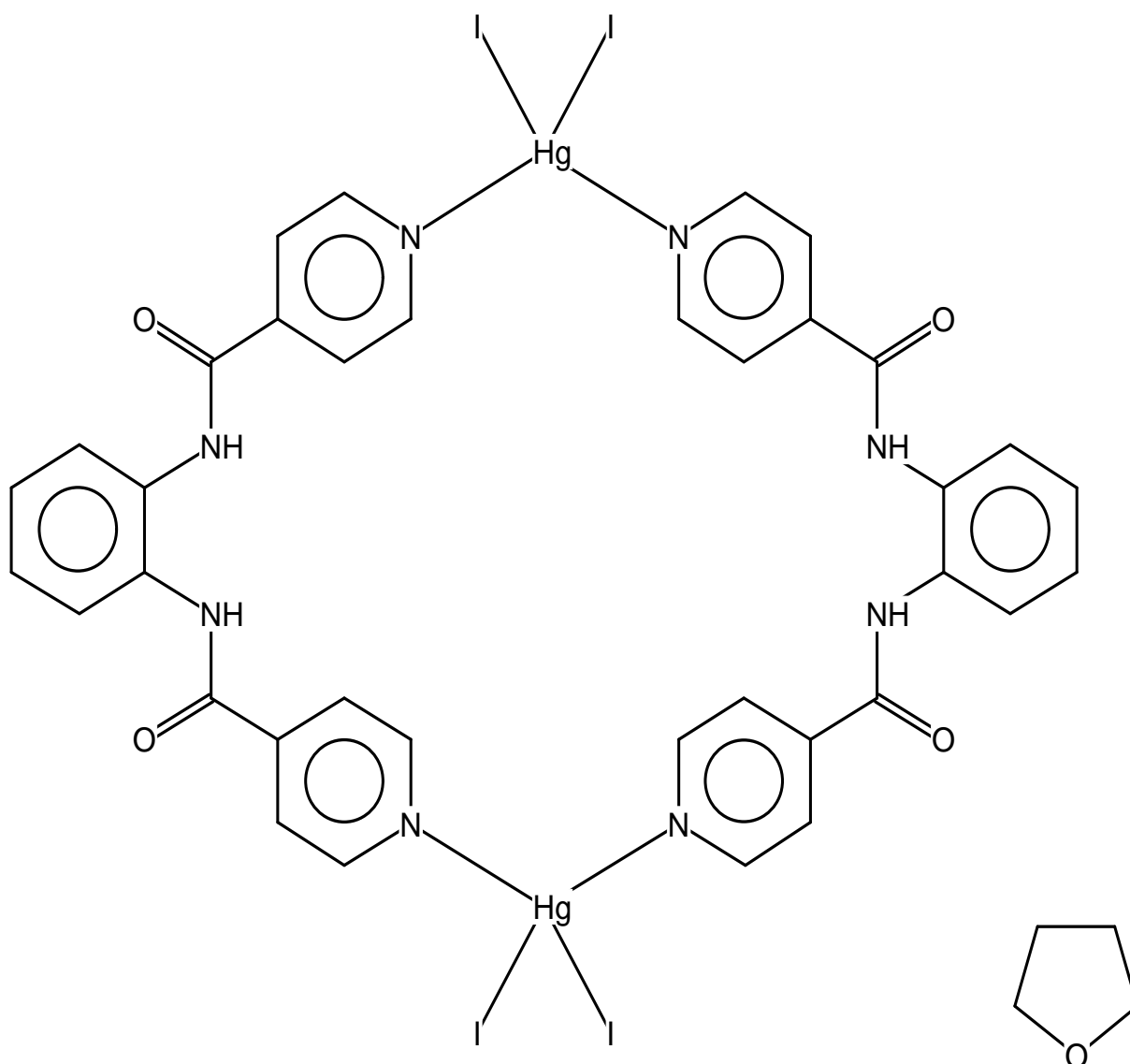
**Formula:** C<sub>36</sub> H<sub>28</sub> Hg<sub>2</sub> I<sub>4</sub> N<sub>8</sub> O<sub>4</sub>·2(C<sub>4</sub> H<sub>8</sub> O<sub>1</sub>)

**Compound Name:** bis(μ<sub>2</sub>-1,2-bis(4-Pyridylcarbonylamino)benzene)-tetraiodo-di-mercury(ii)  
tetrahydrofuran clathrate tetrahydrofuran solvate

**Synonym:** bis(μ<sub>2</sub>-1,2-bis(Isonicotinamido)benzene)-tetraiodo-di-mercury(ii)  
tetrahydrofuran clathrate tetrahydrofuran solvate

**Space Group:** P-1      **Cell:**      **a** 9.338(0)      **b** 12.195(0)      **c** 13.251(0)  
**Space Group No.:** 2      **(Å, °)**      α 104.65(0)      β 103.34(0)      γ 109.63(0)

**R-Factor (%):** 4.89      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 2.175



## Search Overview

**Search:** search49  
**Date/Time done:** Thu May 26 11:45:19 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:** 11

*Summary of queries used. Search found structures that:*

match

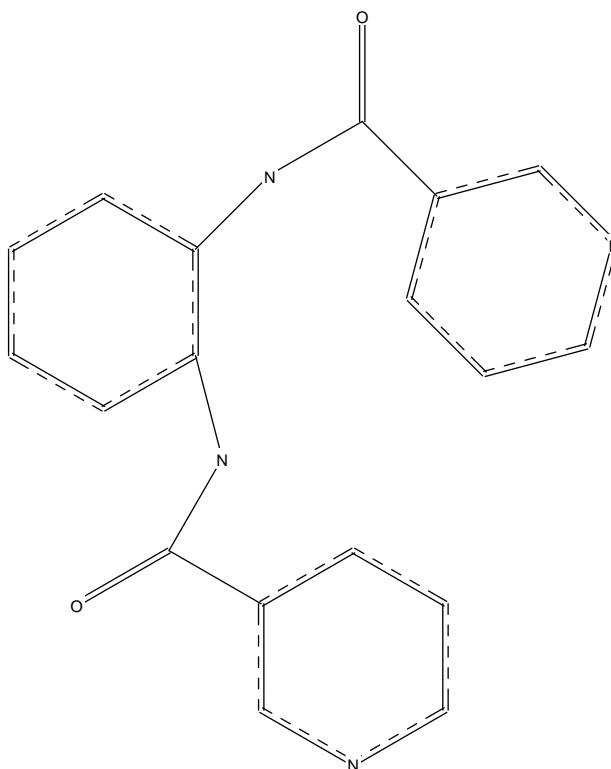
**Query 2**

**Query 3**

**Query 2**

4M

**Query 3**





## Search: search49 (Thu May 26 11:45:19 2011): Hit 1

### COHTID

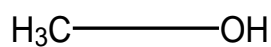
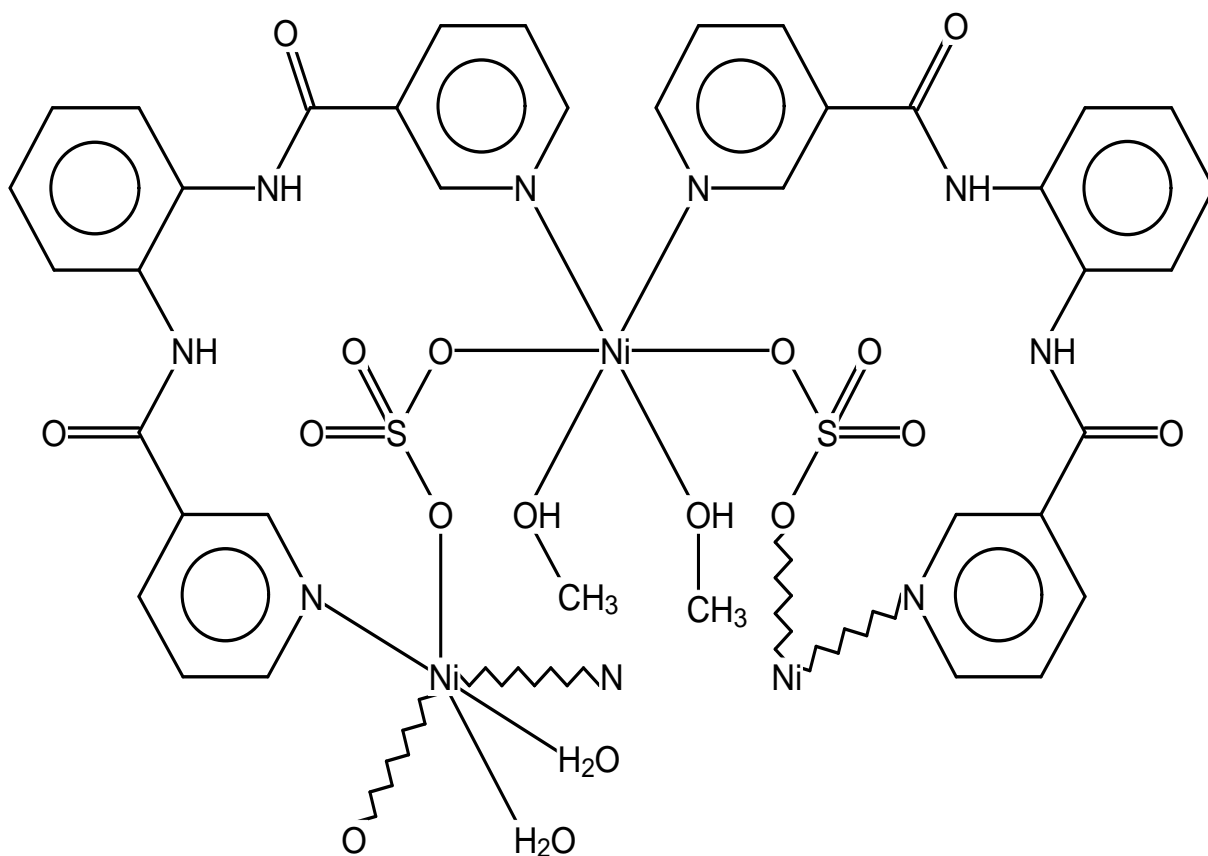
**Reference:** Ben-Lai Wu, Ping Zhang, Yun-Yin Niu, Hong-yun Zhang, Zhong-Jun Li, Hong-Wei Hou (2008) *Inorg.Chim.Acta*, **361**,2203

**Formula:** (C<sub>38</sub> H<sub>40</sub> N<sub>8</sub> Ni<sub>2</sub> O<sub>16</sub> S<sub>2</sub>)<sub>n</sub>,n(C<sub>1</sub> H<sub>4</sub> O<sub>1</sub>)

**Compound Name:** catena-(bis(μ<sub>2</sub>-1,2-bis(3-pyridylcarboxamide)benzene-N,N')-bis(μ<sub>2</sub>-sulfato-O,O')-diaqua-dimethanol-di-nickel(ii) methanol solvate)

**Space Group:** C2/c      **Cell:**    **a** 23.201(5)    **b** 14.156(3)    **c** 18.799(4)  
**Space Group No.:** 15      **(Å, °)**    **α** 90.00      **β** 117.79(3)    **γ** 90.00

**R-Factor (%):** 6.95      **Temperature(K):** 291      **Density(g/cm<sup>3</sup>):** 1.311



## Search: search49 (Thu May 26 11:45:19 2011): Hit 2

COHTOJ

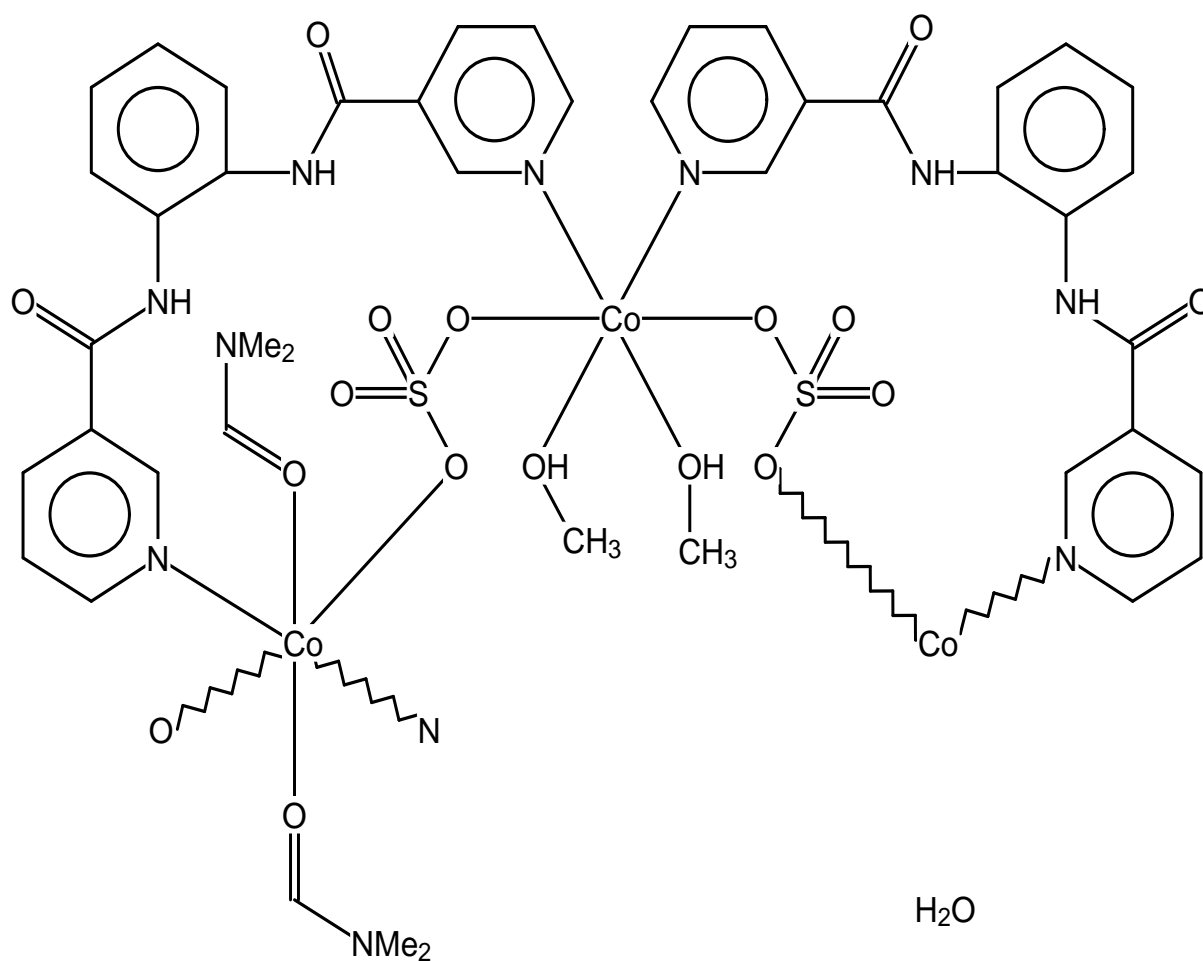
**Reference:** Ben-Lai Wu, Ping Zhang, Yun-Yin Niu, Hong-yun Zhang, Zhong-Jun Li, Hong-Wei Hou (2008) *Inorg.Chim.Acta* ,**361**,2203

**Formula:** (C<sub>44</sub> H<sub>50</sub> Co<sub>2</sub> N<sub>10</sub> O<sub>16</sub> S<sub>2</sub>)<sub>n</sub>,0.5n(H<sub>2</sub> O<sub>1</sub>)

**Compound Name:** catena-(bis( $\mu_2$ -1,2-bis(3-pyridylcarboxamide)benzene-N,N')-bis( $\mu_2$ -sulfato-O,O')-bis(N,N-dimethylformamide-O)-dimethanol-di-cobalt(ii) hemihydrate)

**Space Group:** C2/c      **Cell:**    **a** 23.951(5)    **b** 13.997(3)    **c** 18.913(4)  
**Space Group No.:** 15      **(Å, °)**     $\alpha$  90.00       $\beta$  117.85(3)     $\gamma$  90.00

**R-Factor (%):** 7.14      **Temperature(K):** 291      **Density(g/cm<sup>3</sup>):** 1.381



## Search: search49 (Thu May 26 11:45:19 2011): Hit 3

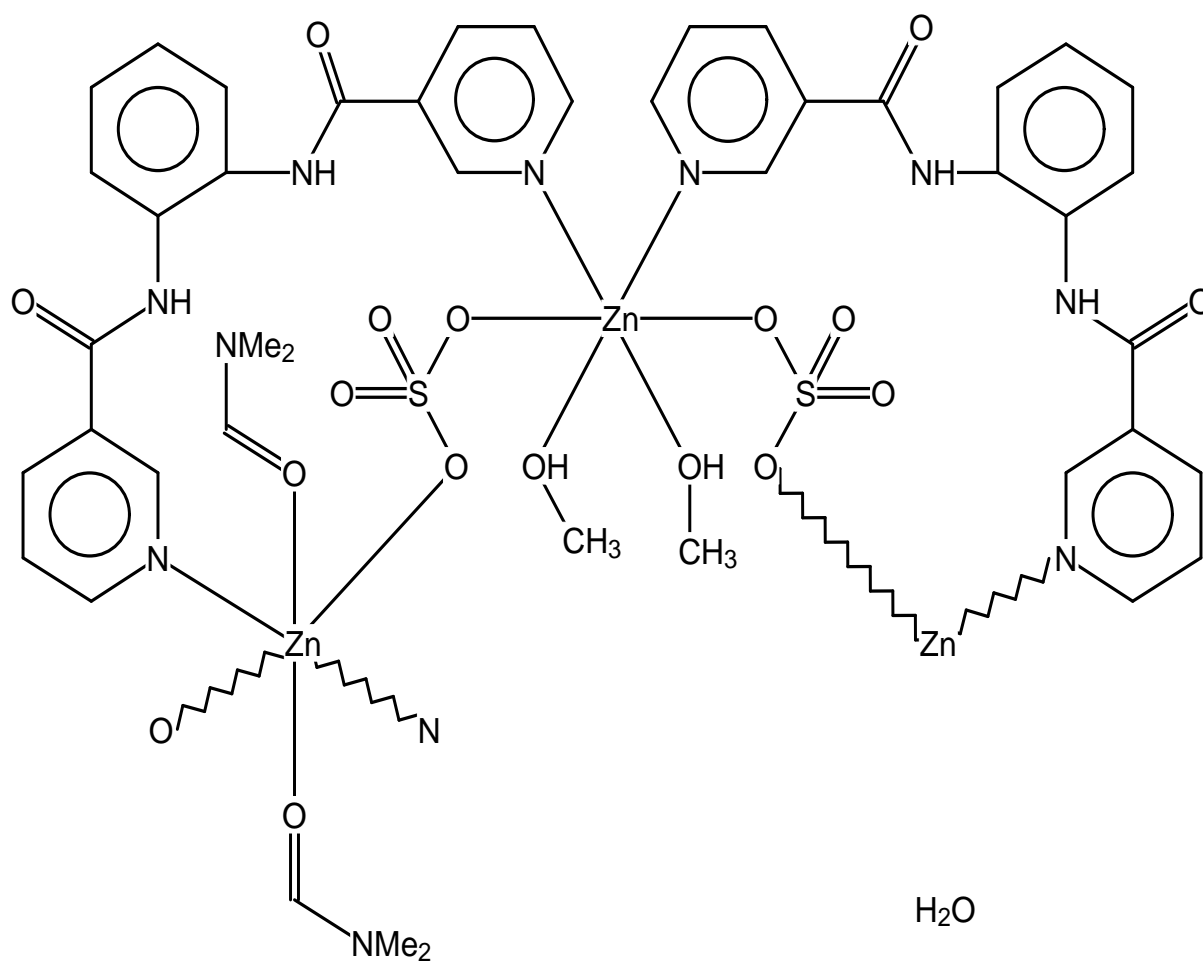
### COHTUP

**Reference:** Ben-Lai Wu, Ping Zhang, Yun-Yin Niu, Hong-yun Zhang, Zhong-Jun Li, Hong-Wei Hou (2008) *Inorg.Chim.Acta*, **361**,2203

**Formula:**  $(C_{44} H_{50} N_{10} O_{16} S_2 Zn_2)_n \cdot 0.5n(H_2 O)_1$

**Compound Name:** catena-(bis( $\mu_2$ -1,2-bis(3-pyridylcarboxamide)benzene-N,N')-bis( $\mu_2$ -sulfato-O,O')-bis(N,N-dimethylformamide-O)-dimethanol-di-zinc(ii) hemihydrate)

<b>Space Group:</b>	C2/c	<b>Cell:</b>	<b>a</b> 23.779(4)	<b>b</b> 13.998(2)	<b>c</b> 18.789(5)
<b>Space Group No.:</b>	15	<b>(Å, °)</b>	$\alpha$ 90.00	$\beta$ 117.65(0)	$\gamma$ 90.00
<b>R-Factor (%):</b>	4.84	<b>Temperature(K):</b>	291	<b>Density(g/cm<sup>3</sup>):</b>	1.413



## Search: search49 (Thu May 26 11:45:19 2011): Hit 4

EXEHUK

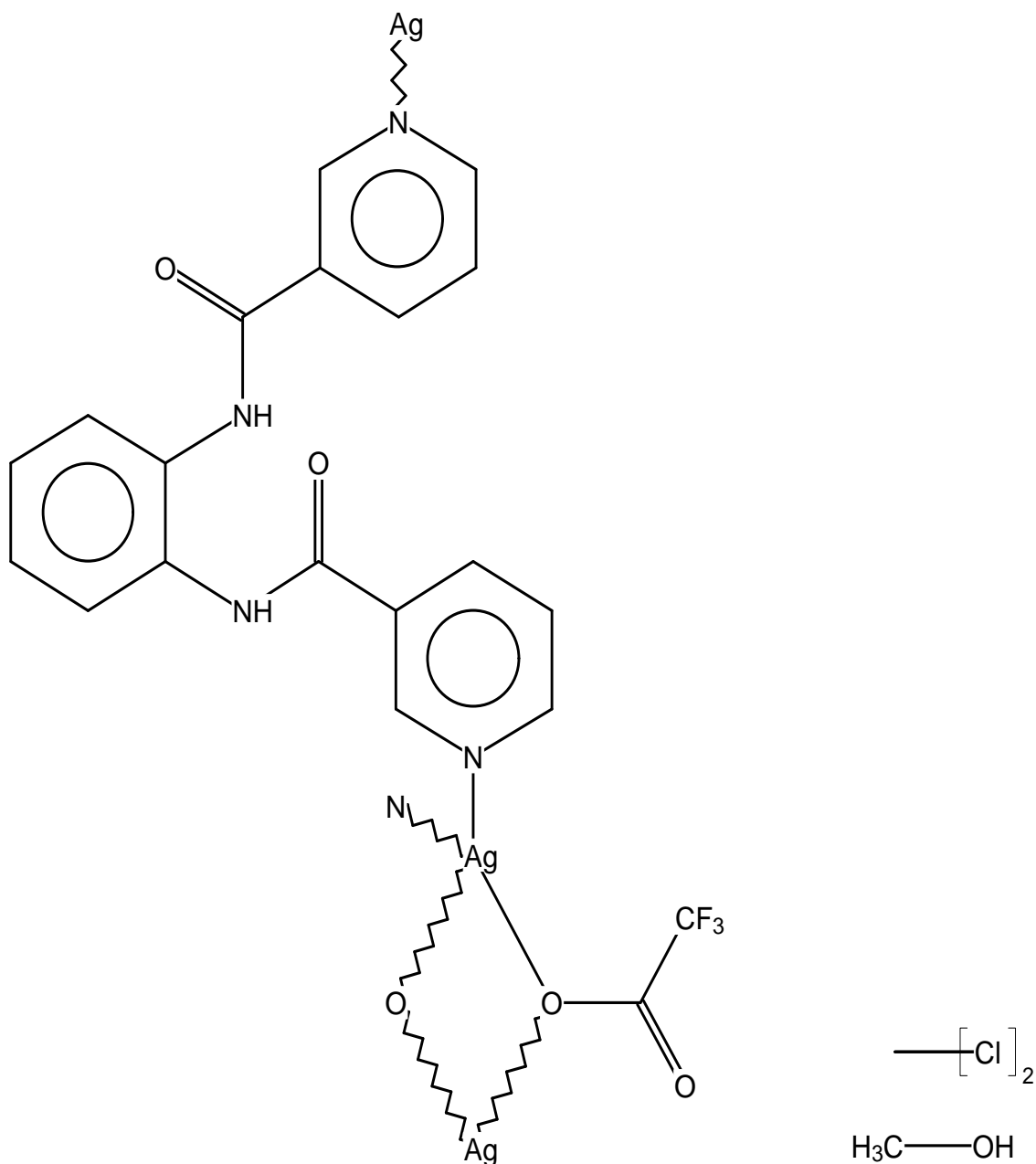
**Reference:** T.J.Burchell, D.J.Eisler, R.J.Puddephatt (2004)  
*Chem. Commun.* ,944

**Formula:**  $(C_{20}H_{14}Ag_1F_3N_4O_4)_n \cdot 0.75n(C_1H_2Cl_2) \cdot 0.5n(C_1H_4O_1)$

**Compound Name:** catena-(( $\mu_2$ -Trifluoroacetato)-( $\mu_2$ -1,2-bis(pyridine-3-carboxamido)benzene)-silver(i) dichloromethane methanol solvate)

**Space Group:** P-1      **Cell:**    **a** 9.370(1)    **b** 12.076(2)    **c** 12.400(3)  
**Space Group No.:** 2      (**Å, °**)     $\alpha$  88.01(3)     $\beta$  85.14(3)     $\gamma$  73.19(3)

**R-Factor (%):** 6.12      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.536



## Search: search49 (Thu May 26 11:45:19 2011): Hit 5

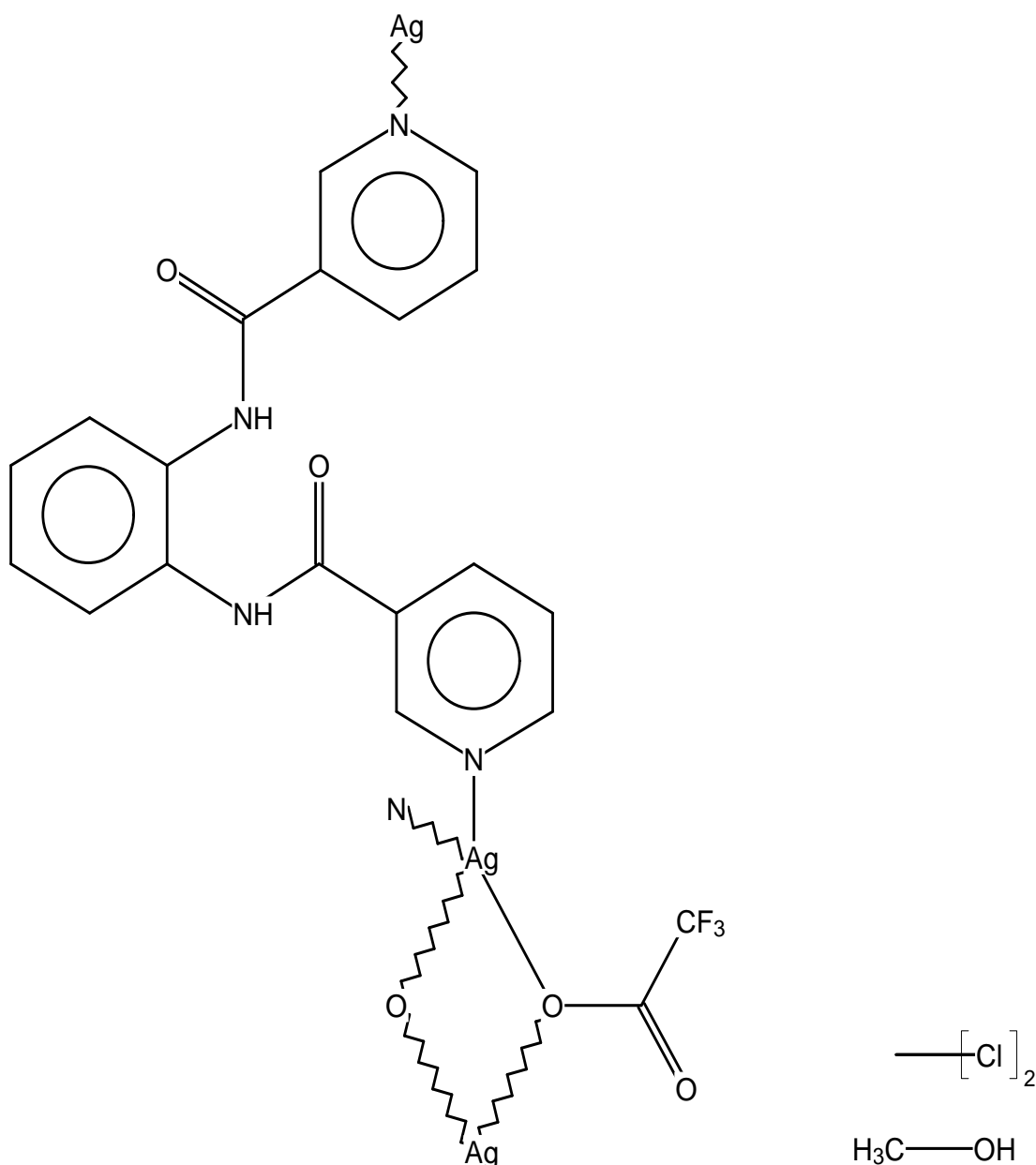
EXEHUK01

**Reference:** T.J.Burchell, D.J.Eisler, R.J.Puddephatt (2006)  
*Cryst.Growth Des.* ,6,974

**Formula:**  $(C_{20}H_{14}Ag_1F_3N_4O_4)_n \cdot 0.75n(C_1H_2Cl_2) \cdot 0.5n(C_1H_4O_1)$

**Compound Name:** catena-(bis(( $\mu_2$ -Trifluoroacetato-O,O)-( $\mu_2$ -1,2-bis(pyridine-3-carboxamido)benzene)-silver(i)) sesquikis(dichloromethane) methanol clathrate)

**Space Group:** P-1      **Cell:**    **a** 9.370(1)    **b** 12.076(2)    **c** 12.400(3)  
**Space Group No.:** 2      **(Å, °)**     $\alpha$  88.01(3)     $\beta$  85.14(3)     $\gamma$  73.19(3)  
**R-Factor (%):** 6.12      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.536



## Search: search49 (Thu May 26 11:45:19 2011): Hit 6

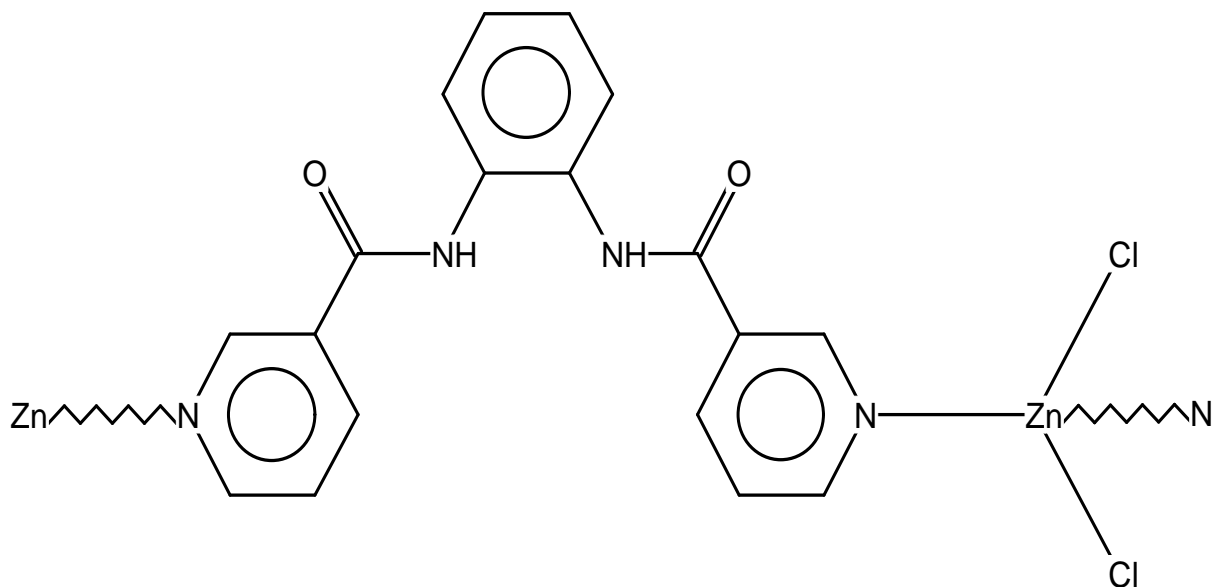
### GIXWUG

**Reference:** Ping Zhang, Yun-Yin Niu, Zong-Pei Zhang, Hong-Yun Zhang, Zhong-Jun Li, Cao-Yuan Niu, Ben-Lai Wu, Hong-Wei Hou (2008) *J.Coord.Chem.* , **61**,285

**Formula:** (C<sub>18</sub> H<sub>14</sub> Cl<sub>2</sub> N<sub>4</sub> O<sub>2</sub> Zn<sub>1</sub>)<sub>n</sub>,n(C<sub>1</sub> H<sub>4</sub> O<sub>1</sub>)

**Compound Name:** catena-((μ<sub>2</sub>-1,2-bis(3-Pyridylcarbonylamino)benzene-N,N')-dichloro-zinc(ii) methanol solvate)

<b>Space Group:</b>	P-1	<b>Cell:</b>	<b>a</b> 7.898(3)	<b>b</b> 11.792(4)	<b>c</b> 11.911(4)
<b>Space Group No.:</b>	2	(Å, °)	α 76.05(0)	β 89.92(0)	γ 78.27(0)
<b>R-Factor (%):</b>	8.92	<b>Temperature(K):</b>	291	<b>Density(g/cm<sup>3</sup>):</b>	1.535



## Search: search49 (Thu May 26 11:45:19 2011): Hit 7

### SORGA1

**Reference:** Ping Zhang, Ben-Lai Wu, Yun-Yin Niu, Hong-Yun Zhang, Cao-Yuan Niu, Hong-Wei Hou (2007)  
*Synth.React.Inorg.,Met.-Org.,Nano-Met.Chem.* ,37,577

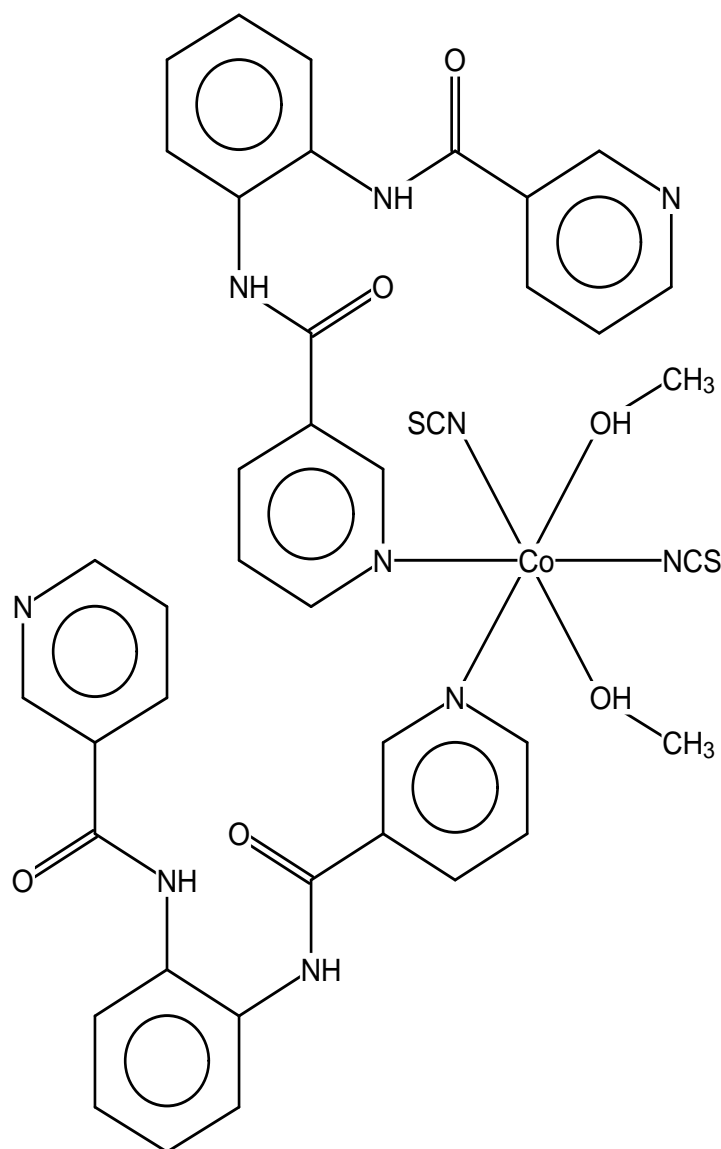
**Formula:** C<sub>40</sub> H<sub>36</sub> Co<sub>1</sub> N<sub>10</sub> O<sub>6</sub> S<sub>2</sub>

**Compound Name:** bis(methanol)-bis(N,N'-(1,2-phenylene)dinicotinamide)-bis(isothiocyanato)-cobalt(ii)

**Synonym:** bis(methanol)-bis(1,2-bis(3-pyridylcarboxamide)benzene)-bis(isothiocyanato)-cobalt(ii)

**Space Group:** P-1      **Cell:**    **a** 8.700(0)    **b** 9.611(1)    **c** 13.767(2)  
**Space Group No.:** 2      **(Å, °)**     $\alpha$  101.39(0)     $\beta$  93.19(0)     $\gamma$  114.52(0)

**R-Factor (%):** 2.98      **Temperature(K):** 291      **Density(g/cm<sup>3</sup>):** 1.434



## Search: search49 (Thu May 26 11:45:19 2011): Hit 8

### SORGA103

**Reference:** Ping Zhang, Ben-Lai Wu, Yun-Yin Niu, Hong-Yun Zhang, Cao-Yuan Niu, Hong-Wei Hou (2008)  
*Synth.React.Inorg.,Met.-Org.,Nano-Met.Chem.* ,**38**,439

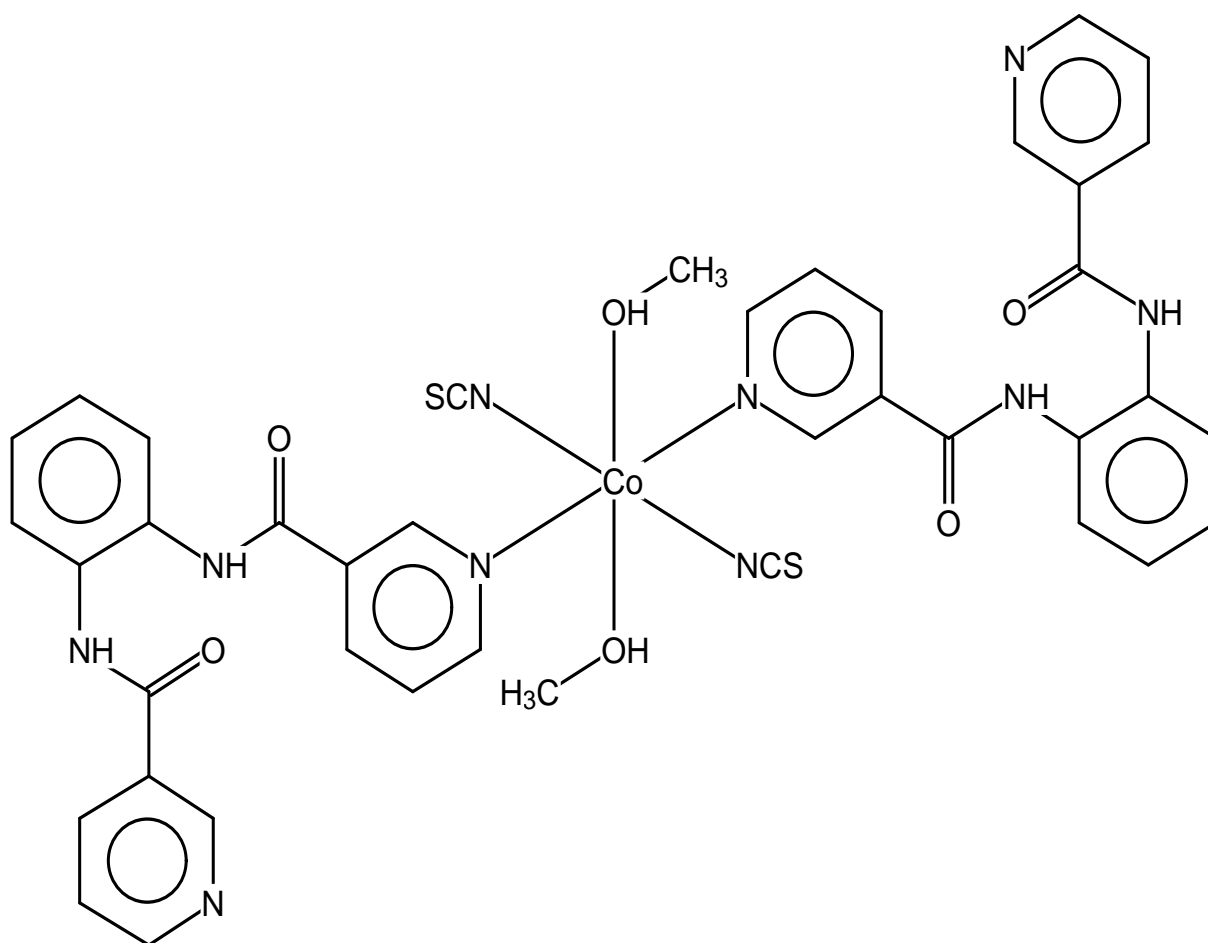
**Formula:** C<sub>40</sub> H<sub>36</sub> Co<sub>1</sub> N<sub>10</sub> O<sub>6</sub> S<sub>2</sub>

**Compound Name:** bis(Isothiocyanato)-bis(methanol)-bis(1,2-bis(3-pyridylcarboxamido) benzene-N)-cobalt(ii)

**Synonym:** bis(Isothiocyanato)-bis(methanol)-bis(N,N'-(1,2-phenylene) dinicotinamide)-cobalt(ii)

**Space Group:** P-1      **Cell:**    **a** 8.700(0)    **b** 9.611(1)    **c** 13.767(2)  
**Space Group No.:** 2      **(Å, °)**     $\alpha$  101.39(0)     $\beta$  93.19(0)     $\gamma$  114.52(0)

**R-Factor (%):** 2.98      **Temperature(K):** 291      **Density(g/cm<sup>3</sup>):** 1.434





## Search: search49 (Thu May 26 11:45:19 2011): Hit 9

SORGA104

**Reference:** Ping Zhang, Ben-Lai Wu, Yun-Yin Niu, Hong-Yun Zhang, Cao-Yuan Niu, Hong-Wei Hou (2008)  
*Synth.React.Inorg.,Met.-Org.,Nano-Met.Chem.* ,**38**,539

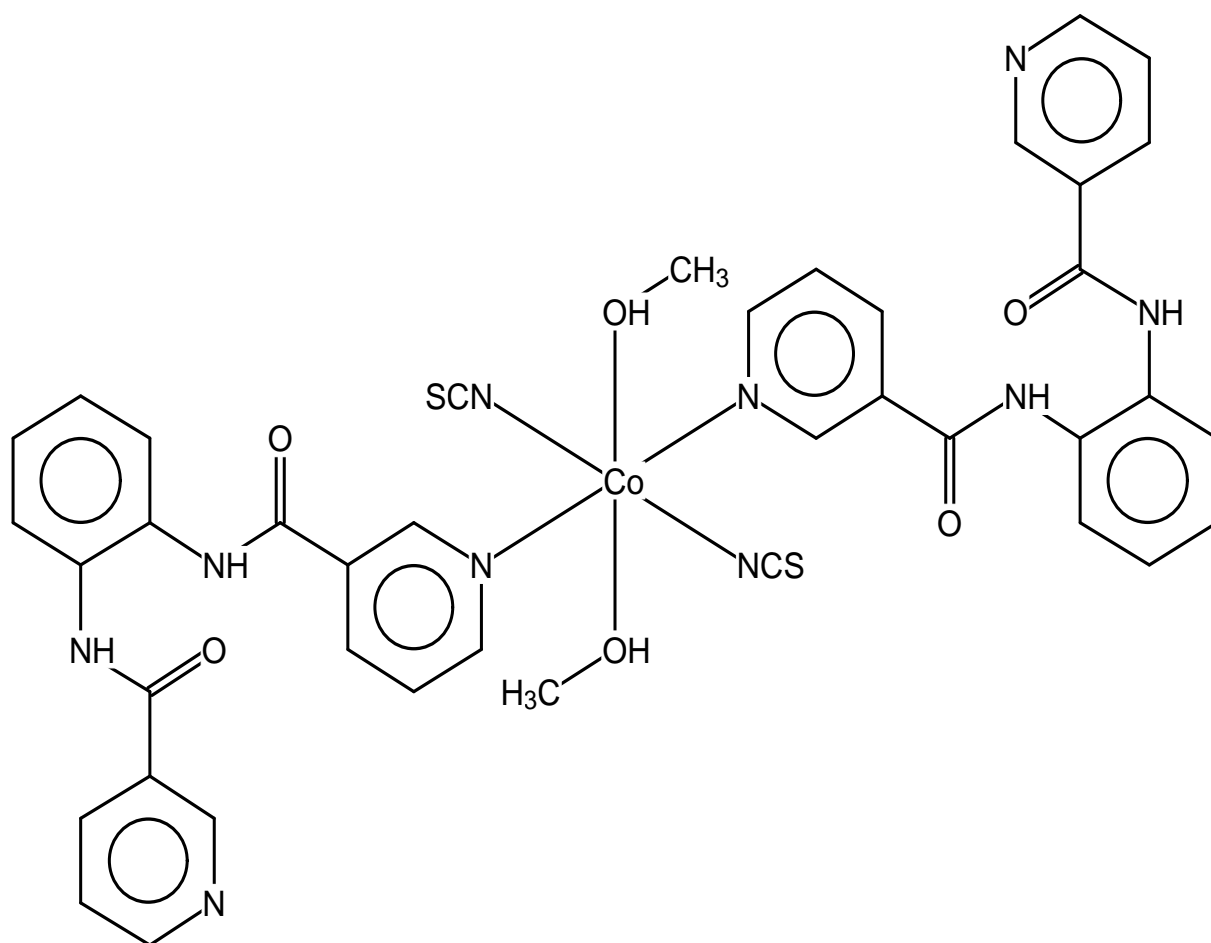
**Formula:** C<sub>40</sub> H<sub>36</sub> Co<sub>1</sub> N<sub>10</sub> O<sub>6</sub> S<sub>2</sub>

**Compound Name:** bis(Isothiocyanato)-bis(methanol)-bis(1,2-bis(3-pyridylcarboxamido) benzene-N)-cobalt(ii)

**Synonym:** bis(Isothiocyanato)-bis(methanol)-bis(N,N'-(1,2-phenylene) dinicotinamide)-cobalt(ii)

**Space Group:** P-1      **Cell:**    **a** 8.700(0)    **b** 9.611(1)    **c** 13.767(2)  
**Space Group No.:** 2      **(Å, °)**     $\alpha$  101.39(0)     $\beta$  93.19(0)     $\gamma$  114.52(0)

**R-Factor (%):** 2.98      **Temperature(K):** 291      **Density(g/cm<sup>3</sup>):** 1.434



## Search: search49 (Thu May 26 11:45:19 2011): Hit 10

### TEHMEZ

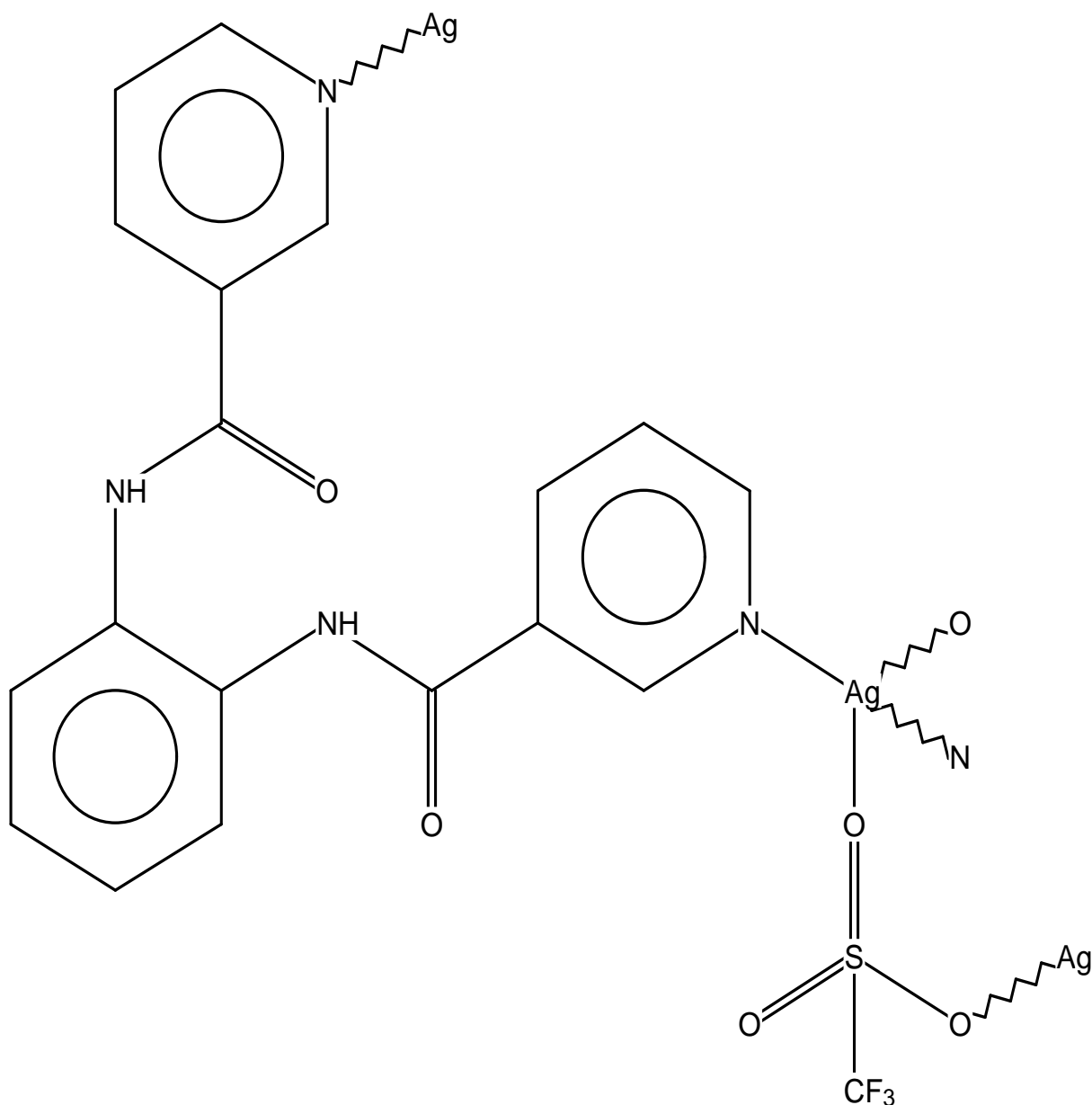
**Reference:** T.J.Burchell, D.J.Eisler, R.J.Puddephatt (2006)  
*Cryst.Growth Des.* ,6,974

**Formula:** (C<sub>19</sub> H<sub>14</sub> Ag<sub>1</sub> F<sub>3</sub> N<sub>4</sub> O<sub>5</sub> S<sub>1</sub>)<sub>n</sub>

**Compound Name:** catena-((μ<sub>2</sub>-Trifluoromethanesulfonato)-(μ<sub>2</sub>-1,2-bis(pyridine-3-carboxamido)benzene)-silver(i))

**Space Group:** P21/c      **Cell:**    **a** 11.470(2)    **b** 19.039(4)    **c** 9.852(2)  
**Space Group No.:** 14      **(Å, °)**    **α** 90.00      **β** 99.69(3)    **γ** 90.00

**R-Factor (%):** 4.77      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.802



## Search: search49 (Thu May 26 11:45:19 2011): Hit 11

### TEHMID

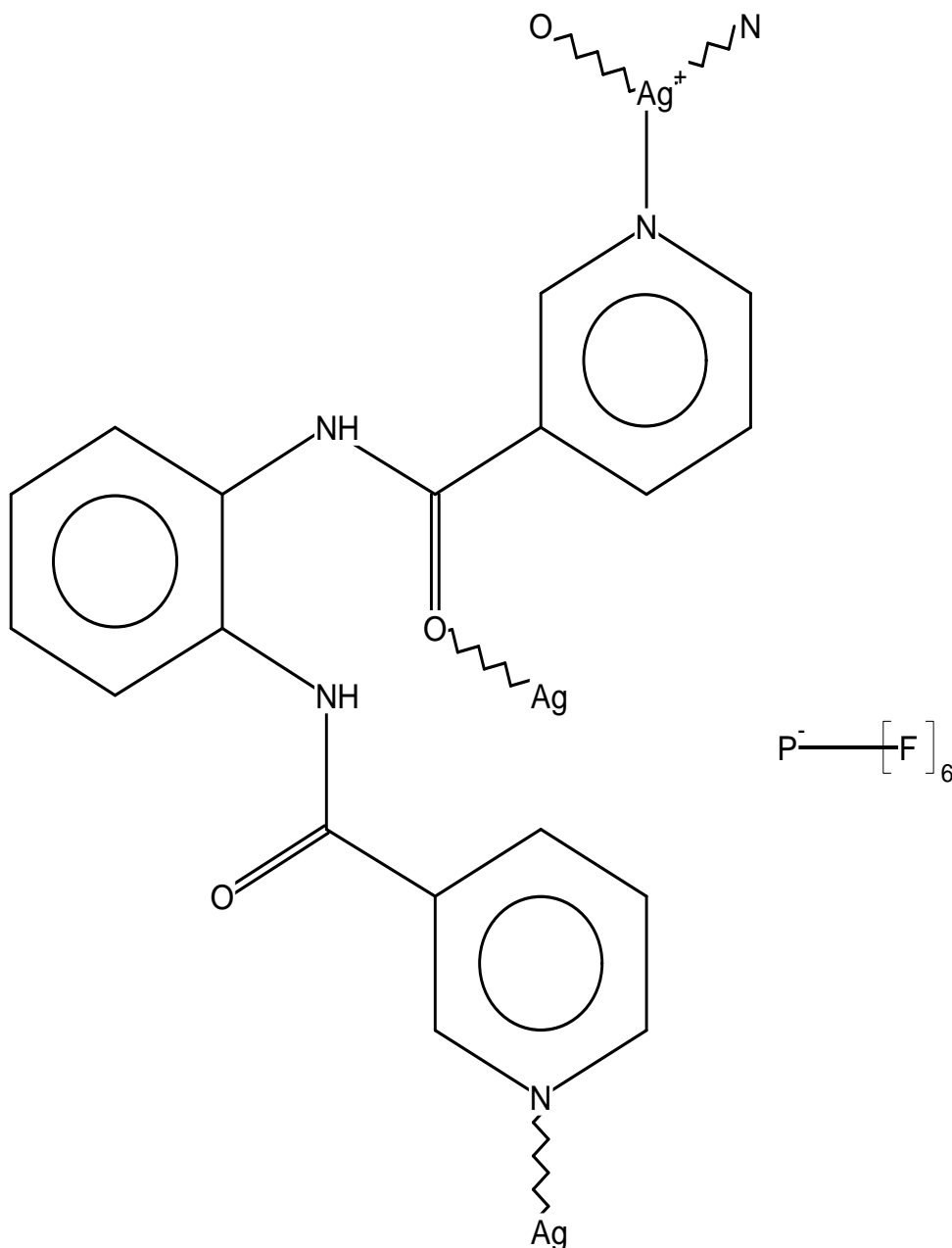
**Reference:** T.J.Burchell, D.J.Eisler, R.J.Puddephatt (2006)  
*Cryst.Growth Des.* ,6,974

**Formula:** (C<sub>18</sub> H<sub>14</sub> Ag<sub>1</sub> N<sub>4</sub> O<sub>2</sub><sup>1+</sup>)<sub>n</sub>,n(F<sub>6</sub> P<sub>1</sub><sup>1-</sup>)

**Compound Name:** catena-((μ<sub>3</sub>-1,2-bis(Pyridine-3-carboxamido)benzene)-silver(i) hexafluorophosphate)

**Space Group:** P21      **Cell:**    **a** 8.717(1)    **b** 13.711(3)    **c** 9.266(1)  
**Space Group No.:** 4      **(Å, °)**    **α** 90.00      **β** 112.10(3)    **γ** 90.00

**R-Factor (%):** 4.66      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.849



## Search Overview

**Search:** search50  
**Date/Time done:** Thu May 26 11:47:06 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:** 3

*Summary of queries used. Search found structures that:*

match

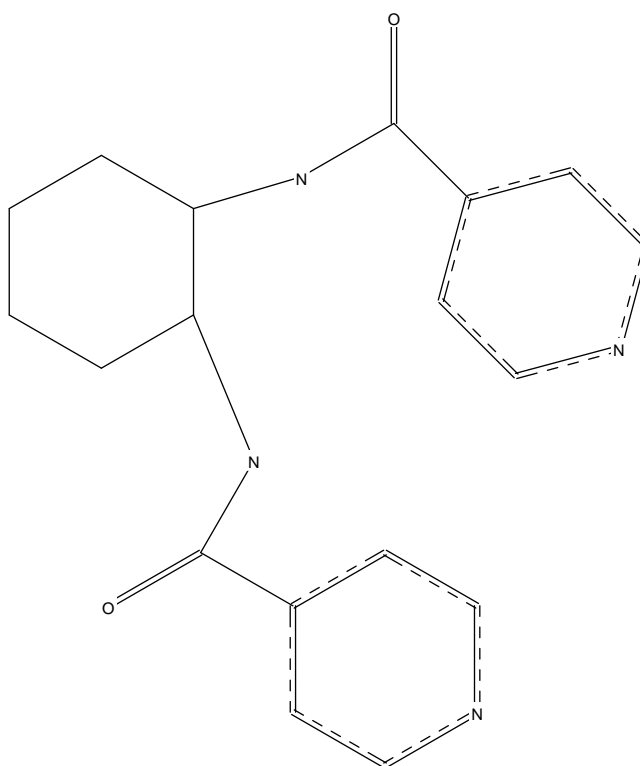
**Query 2**

**Query 3**

**Query 2**

4M

**Query 3**



## Search: search50 (Thu May 26 11:47:06 2011): Hit 1

BOFDOQ

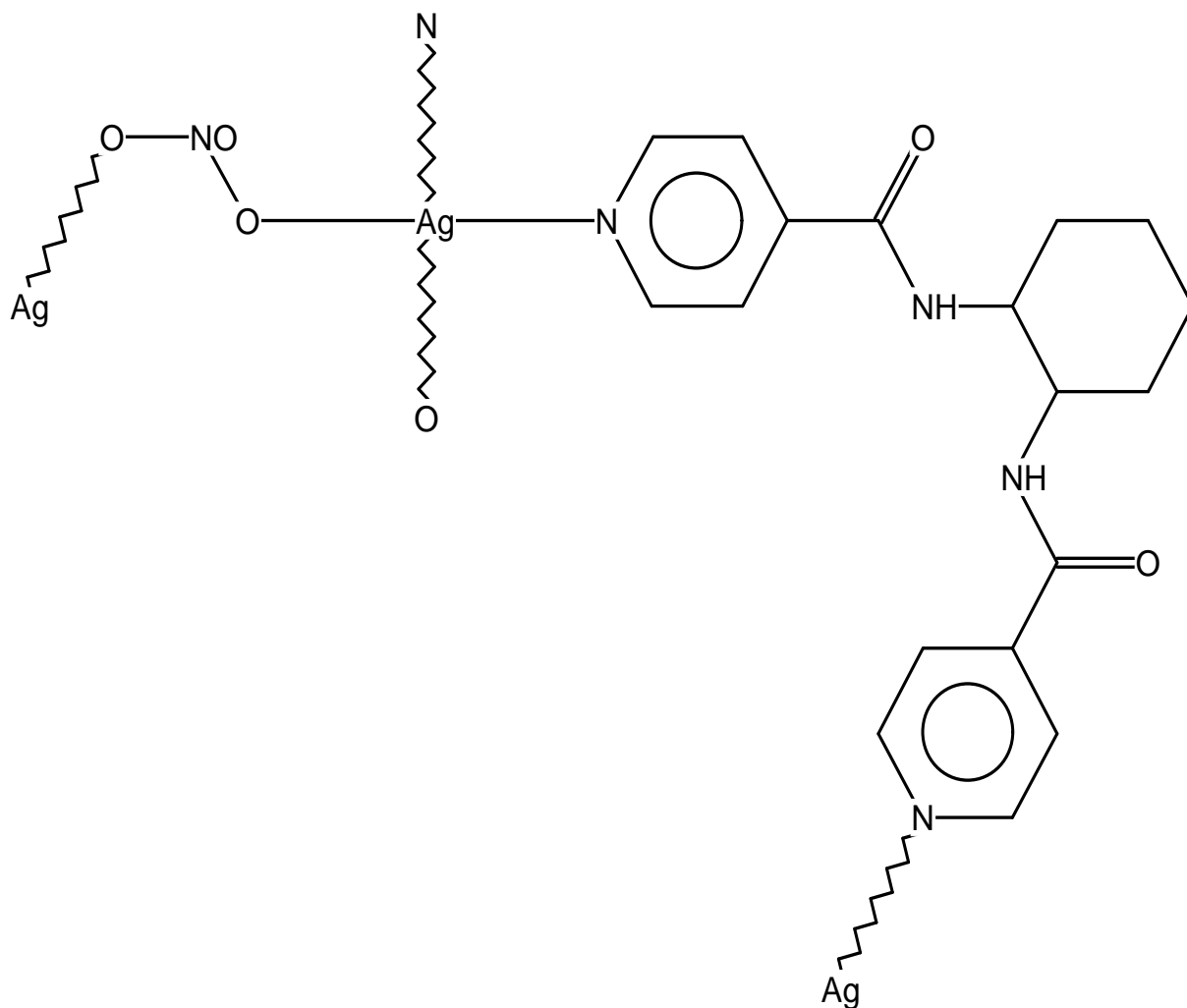
**Reference:** S.P.Anthony (2008) *Inorg.Chem.Commun.* ,11,791

**Formula:** (C<sub>18</sub> H<sub>20</sub> Ag<sub>1</sub> N<sub>5</sub> O<sub>5</sub>)<sub>n</sub>

**Compound Name:** catena-((μ<sub>2</sub>-(R,R)-N,N'-1,2-Cyclohexanediyl)diisonicotinamide)-(μ<sub>2</sub>-nitrate)-silver(i)

**Space Group:** P21212    **Cell:**    **a** 5.199(0)    **b** 12.695(0)    **c** 14.428(1)  
**Space Group No.:** 18    **(Å, °)**    **α** 90.00    **β** 90.00    **γ** 90.00

**R-Factor (%):** 3.41    **Temperature(K):** 273    **Density(g/cm<sup>3</sup>):** 1.724



## Search: search50 (Thu May 26 11:47:06 2011): Hit 2

BOFDUW

**Reference:** S.P.Anthony (2008) *Inorg.Chem.Commun.* ,11,791

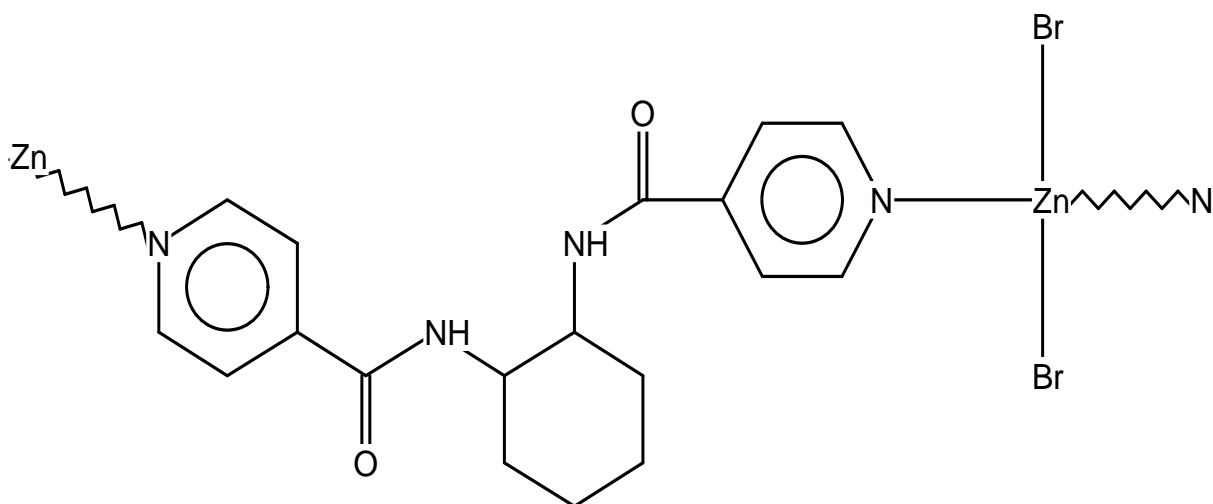
**Formula:**  $(C_{18} H_{20} Br_2 N_4 O_2 Zn_1)_n$

**Compound Name:** catena-(( $\mu_2$ -(R,R)-N,N'-1,2-Cyclohexanediyl)diisonicotinamide)-dibromo-zinc(ii)

**Space Group:** P21212      **Cell:**      **a** 15.112(1)      **b** 25.855(3)      **c** 5.069(0)

**Space Group No.:** 18      **(Å, °)**       $\alpha$  90.00       $\beta$  90.00       $\gamma$  90.00

**R-Factor (%):** 3.55      **Temperature(K):** 273      **Density(g/cm<sup>3</sup>):** 1.843



## Search: search50 (Thu May 26 11:47:06 2011): Hit 3

BOFFAE

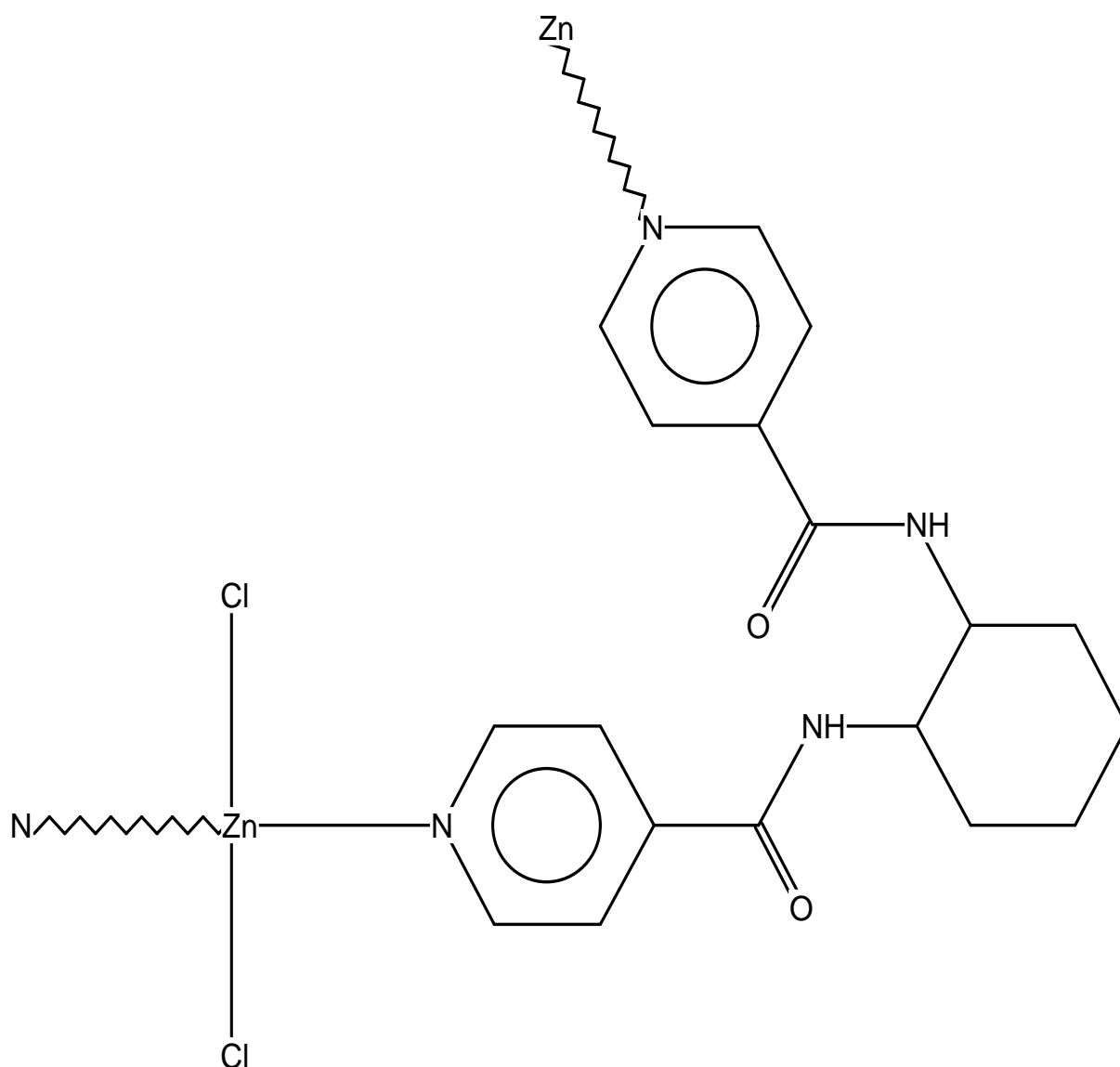
**Reference:** S.P.Anthony (2008) *Inorg.Chem.Commun.* ,11,791

**Formula:** (C<sub>18</sub> H<sub>20</sub> Cl<sub>2</sub> N<sub>4</sub> O<sub>2</sub> Zn<sub>1</sub>)<sub>n</sub>

**Compound Name:** catena-((μ<sub>2</sub>-(R,R)-N,N'-1,2-cyclohexanediyl)diisonicotinamide)-dichloro-zinc(ii)

**Space Group:** P21212    **Cell:**    **a** 15.082(0)    **b** 25.348(1)    **c** 5.057(0)  
**Space Group No.:** 18    **(Å, °)**    **α** 90.00    **β** 90.00    **γ** 90.00

**R-Factor (%):** 4.75    **Temperature(K):** 273    **Density(g/cm<sup>3</sup>):** 1.583



## Search Overview

**Search:** search2  
**Date/Time done:** Wed Jul 13 12:47:53 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

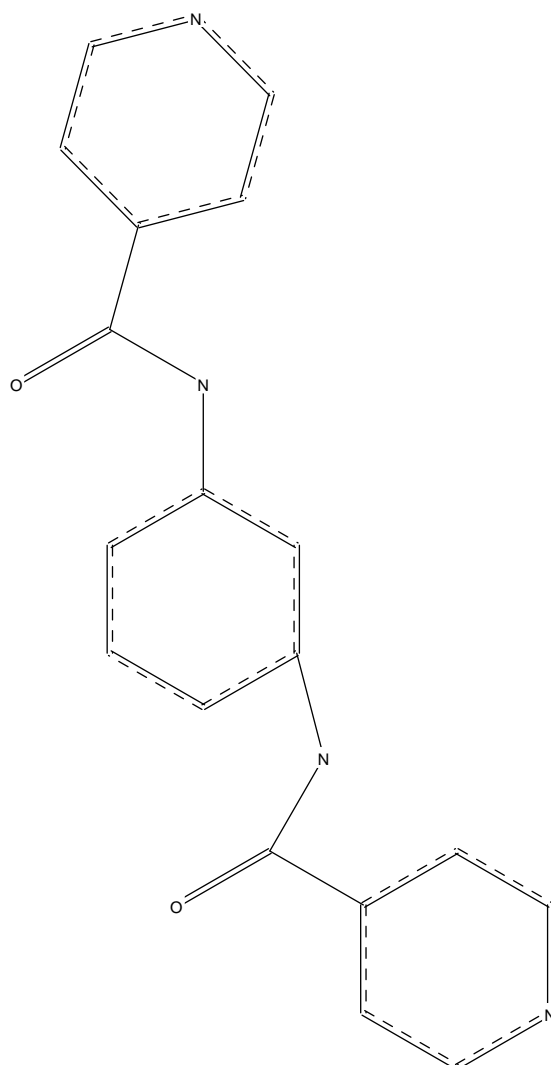
**Query 1**

**Query 2**

**Query 1**

4M

**Query 2**





## Search: search2 (Wed Jul 13 12:47:53 2011): Hit 1

### KEHGIO

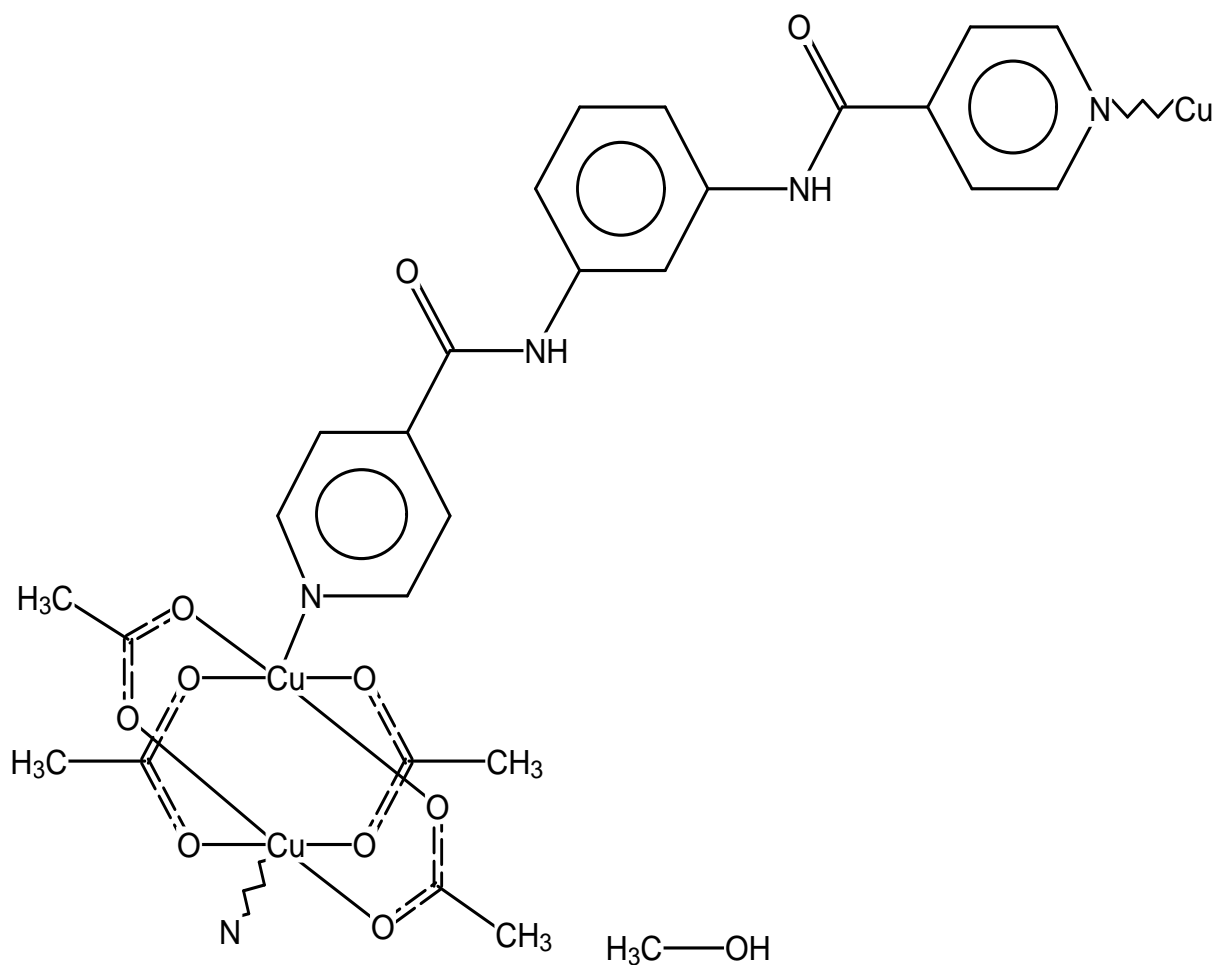
**Reference:** J.Pansanel, A.Jouaiti, S.Ferlay, M.W.Hosseini,  
J.-M.Planeix, N.Kyritsakas (2006) *New J.Chem.* ,**30**,683

**Formula:**  $(C_{26} H_{26} Cu_2 N_4 O_{10})_n, 2n(C_1 H_4 O_1)$

**Compound Name:** catena-(tetrakis( $\mu_2$ -Acetato)-( $\mu_2$ -1,3-bis(isonicotinoylamino)benzene)-  
di-copper methanol solvate)

**Space Group:** C2/c      **Cell:**      **a** 33.799(1)      **b** 12.745(0)      **c** 8.567(0)  
**Space Group No.:** 15      **(Å, °)**       $\alpha$  90.00       $\beta$  95.30(0)       $\gamma$  90.00

**R-Factor (%):** 10.50      **Temperature(K):** 173      **Density(g/cm<sup>3</sup>):** 1.348



## Search Overview

**Search:** search1  
**Date/Time done:** Thu May 26 12:00:44 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:** 6

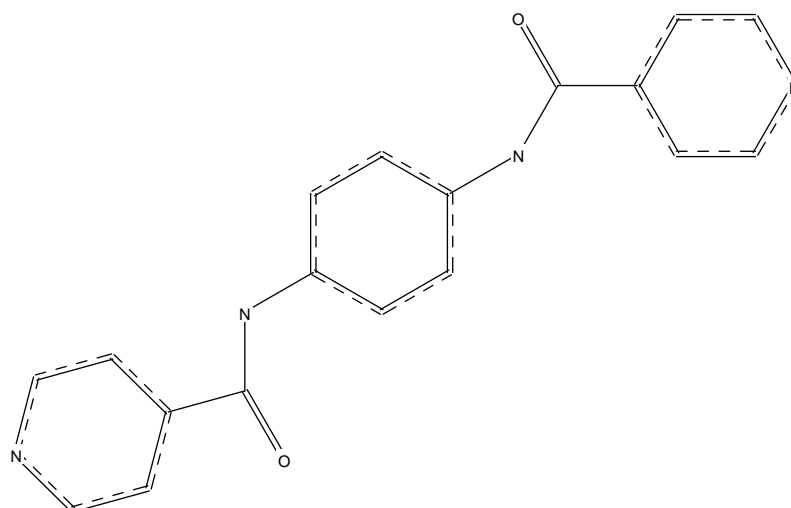
*Summary of queries used. Search found structures that:*

match

**Query 1**

**Query 2**

**Query 1**



**Query 2**

4M

## Search: search1 (Thu May 26 12:00:44 2011): Hit 1

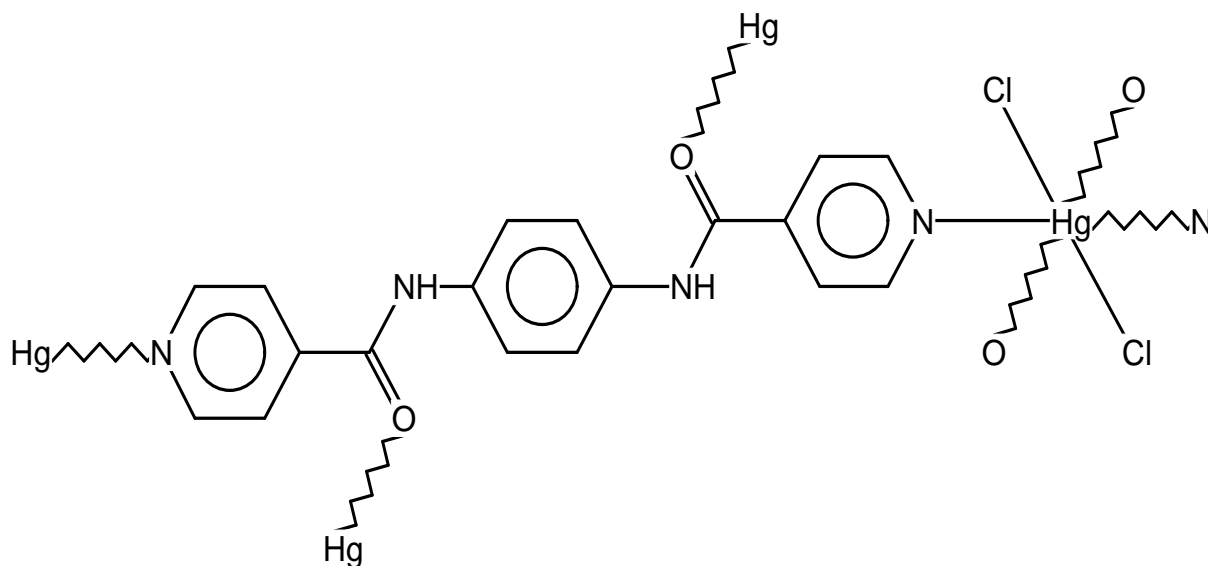
### ACIXAM

**Reference:** J.Pansanel, A.Jouaiti, S.Ferlay, M.W.Hosseini,  
J.-M.Planeix, N.Kyritsakas (2006) *New J.Chem.* ,**30**,71

**Formula:** (C<sub>18</sub> H<sub>14</sub> Cl<sub>2</sub> Hg<sub>1</sub> N<sub>4</sub> O<sub>2</sub>)<sub>n</sub>

**Compound Name:** catena-((μ<sub>4</sub>-N,N'-bis((4-Pyridyl)carbonyl)-1,4-phenylenediamine-N'',N''',O,O')-dichloro-mercury(ii))

<b>Space Group:</b>	P21/n	<b>Cell:</b>	<b>a</b> 8.334(0)	<b>b</b> 9.237(0)	<b>c</b> 11.446(0)
<b>Space Group No.:</b>	14	<b>(Å, °)</b>	<b>α</b> 90.00	<b>β</b> 94.21(0)	<b>γ</b> 90.00
<b>R-Factor (%):</b>	1.70	<b>Temperature(K):</b>	173	<b>Density(g/cm<sup>3</sup>):</b>	2.229



## Search: search1 (Thu May 26 12:00:44 2011): Hit 2

### BESJEP

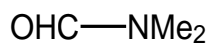
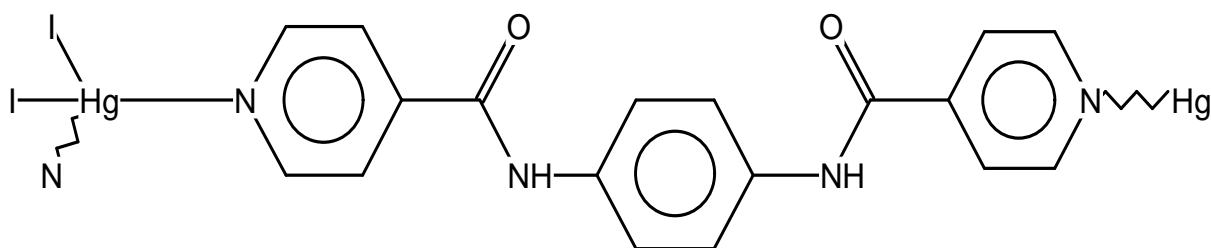
**Reference:** Yun-Yin Niu, Ying-Lin Song, Jie Wu, Hongwei Hou,  
Yu Zhu, Xia Wang (2004) *Inorg.Chem.Commun.* ,7,471

**Formula:** (C<sub>18</sub> H<sub>14</sub> Hg<sub>1</sub> I<sub>2</sub> N<sub>4</sub> O<sub>2</sub>)<sub>n</sub>,2n(C<sub>3</sub> H<sub>7</sub> N<sub>1</sub> O<sub>1</sub>)

**Compound Name:** catena-((μ<sub>2</sub>-N,N'-bis(4-pyridylformamide)-1,4-benzene)-diiodo-mercury dimethylformamide solvate)

**Space Group:** P21/c      **Cell:**      **a** 11.389(2)      **b** 11.392(2)      **c** 24.216(5)  
**Space Group No.:** 14      **(Å, °)**      **α** 90.00      **β** 102.21(3)      **γ** 90.00

**R-Factor (%):** 4.33      **Temperature(K):** 291      **Density(g/cm<sup>3</sup>):** 1.988



## Search: search1 (Thu May 26 12:00:44 2011): Hit 3

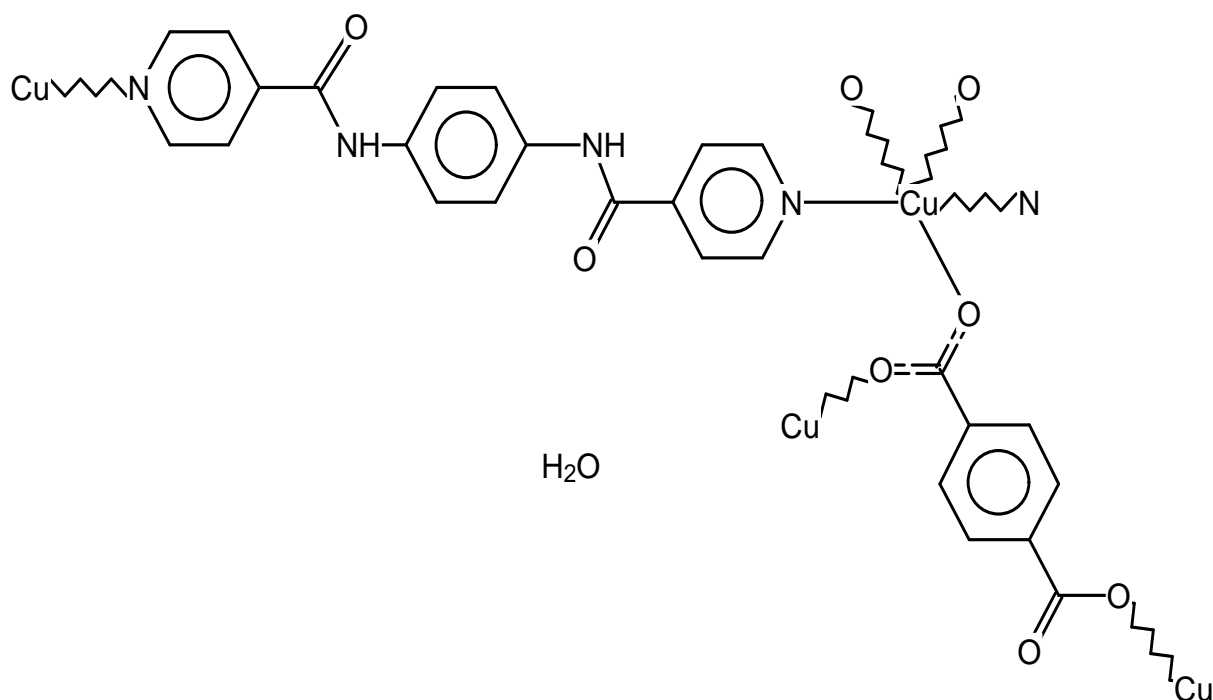
### BOWSIQ

**Reference:** Feng Luo, Yun-xia Che, Ji-min Zheng (2009)  
*Microporous and Mesoporous Materials*, **117**,486

**Formula:**  $(C_{26} H_{18} Cu_1 N_4 O_6)_n \cdot 3n(H_2 O_1)$

**Compound Name:** catena-[( $\mu_2$ -Benzene-1,4-dicarboxylato)-( $\mu_2$ -N,N'-bis(4-pyridylformamide)-1,4-benzene)-copper(ii) trihydrate clathrate]

<b>Space Group:</b>	lbca	<b>Cell:</b>	<b>a</b> 15.378(3)	<b>b</b> 19.560(4)	<b>c</b> 39.822(8)
<b>Space Group No.:</b>	73	<b>(Å, °)</b>	$\alpha$ 90.00	$\beta$ 90.00	$\gamma$ 90.00
<b>R-Factor (%):</b>	8.19	<b>Temperature(K):</b>	298	<b>Density(g/cm<sup>3</sup>):</b>	1.331



## Search: search1 (Thu May 26 12:00:44 2011): Hit 4

KEHGOU

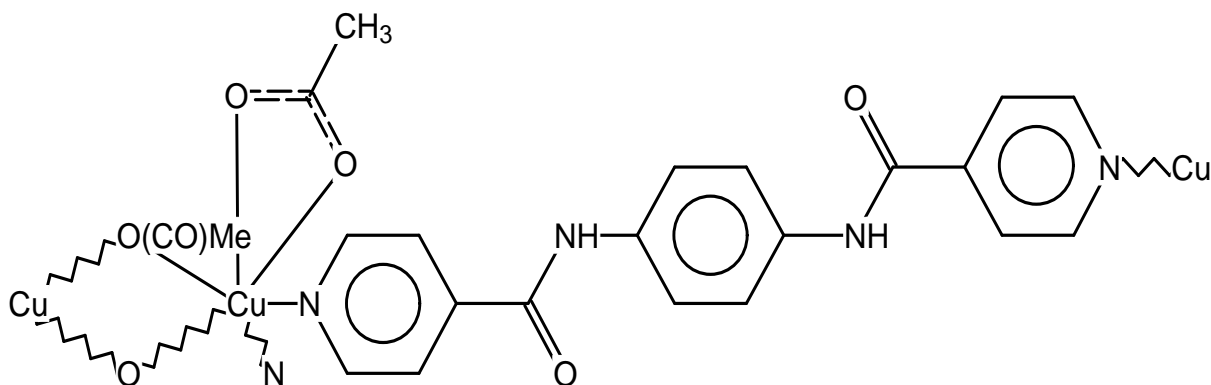
**Reference:** J.Pansanel, A.Jouaiti, S.Ferlay, M.W.Hosseini,  
J.-M.Planeix, N.Kyritsakas (2006) *New J.Chem.* ,**30**,683

**Formula:** (C<sub>22</sub> H<sub>20</sub> Cu<sub>1</sub> N<sub>4</sub> O<sub>6</sub>)<sub>n</sub>

**Compound Name:** catena-((μ<sub>2</sub>-Acetato)-(μ<sub>2</sub>-1,4-bis(isonicotinoylamino)benzene)-(acetato-O,O')-di-copper)

**Space Group:** P21/n      **Cell:**      **a** 13.667(1)      **b** 11.591(0)      **c** 14.152(1)  
**Space Group No.:** 14      **(Å, °)**      **α** 90.00      **β** 117.79(0)      **γ** 90.00

**R-Factor (%):** 3.49      **Temperature(K):** 173      **Density(g/cm<sup>3</sup>):** 1.674



## Search: search1 (Thu May 26 12:00:44 2011): Hit 5

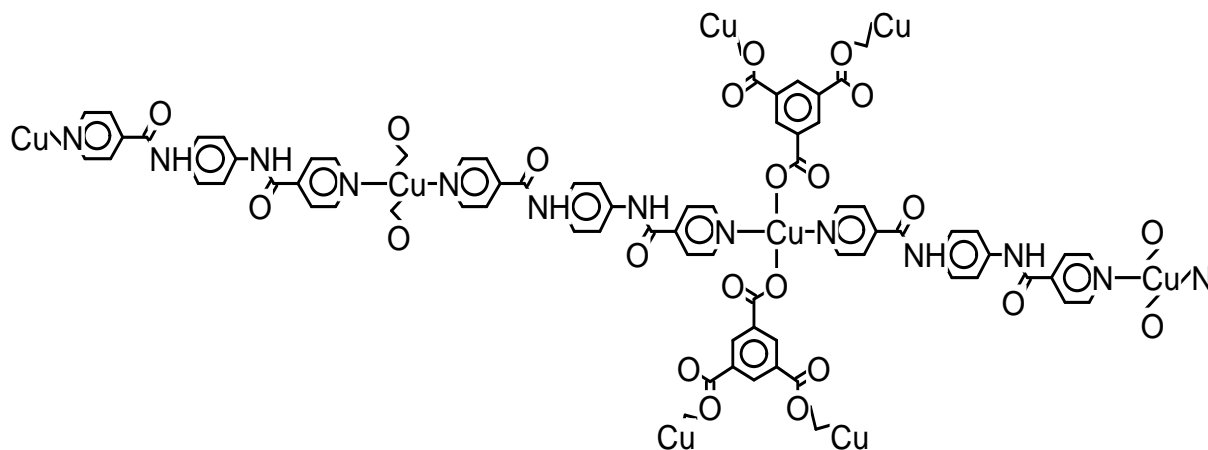
### NIMRAD

**Reference:** Feng Luo, Ji-min Zheng, S.R.Batten (2007)  
*Chem. Commun.* ,3744

**Formula:**  $(C_{72} H_{48} Cu_3 N_{12} O_{18})_n \cdot 5n(H_2 O)_1$

**Compound Name:** catena-(bis( $\mu_3$ -Benzene-1,3,5-tricarboxylato)-tris( $\mu_2$ -1,4-bis(isonicotinamido)benzene)-tri-copper(ii) pentahydrate clathrate)

<b>Space Group:</b>	R-3	<b>Cell:</b>	<b>a</b> 18.604(3)	<b>b</b> 18.604(3)	<b>c</b> 19.756(4)
<b>Space Group No.:</b>	148	<b>(Å, °)</b>	$\alpha$ 90.00	$\beta$ 90.00	$\gamma$ 120.00
<b>R-Factor (%):</b>	5.40	<b>Temperature(K):</b>	298	<b>Density(g/cm<sup>3</sup>):</b>	1.388



H<sub>2</sub>O

## Search: search1 (Thu May 26 12:00:44 2011): Hit 6

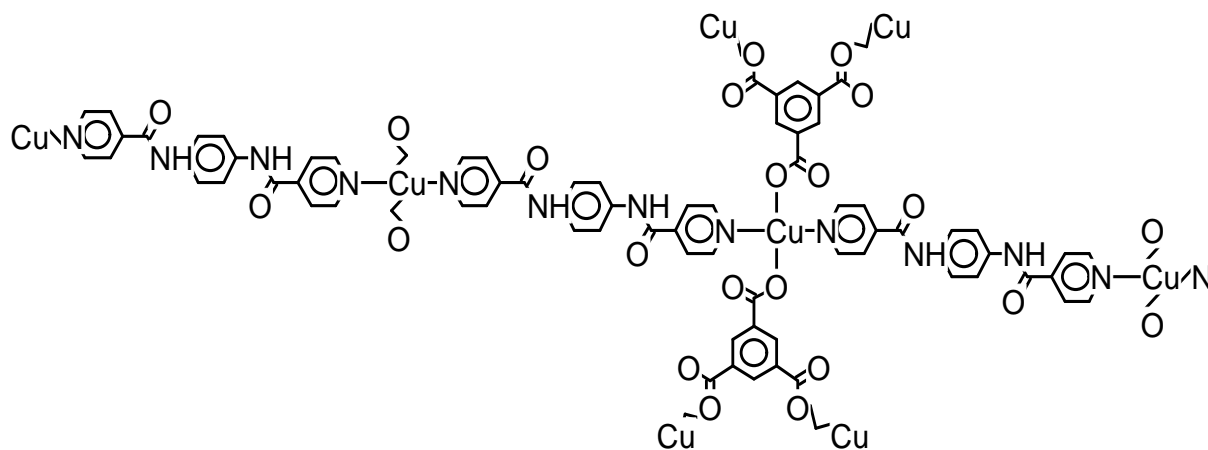
NIQXUH

**Reference:** Feng Luo, Ji-min Zheng, S.R.Batten (2007)  
*Chem.Commun.* ,3744

**Formula:** (C<sub>72</sub> H<sub>48</sub> Cu<sub>3</sub> N<sub>12</sub> O<sub>18</sub>)<sub>n</sub>

**Compound Name:** catena-(bis(μ<sub>3</sub>-Benzene-1,3,5-tricarboxylato)-tris(μ<sub>2</sub>-1,4-bis(isonicotinamido)benzene)-tri-copper(ii))

<b>Space Group:</b>	R-3	<b>Cell:</b>	<b>a</b> 18.594(1)	<b>b</b> 18.594(1)	<b>c</b> 19.761(3)
<b>Space Group No.:</b>	148	<b>(Å, °)</b>	<b>α</b> 90.00	<b>β</b> 90.00	<b>γ</b> 120.00
<b>R-Factor (%):</b>	6.17	<b>Temperature(K):</b>	294	<b>Density(g/cm<sup>3</sup>):</b>	1.313





## Search Overview

**Search:** search2  
**Date/Time done:** Thu May 26 12:03:45 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:** 3

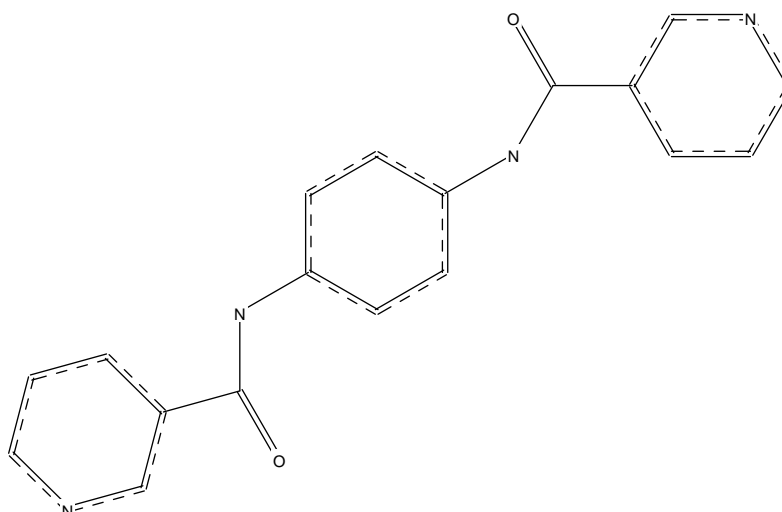
*Summary of queries used. Search found structures that:*

match

**Query 1**

**Query 2**

**Query 1**



**Query 2**

4M

## Search: search2 (Thu May 26 12:03:45 2011): Hit 1

ACIWUF

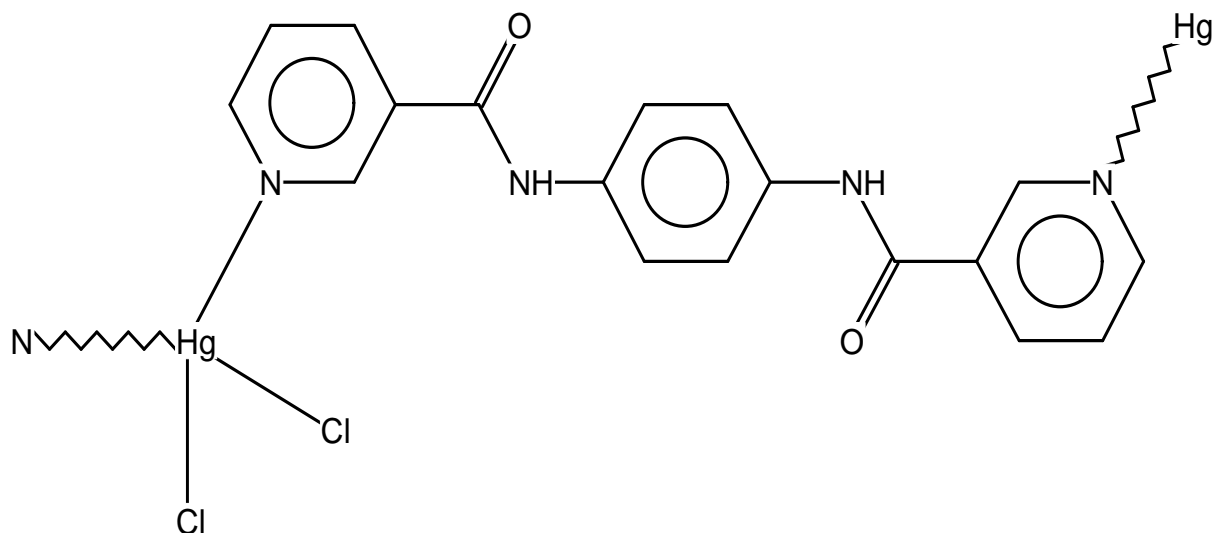
**Reference:** J.Pansanel, A.Jouaiti, S.Ferlay, M.W.Hosseini,  
J.-M.Planeix, N.Kyritsakas (2006) *New J.Chem.* ,**30**,71

**Formula:** (C<sub>18</sub> H<sub>14</sub> Cl<sub>2</sub> Hg<sub>1</sub> N<sub>4</sub> O<sub>2</sub>)<sub>n</sub>

**Compound Name:** catena-((μ<sub>2</sub>-N,N'-bis((3-Pyridyl)carbonyl)-1,4-phenylenediamine-N'',N''')-  
dichloro-mercury(ii))

**Space Group:** P2/c      **Cell:**    **a** 13.045(0)    **b** 5.026(1)    **c** 13.777(2)  
**Space Group No.:** 13      **(Å, °)**    **α** 90.00      **β** 96.00(0)    **γ** 90.00

**R-Factor (%):** 3.28      **Temperature(K):** 173      **Density(g/cm<sup>3</sup>):** 2.181



## Search: search2 (Thu May 26 12:03:45 2011): Hit 2

### DEYTAD

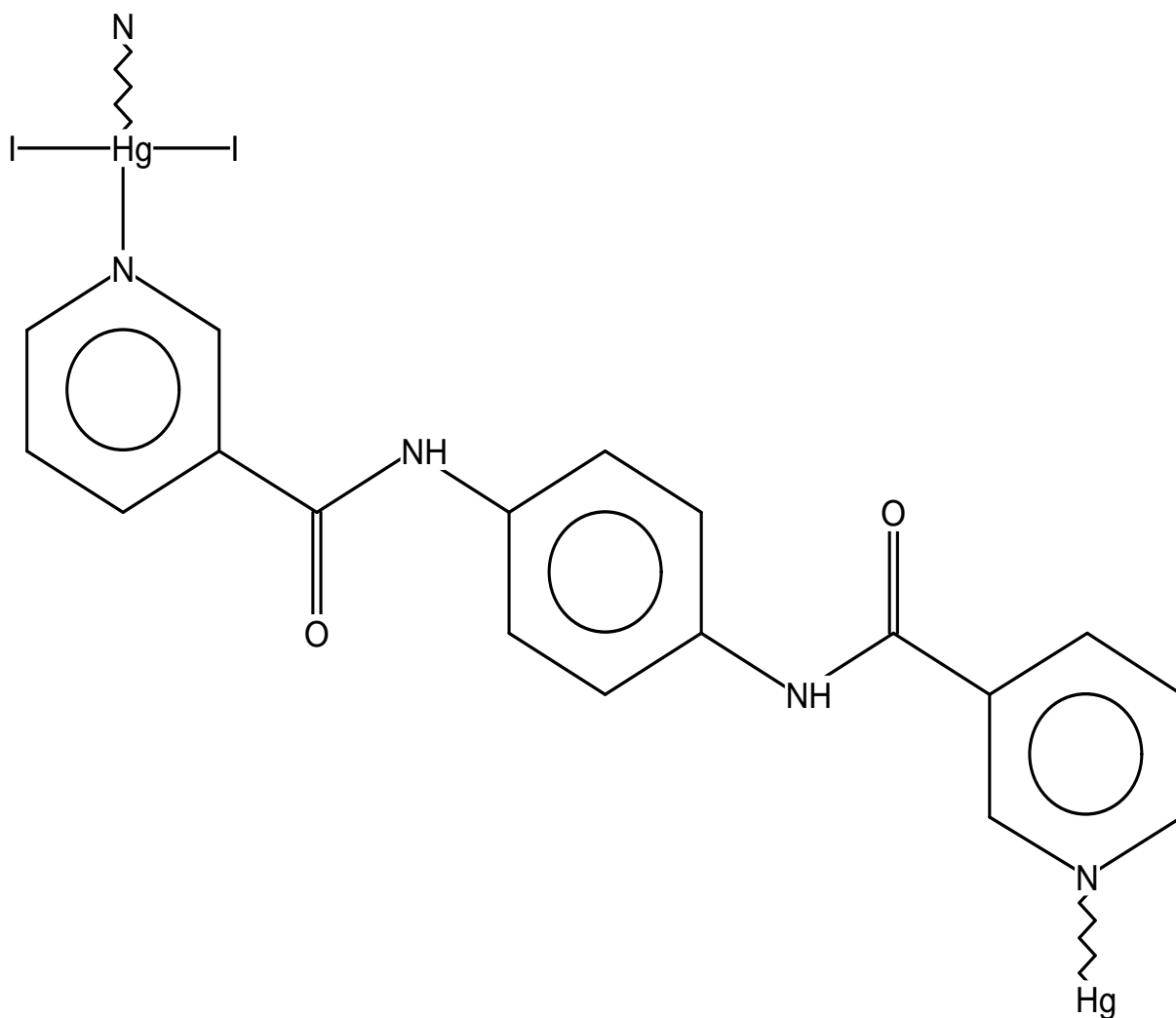
**Reference:** Ying-Gui Zhu, Feng Gao (2007)  
*Acta Crystallogr., Sect. E: Struct. Rep. Online* ,**63**,m778

**Formula:** (C<sub>18</sub> H<sub>14</sub> Hg<sub>1</sub> I<sub>2</sub> N<sub>4</sub> O<sub>2</sub>)<sub>n</sub>

**Compound Name:** catena-((μ<sub>2</sub>-N,N'-p-Phenylene-bis(pyridine-3-carboxamide)-N,N')-diiodo-mercury(ii))

**Space Group:** C2/c      **Cell:**    **a** 16.035(4)    **b** 5.047(1)    **c** 25.060(7)  
**Space Group No.:** 15      **(Å, °)**    **α** 90.00      **β** 95.56(0)    **γ** 90.00

**R-Factor (%):** 3.44      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 2.543



## Search: search2 (Thu May 26 12:03:45 2011): Hit 3

### SECQAT

**Reference:** M.Sarkar, K.Biradha (2006) *Eur.J.Inorg.Chem.* ,531

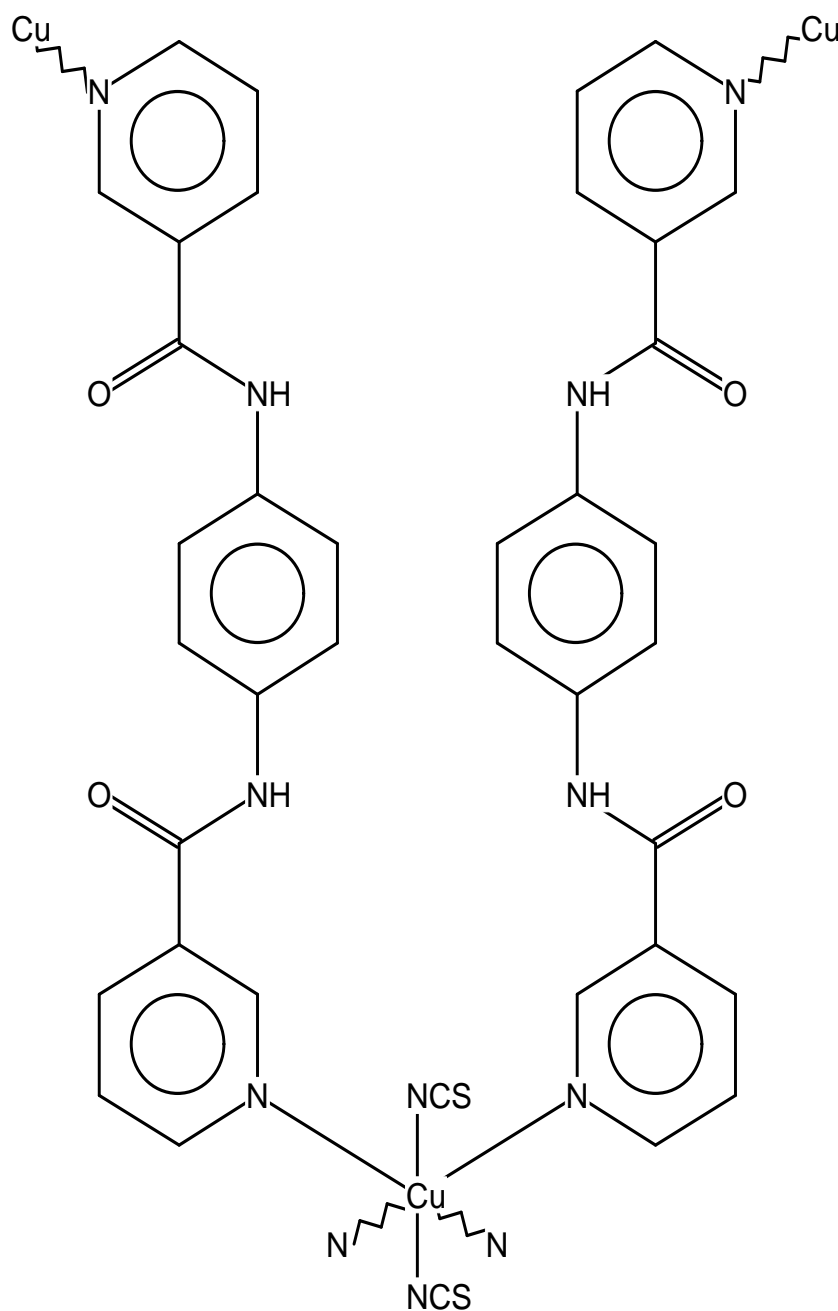
**Formula:**  $(C_{38} H_{28} Cu_1 N_{10} O_4 S_2)_n$

**Compound Name:** catena-(bis( $\mu_2$ -1,4-bis(3-pyridinecarboxamido)benzene-N,N')-(isothiocyanato)-copper(ii))

**Space Group:** P-1      **Cell:**      **a** 8.259(1)      **b** 9.613(1)      **c** 12.656(3)

**Space Group No.:** 2      **(Å, °)**       $\alpha$  85.70(3)       $\beta$  74.66(3)       $\gamma$  71.18(3)

**R-Factor (%):** 5.22      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.478



## Search Overview

**Search:** search5  
**Date/Time done:** Wed Jul 13 08:20:34 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:** 6

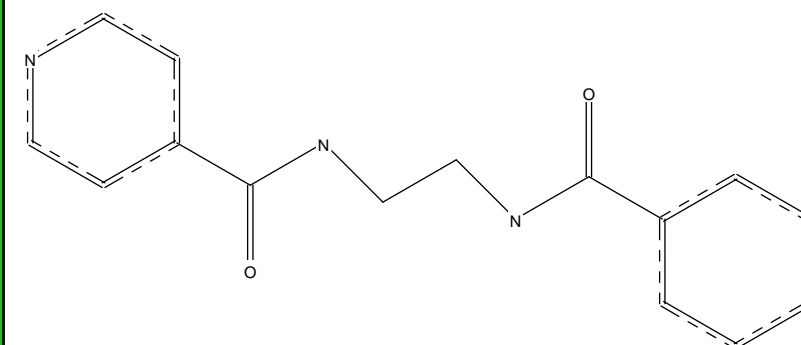
*Summary of queries used. Search found structures that:*

match

**Query 1**

**Query 2**

**Query 1**



**Query 2**

4M

## Search: search5 (Wed Jul 13 08:20:34 2011): Hit 1

### AREZUS

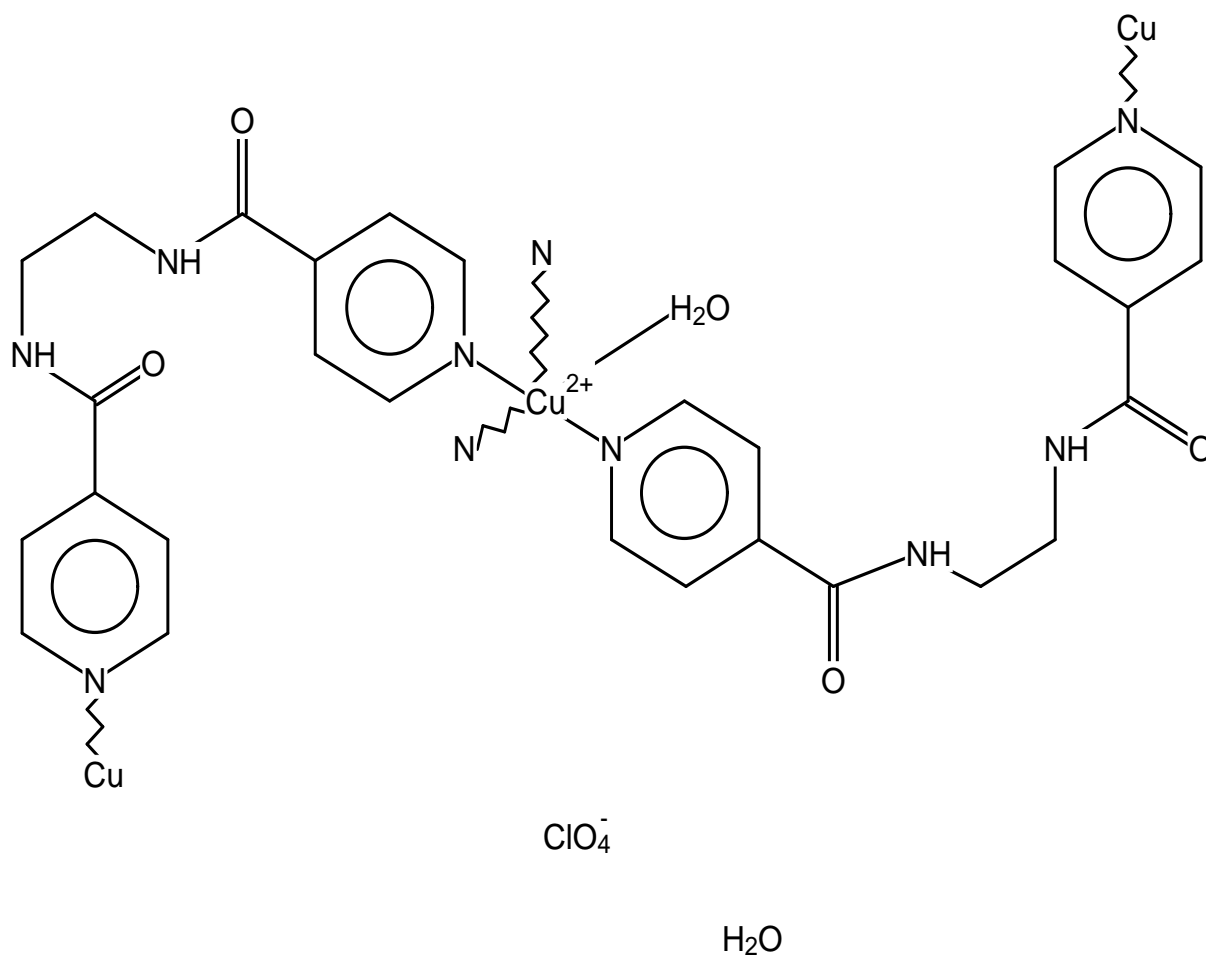
**Reference:** Chun-Hua Ge, Xiang-Dong Zhang, Peng Zhang,  
Wei Guan, Fang Guo, Qi-Tao Liu (2003) *Polyhedron*, **22**,3493

**Formula:**  $(C_{28} H_{30} Cu_1 N_8 O_5^{2+})_n, 2n(Cl_1 O_4^{1-}), 6n(H_2 O_1)$

**Compound Name:** catena-(bis( $\mu_2$ -1,2-bis(4-pyridinecarboxamido)ethane)-aqua-copper(ii) diperchlorate hexahydrate)

**Space Group:** P21/n      **Cell:**      **a** 12.732(4)      **b** 13.164(4)      **c** 23.024(8)  
**Space Group No.:** 14      **(Å, °)**       $\alpha$  90.00       $\beta$  92.66(0)       $\gamma$  90.00

**R-Factor (%):** 7.03      **Temperature(K):** 273      **Density(g/cm<sup>3</sup>):** 1.601



## Search: search5 (Wed Jul 13 08:20:34 2011): Hit 2

### ARIBAE

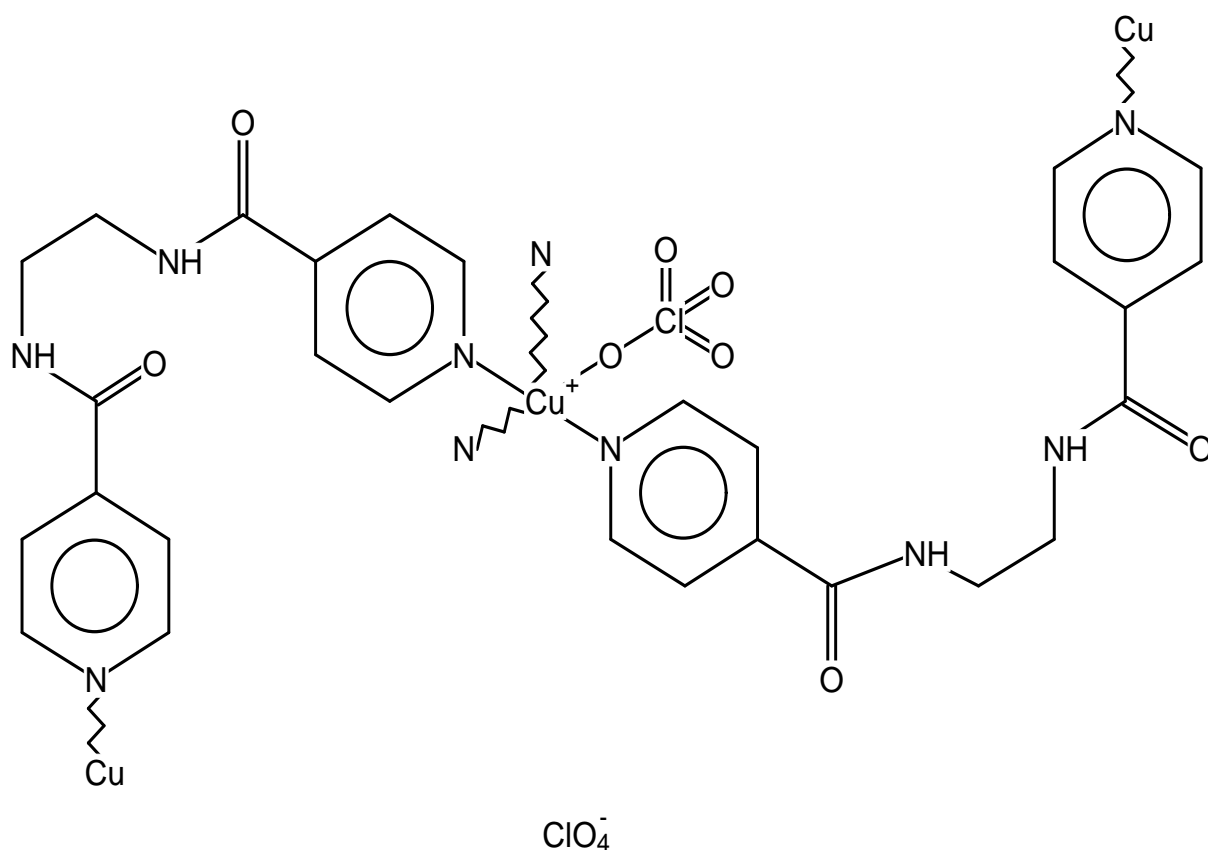
**Reference:** Chun-Hua Ge, Xiang-Dong Zhang, Peng Zhang,  
Wei Guan, Fang Guo, Qi-Tao Liu (2003) *Polyhedron*, **22**,3493

**Formula:** (C<sub>28</sub> H<sub>28</sub> Cl<sub>1</sub> Cu<sub>1</sub> N<sub>8</sub> O<sub>8</sub> 1<sup>+</sup>)<sub>n</sub>,n(Cl<sub>1</sub> O<sub>4</sub> 1<sup>-</sup>)

**Compound Name:** catena-(bis(μ<sub>2</sub>-1,2-bis(4-pyridinecarboxamido)ethane)-perchlorato-copper(ii) perchlorate)

**Space Group:** Pca21      **Cell:**      **a** 16.880(5)      **b** 9.483(3)      **c** 22.044(7)  
**Space Group No.:** 29      **(Å, °)**      **α** 90.00      **β** 90.00      **γ** 90.00

**R-Factor (%):** 6.86      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.512



## Search: search5 (Wed Jul 13 08:20:34 2011): Hit 3

### DIKHOV

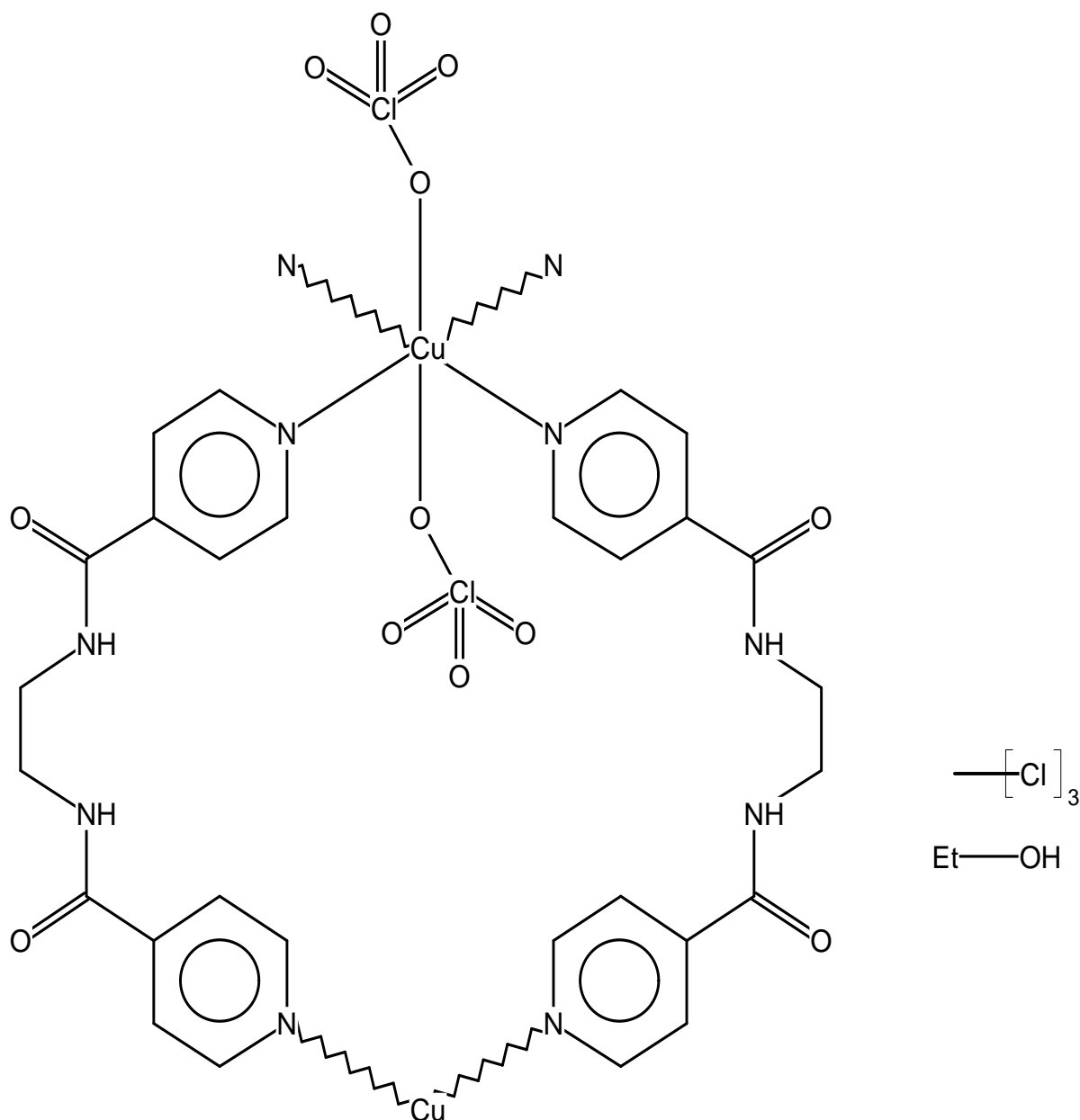
**Reference:** M.Sarkar, K.Biradha (2007) *Cryst.Growth Des.* ,7,1318

**Formula:**  $(C_{28} H_{28} Cl_2 Cu_1 N_8 O_{12})_n, 2n(C_1 H_1 Cl_3), 2n(C_2 H_6 O_1)$

**Compound Name:** catena-(bis( $\mu_2$ -1,2-bis((4-Pyridyl)carbonylamino)ethane)-bis(perchlorato-O)-copper(ii) chloroform ethanol clathrate)

**Space Group:** C2/m      **Cell:**      **a** 9.591(1)      **b** 21.013(4)      **c** 12.284(3)  
**Space Group No.:** 12      **(Å, °)**       $\alpha$  90.00       $\beta$  101.78(3)       $\gamma$  90.00

**R-Factor (%):** 7.76      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.554





## Search: search5 (Wed Jul 13 08:20:34 2011): Hit 4

DIKJEN

**Reference:** M.Sarkar, K.Biradha (2007) *Cryst.Growth Des.* ,7,1318

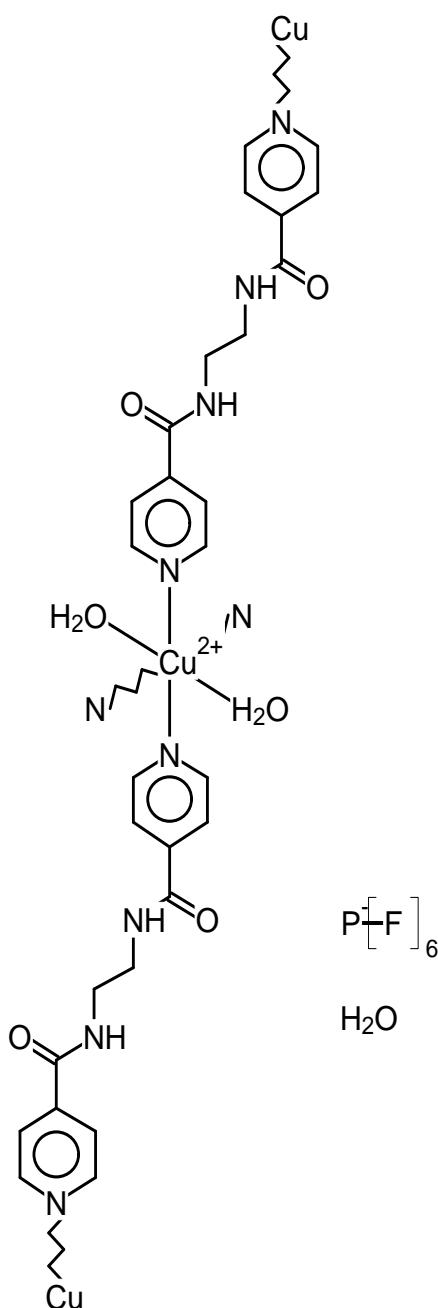
**Formula:**  $(C_{28} H_{32} Cu_1 N_8 O_6^{2+})_n, 2n(F_6 P_1^{1-}), 2n(H_2 O_1)$

**Compound Name:** catena-(bis( $\mu_2$ -1,2-bis((4-Pyridyl)carbonylamino)ethane)-diaqua-copper(ii) bis(hexafluorophosphate) dihydrate)

**Space Group:** P-1      **Cell:**      **a** 11.787(2)      **b** 15.941(3)      **c** 16.312(3)

**Space Group No.:** 2      **(Å, °)**       $\alpha$  65.77(3)       $\beta$  75.63(3)       $\gamma$  86.96(3)

**R-Factor (%):** 7.90      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.187



## Search: search5 (Wed Jul 13 08:20:34 2011): Hit 5

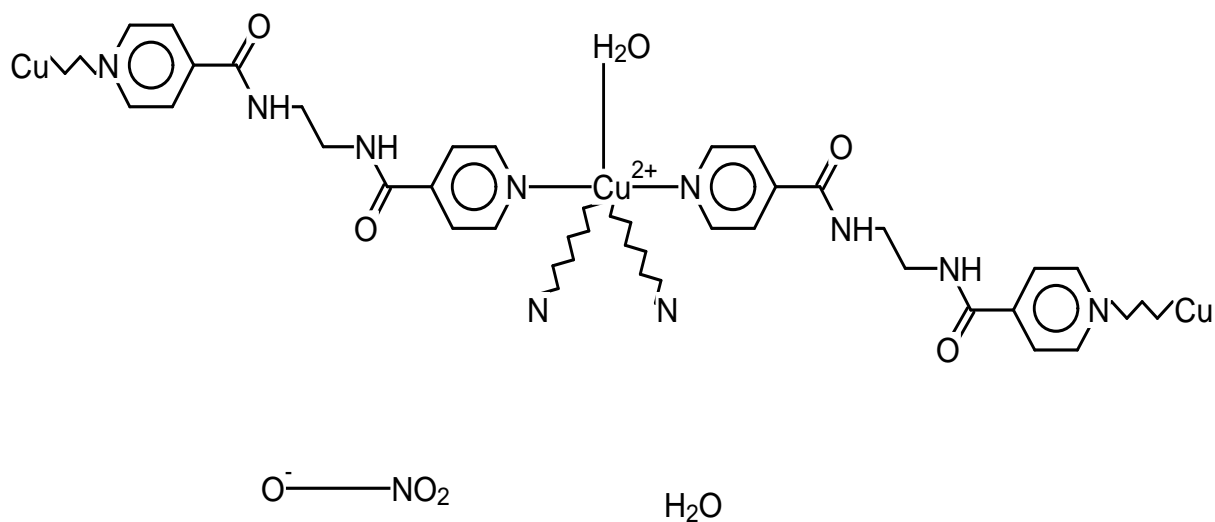
### ESEQAU

**Reference:** Chun-Hua Ge, Xiang-Dong Zhang, Fang Guo,  
Li-Tian Zhang, Zhan Yu, Wen-Sheng Guo, Qi-Tao Liu (2003)  
*Chin.J.Chem.* ,**21**,581

**Formula:**  $(C_{28} H_{30} Cu_1 N_8 O_5^{2+})_n, 2n(N_1 O_3^{1-}), 6n(H_2 O_1)$

**Compound Name:** catena-(bis( $\mu_2$ -1,2-bis(4-Pyridinecarboxamido)ethane-N,N')-aqua-copper(ii) dinitrate hexahydrate)

<b>Space Group:</b>	P21/n	<b>Cell:</b>	<b>a</b> 12.896(3)	<b>b</b> 12.552(8)	<b>c</b> 22.903(19)
<b>Space Group No.:</b>	14	(Å, °)	$\alpha$ 90.00	$\beta$ 93.04(5)	$\gamma$ 90.00
<b>R-Factor (%):</b>	4.03	<b>Temperature(K):</b>	293	<b>Density(g/cm<sup>3</sup>):</b>	1.533



## Search: search5 (Wed Jul 13 08:20:34 2011): Hit 6

TEHJIA

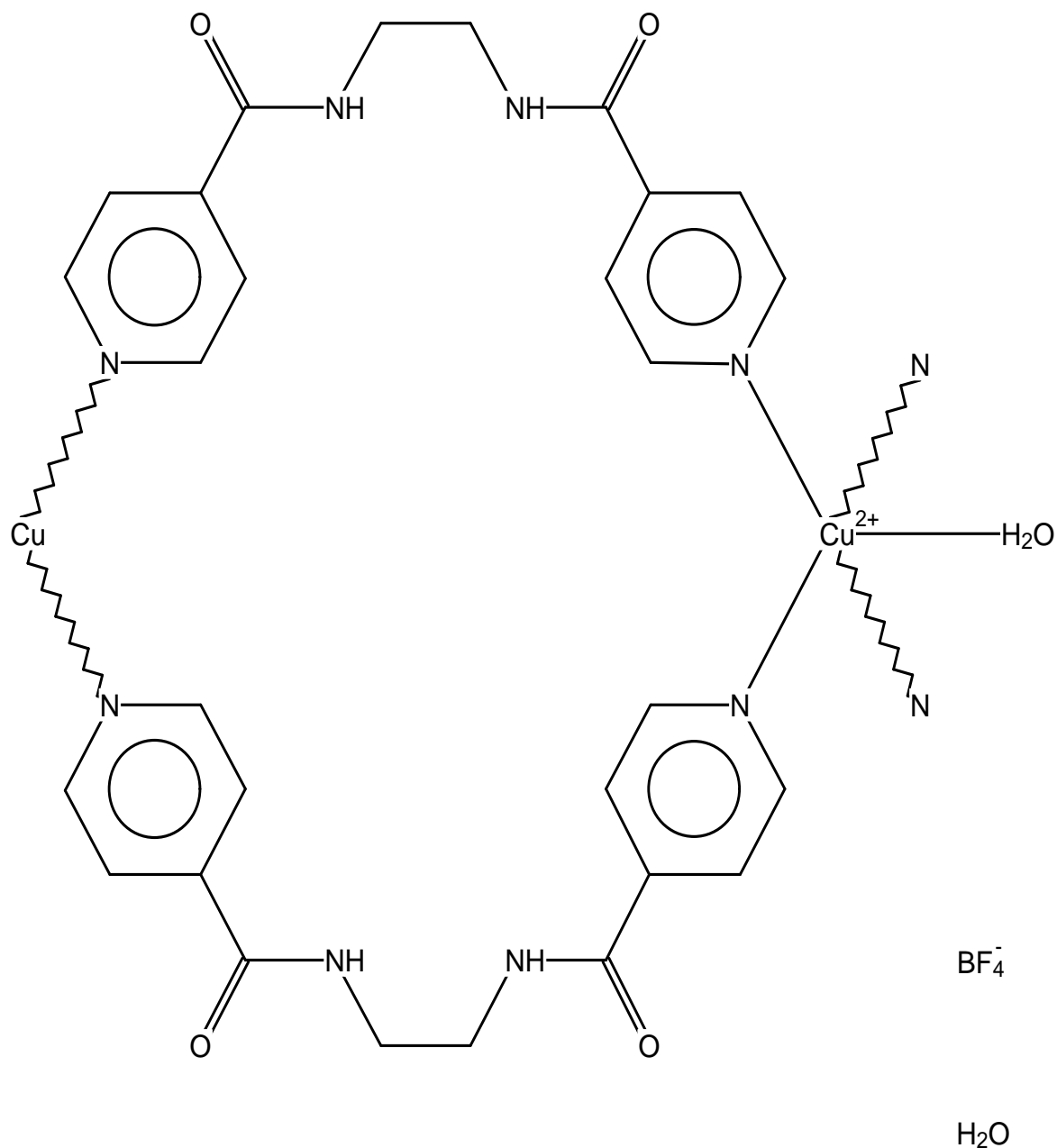
**Reference:** Chun Hua Ge, Xiang Dong Zhang, Wei Guan, Qi Tao Liu, Zhan Yu, Li Yan Liu (2004) *Chin.Chem.Lett.* ,15,183

**Formula:**  $(C_{28}H_{30}Cu_1N_8O_5^{2+})_n, 2n(BF_4^{-}), 6n(H_2O_1)$

**Compound Name:** catena-[bis( $\mu_2$ -1,2-bis(4-Pyridinecarboxamido)ethane)-aqua-copper(ii) bis(tetrafluoroborate) hexahydrate]

**Space Group:** P21/n      **Cell:**      **a** 12.813(5)      **b** 12.734(5)      **c** 22.911(10)  
**Space Group No.:** 14      **(Å, °)**       $\alpha$  90.00       $\beta$  92.78(0)       $\gamma$  90.00

**R-Factor (%):** 6.22      **Temperature(K):** 295      **Density(g/cm<sup>3</sup>):** 1.608



## Search Overview

**Search:** search8  
**Date/Time done:** Wed Jul 13 08:30:33 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:** 6

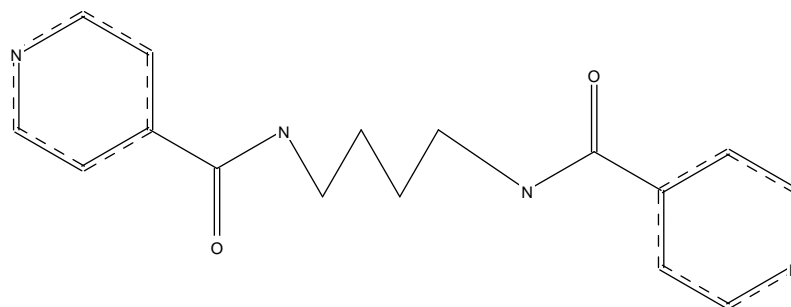
*Summary of queries used. Search found structures that:*

match

**Query 1**

**Query 2**

**Query 1**



**Query 2**

4M

## Search: search8 (Wed Jul 13 08:30:33 2011): Hit 1

### CEMKOV

**Reference:** M.Sarkar, K.Biradha (2006) *Cryst.Growth Des.* ,6,1742

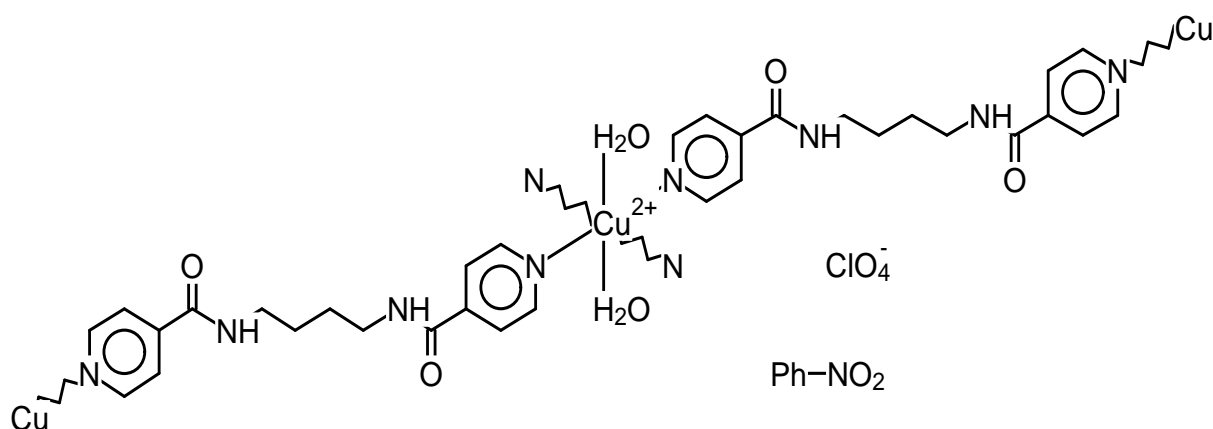
**Formula:**  $(C_{32} H_{40} Cu_1 N_8 O_6^{2+})_n, 2n(Cl_1 O_4^{1-}), 3n(C_6 H_5 N_1 O_2)$

**Compound Name:** catena-(bis( $\mu_2$ -N,N'-bis(4-Pyridylcarbonyl)butane-1,4-diamine-N'',N''')-diaqua-copper(ii) diperchlorate nitrobenzene solvate)

**Space Group:** Pbcn      **Cell:**      **a** 18.567(4)      **b** 9.934(2)      **c** 30.764(6)

**Space Group No.:** 60      **(Å, °)**       $\alpha$  90.00       $\beta$  90.00       $\gamma$  90.00

**R-Factor (%):** 8.39      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.480



## Search: search8 (Wed Jul 13 08:30:33 2011): Hit 2

CEMKOV01

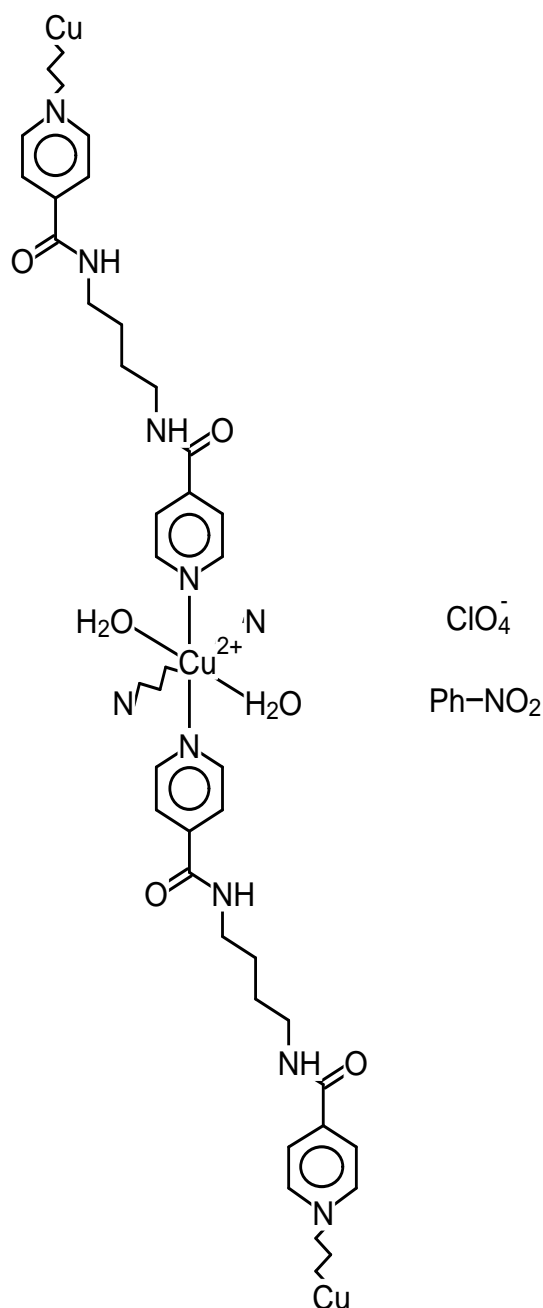
**Reference:** M.Sarkar, K.Biradha (2007) *Cryst.Growth Des.* ,7,1318

**Formula:**  $(C_{32} H_{40} Cu_1 N_8 O_6^{2+})_n, 2n(Cl_1 O_4^{1-}), 3n(C_6 H_5 N_1 O_2)$

**Compound Name:** catena-(bis( $\mu_2$ -1,4-bis((4-Pyridyl)carbonylamino)butane)-diaqua-copper(ii) diperchlorate nitrobenzene clathrate)

**Space Group:** Pbcn      **Cell:**      **a** 18.567(4)      **b** 9.934(2)      **c** 30.764(6)  
**Space Group No.:** 60      **(Å, °)**       $\alpha$  90.00       $\beta$  90.00       $\gamma$  90.00

**R-Factor (%):** 8.39      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.480



## Search: search8 (Wed Jul 13 08:30:33 2011): Hit 3

### CEMKUB

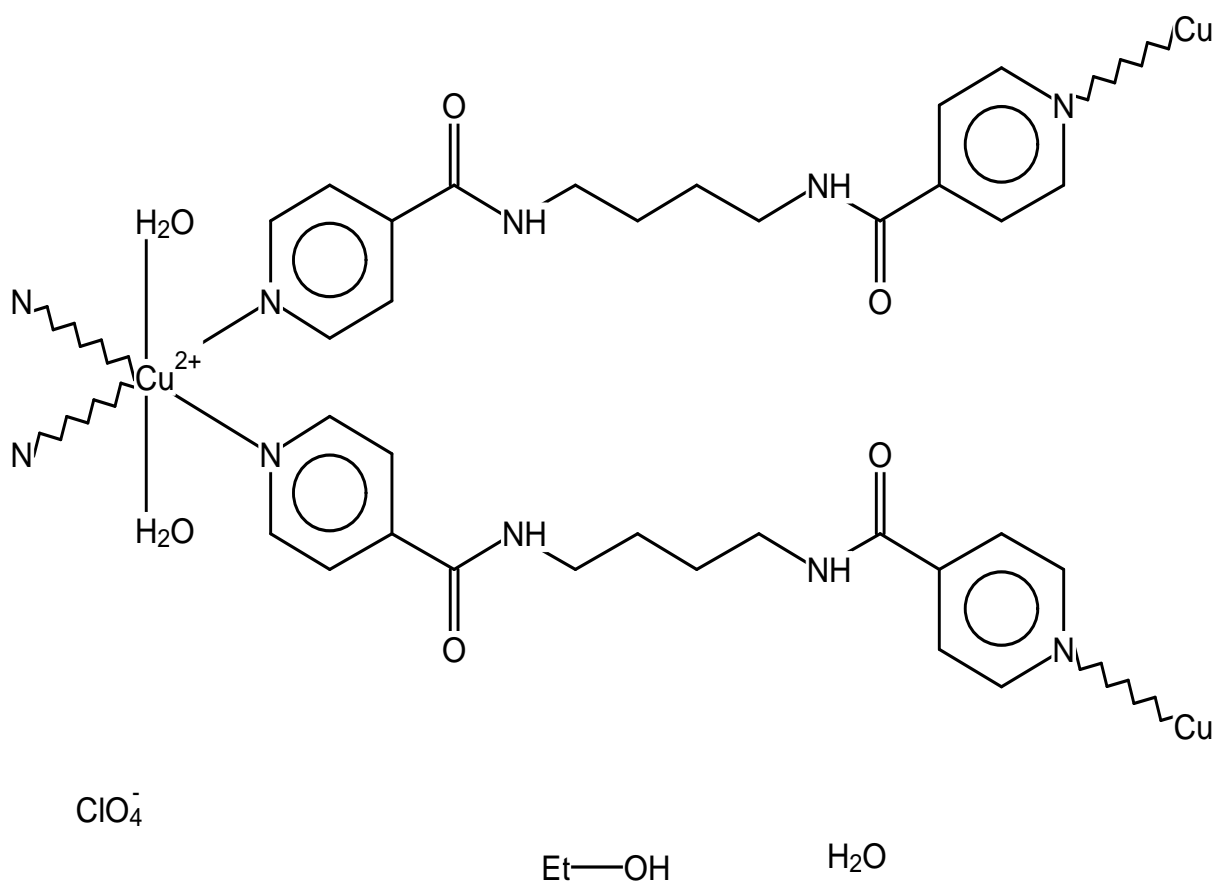
**Reference:** M.Sarkar, K.Biradha (2006) *Cryst.Growth Des.* ,6,1742

**Formula:**  $(C_{32} H_{40} Cu_1 N_8 O_6^{2+})_n, 2n(Cl_1 O_4^{1-}), n(C_2 H_6 O_1), n(H_2 O_1)$

**Compound Name:** catena-(bis( $\mu_2$ -N,N'-bis(4-Pyridylcarbonyl)butane-1,4-diamine-N'',N''')-diaqua-copper(ii) diperchlorate ethanol solvate monohydrate)

**Space Group:** P31      **Cell:**      **a** 17.943(3)      **b** 17.943(3)      **c** 13.252(3)  
**Space Group No.:** 144      **(Å, °)**       $\alpha$  90.00       $\beta$  90.00       $\gamma$  120.00

**R-Factor (%):** 7.67      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.293



## Search: search8 (Wed Jul 13 08:30:33 2011): Hit 4

### CEMKUB01

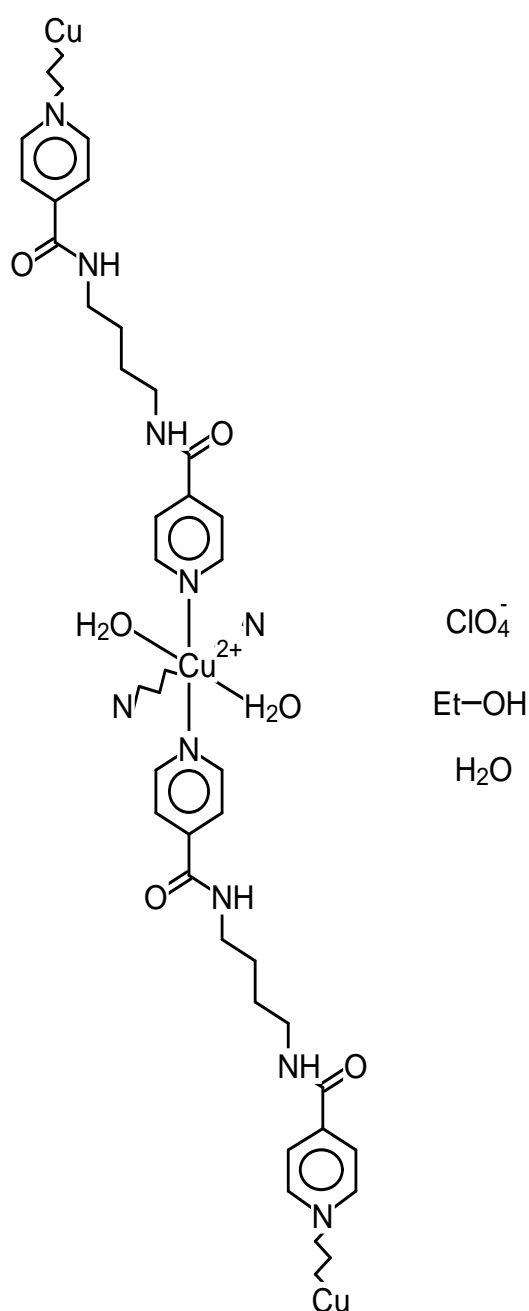
**Reference:** M.Sarkar, K.Biradha (2007) *Cryst.Growth Des.* ,7,1318

**Formula:**  $(C_{32} H_{40} Cu_1 N_8 O_6^{2+})_n, 2n(Cl_1 O_4^{1-}), n(C_2 H_6 O_1), n(H_2 O_1)$

**Compound Name:** catena-(bis( $\mu_2$ -1,4-bis((4-Pyridyl)carbonylamino)butane)-diaqua-copper(ii) diperchlorate ethanol clathrate monohydrate)

**Space Group:** P31      **Cell:**      **a** 17.943(3)      **b** 17.943(3)      **c** 13.252(3)  
**Space Group No.:** 144      **(Å, °)**       $\alpha$  90.00       $\beta$  90.00       $\gamma$  120.00

**R-Factor (%):** 7.67      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.293





## Search: search8 (Wed Jul 13 08:30:33 2011): Hit 5

CEMLAI

**Reference:** M.Sarkar, K.Biradha (2006) *Cryst.Growth Des.* ,6,1742

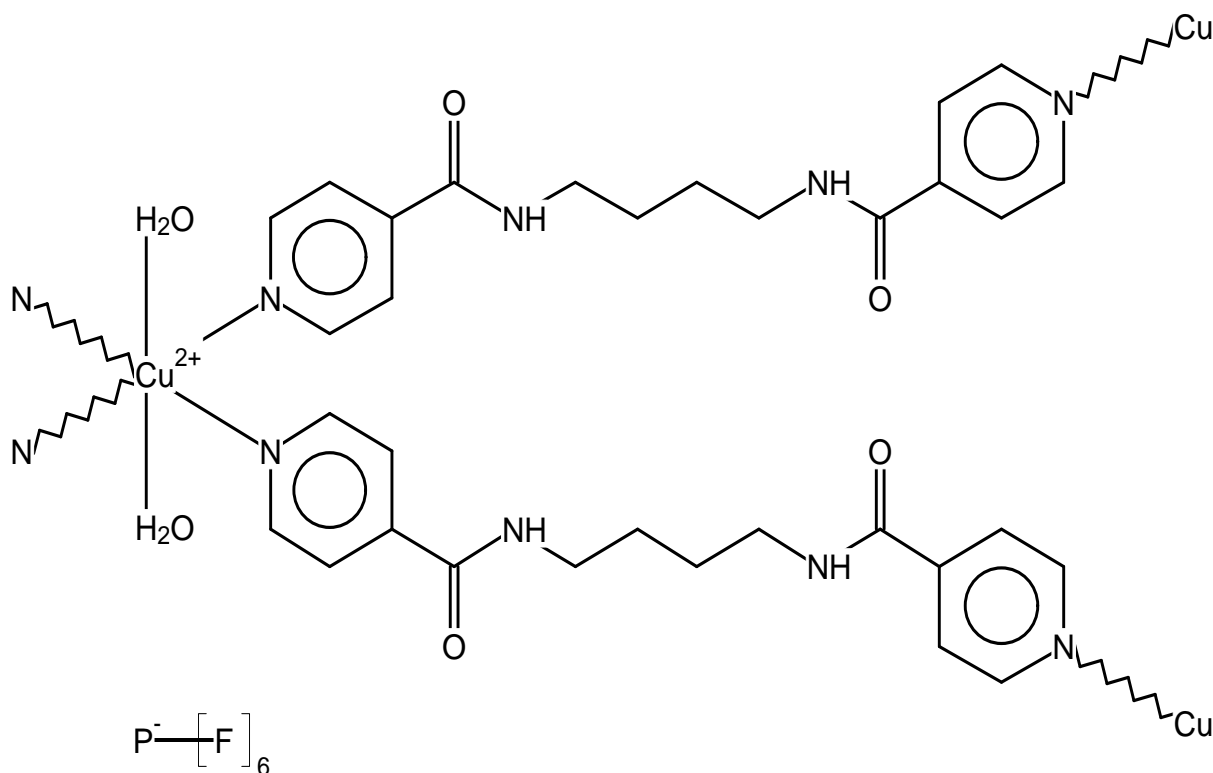
**Formula:**  $(C_{32} H_{40} Cu_1 N_8 O_6^{2+})_n, 2n(F_6 P_1^{1-})$

**Compound Name:** catena-(bis( $\mu_2$ -N,N'-bis(4-Pyridylcarbonyl)butane-1,4-diamine-N'',N''')-diaqua-copper(ii) bis(hexafluorophosphate))

**Space Group:** I-4      **Cell:**    **a** 12.493(1)    **b** 12.493(1)    **c** 31.885(6)

**Space Group No.:** 82      **(Å, °)**     $\alpha$  90.00       $\beta$  90.00       $\gamma$  90.00

**R-Factor (%):** 4.92      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.316



## Search: search8 (Wed Jul 13 08:30:33 2011): Hit 6

CEMLAI01

**Reference:** M.Sarkar, K.Biradha (2007) *Cryst.Growth Des.* ,7,1318

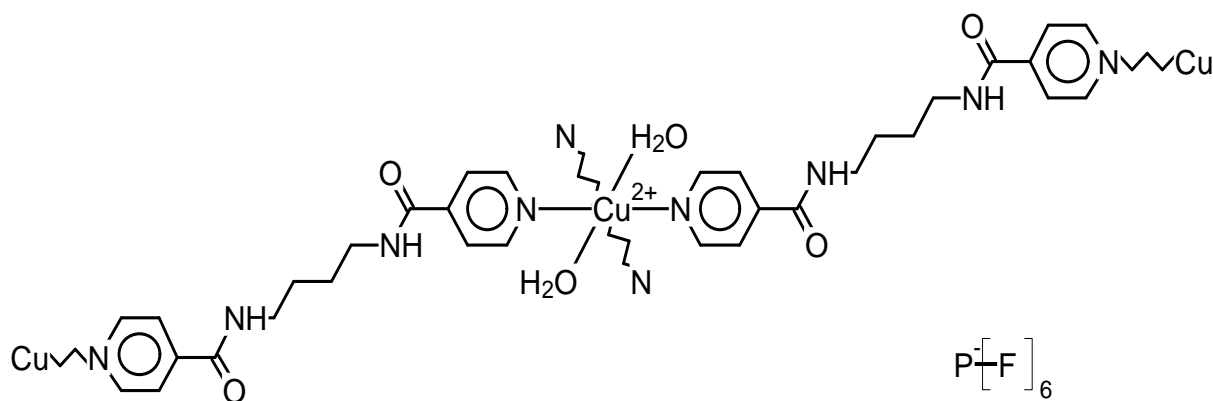
**Formula:**  $(C_{32} H_{40} Cu_1 N_8 O_6^{2+})_n, 2n(F_6 P_1^{1-})$

**Compound Name:** catena-(bis( $\mu_2$ -1,4-bis((4-Pyridyl)carbonylamino)butane)-diaqua-copper(ii) bis(hexafluorophosphate))

**Space Group:** I-4      **Cell:**      **a** 12.493(1)      **b** 12.493(1)      **c** 31.885(6)

**Space Group No.:** 82      **(Å, °)**       $\alpha$  90.00       $\beta$  90.00       $\gamma$  90.00

**R-Factor (%):** 4.92      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.316



## Search Overview

**Search:** search4  
**Date/Time done:** Wed Jul 13 08:18:56 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:** 16

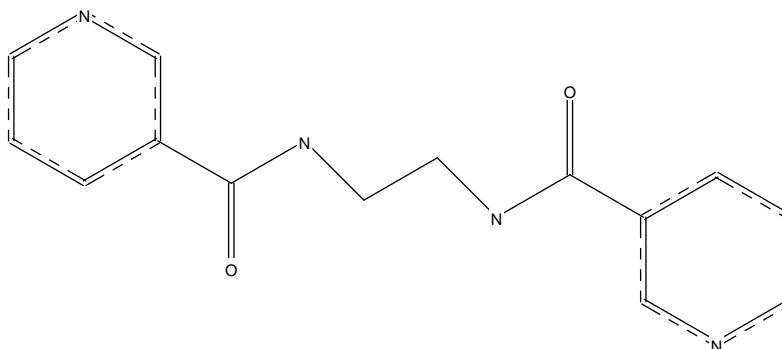
*Summary of queries used. Search found structures that:*

match

**Query 1**

**Query 2**

**Query 1**



**Query 2**

4M

## Search: search4 (Wed Jul 13 08:18:56 2011): Hit 1

ACUQUK

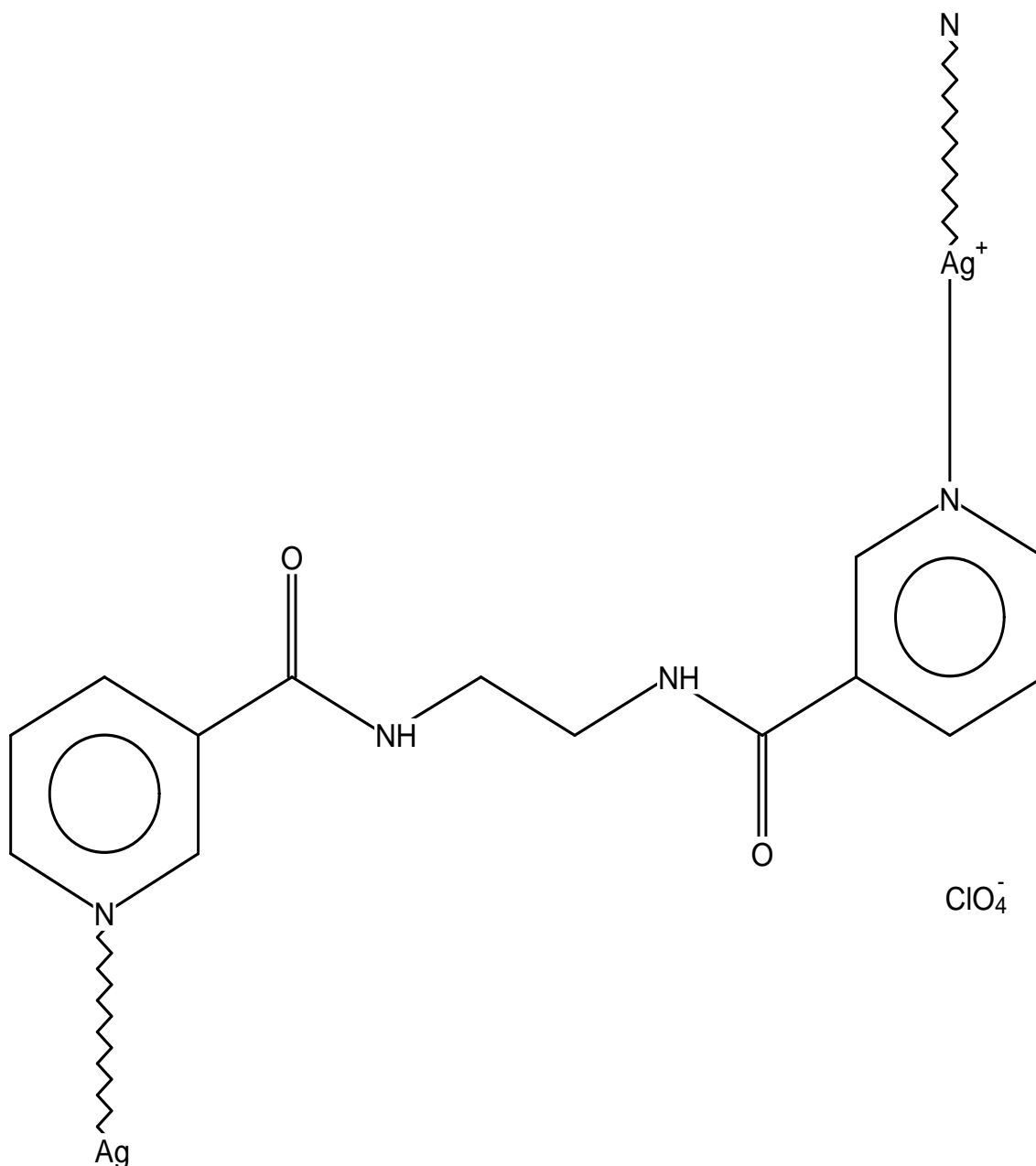
**Reference:** S.Muthu, J.H.K.Yip, J.J.Vittal (2001)  
*J.Chem.Soc.,Dalton Trans.* ,3577

**Formula:** (C<sub>14</sub> H<sub>14</sub> Ag<sub>1</sub> N<sub>4</sub> O<sub>2</sub><sup>1+</sup>)<sub>n</sub>,n(Cl<sub>1</sub> O<sub>4</sub><sup>1-</sup>)

**Compound Name:** catena-((μ<sub>2</sub>-1,2-bis((Pyrid-3-yl)carbonylamino)ethane-N,N')-silver(i) perchlorate)

**Space Group:** C2/c      **Cell:**    **a** 24.065(0)    **b** 5.124(0)    **c** 13.928(0)  
**Space Group No.:** 15      **(Å, °)**    **α** 90.00      **β** 110.76(0)    **γ** 90.00

**R-Factor (%):** 2.31      **Temperature(K):** 223      **Density(g/cm<sup>3</sup>):** 1.975



## Search: search4 (Wed Jul 13 08:18:56 2011): Hit 2

ACUQUK01

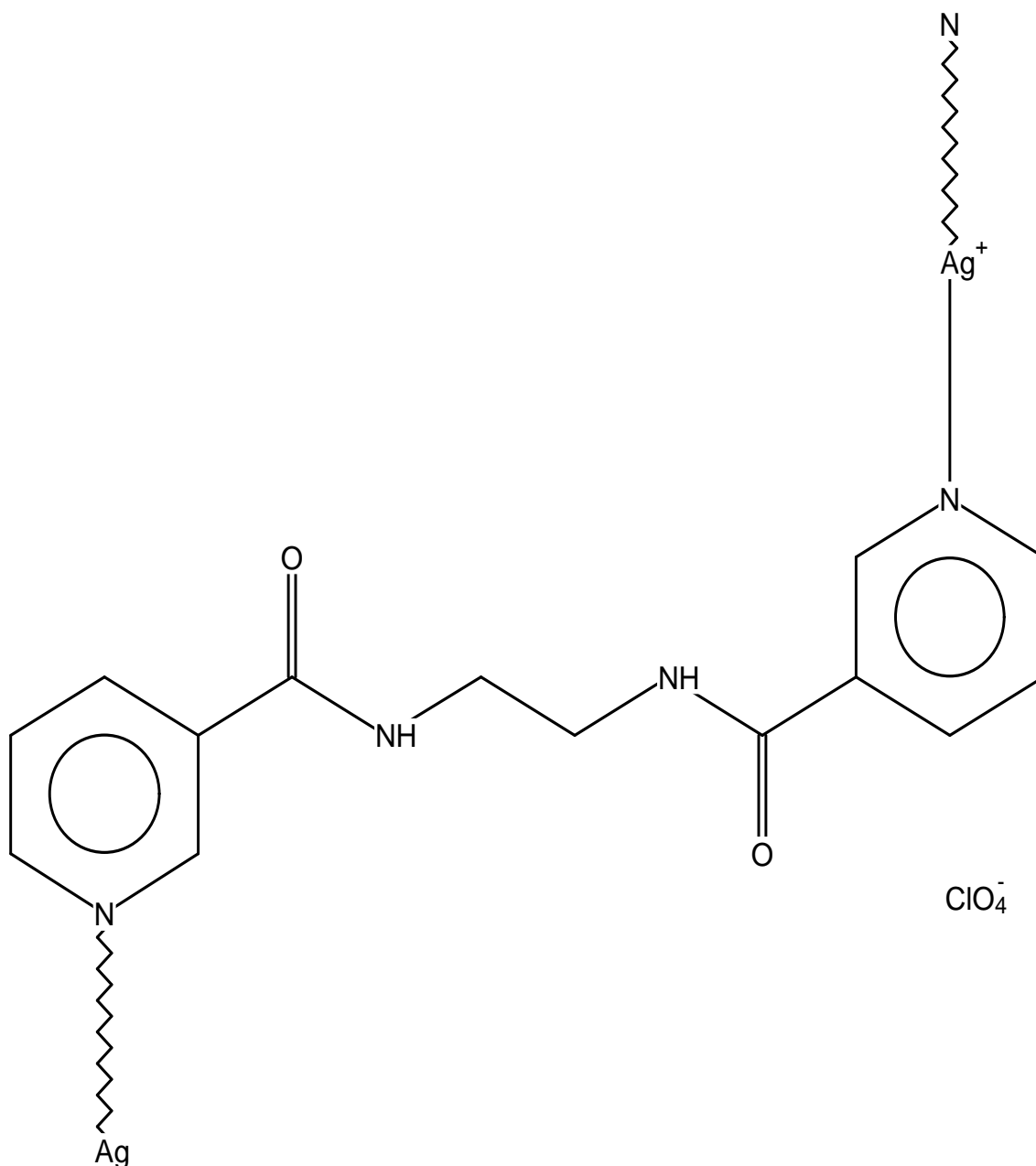
**Reference:** S.Muthu, J.H.K.Yip, J.J.Vittal (2001)  
*J.Chem.Soc.,Dalton Trans.* ,3577

**Formula:** (C<sub>14</sub> H<sub>14</sub> Ag<sub>1</sub> N<sub>4</sub> O<sub>2</sub><sup>1+</sup>)<sub>n</sub>,n(Cl<sub>1</sub> O<sub>4</sub><sup>1-</sup>)

**Compound Name:** catena-((μ<sub>2</sub>-1,2-bis((Pyrid-3-yl)carbonylamino)ethane-N,N')-silver(i) perchlorate)

**Space Group:** C2/c      **Cell:**    **a** 5.113(0)    **b** 13.274(0)    **c** 24.268(0)  
**Space Group No.:** 15      **(Å, °)**    **α** 90.00      **β** 95.28(0)    **γ** 90.00

**R-Factor (%):** 2.53      **Temperature(K):** 223      **Density(g/cm<sup>3</sup>):** 1.934



## Search: search4 (Wed Jul 13 08:18:56 2011): Hit 3

### ACURAR

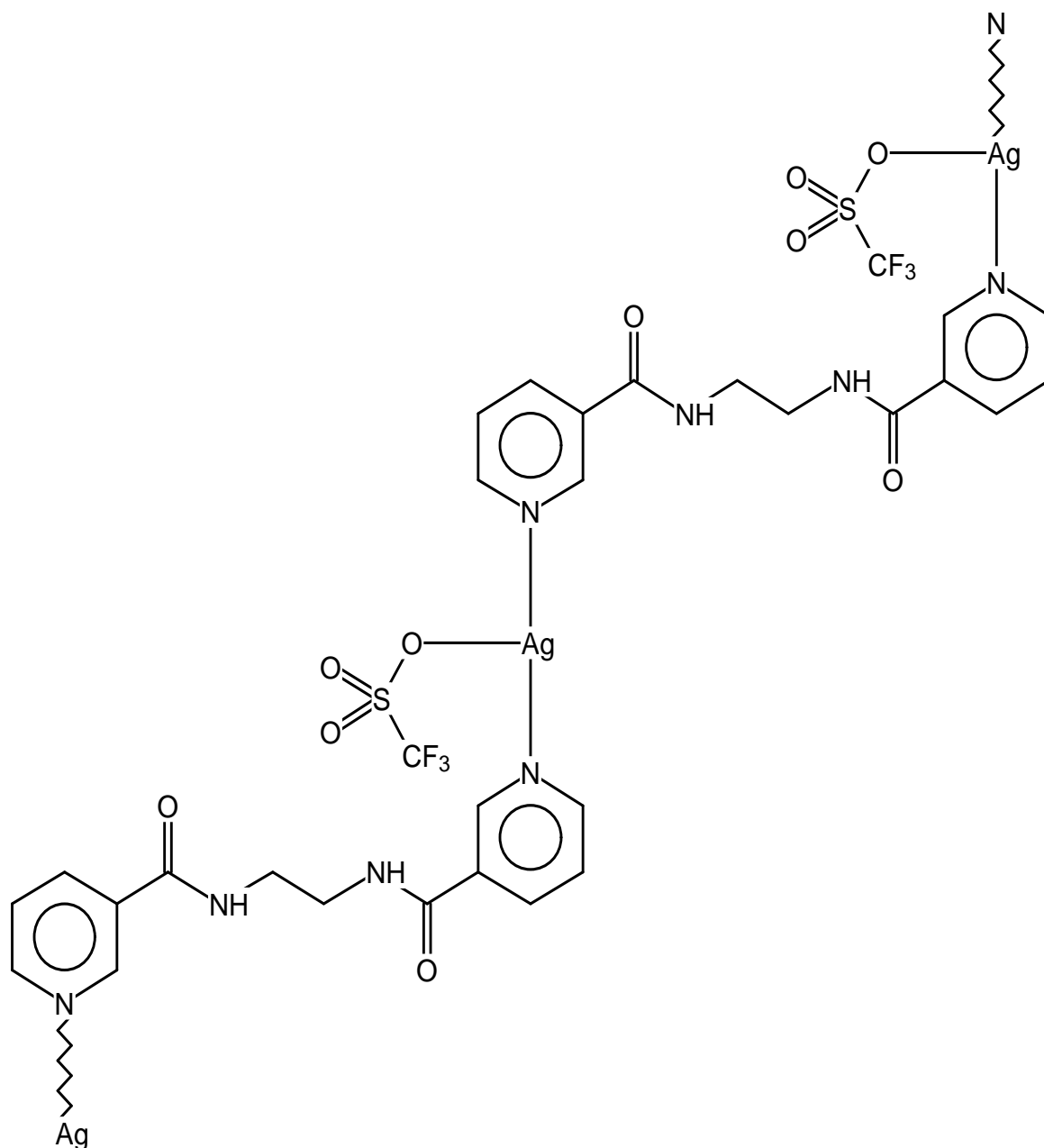
**Reference:** S.Muthu, J.H.K.Yip, J.J.Vittal (2001)  
*J.Chem.Soc.,Dalton Trans.* ,3577

**Formula:** (C<sub>30</sub> H<sub>28</sub> Ag<sub>2</sub> F<sub>6</sub> N<sub>8</sub> O<sub>10</sub> S<sub>2</sub>)<sub>n</sub>

**Compound Name:** catena-(bis(μ<sub>2</sub>-1,2-bis((Pyrid-3-yl)carbonylamino)ethane-N,N')-bis(trifluoromethanesulfonato-O)-di-silver(i))

**Space Group:** P-1      **Cell:**      **a** 9.130(0)      **b** 9.632(0)      **c** 9.865(0)  
**Space Group No.:** 2      **(Å, °)**      **α** 86.83(0)      **β** 87.10(0)      **γ** 89.49(0)

**R-Factor (%):** 2.53      **Temperature(K):** 223      **Density(g/cm<sup>3</sup>):** 2.024



## Search: search4 (Wed Jul 13 08:18:56 2011): Hit 4

### ACUREV

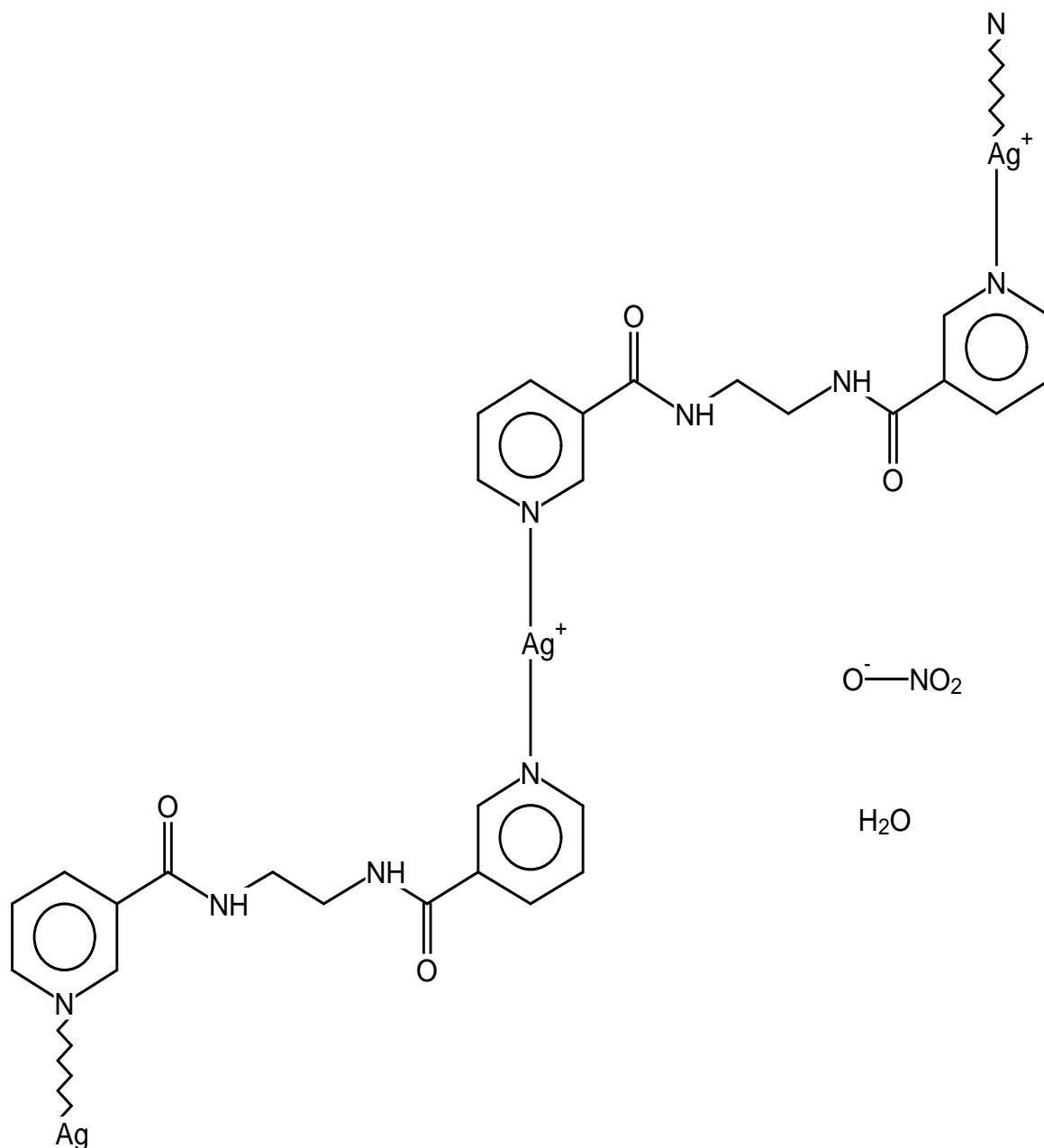
**Reference:** S.Muthu, J.H.K.Yip, J.J.Vittal (2001)  
*J.Chem.Soc.,Dalton Trans.* ,3577

**Formula:**  $(C_{28} H_{28} Ag_2 N_8 O_4^{2+})_n, 2n(N_1 O_3^{1-}), 2.5n(H_2 O_1)$

**Compound Name:** catena-(bis( $\mu_2$ -1,2-bis((Pyrid-3-yl)carbonylamino)ethane-N,N')-di-silver(i) dinitrate hydrate)

**Space Group:** P-1      **Cell:**    **a** 9.086(0)    **b** 9.562(0)    **c** 10.184(0)  
**Space Group No.:** 2      **(Å, °)**     $\alpha$  92.61(0)     $\beta$  98.04(0)     $\gamma$  97.39(0)

**R-Factor (%):** 2.62      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.772



## Search: search4 (Wed Jul 13 08:18:56 2011): Hit 5

### ACURIZ

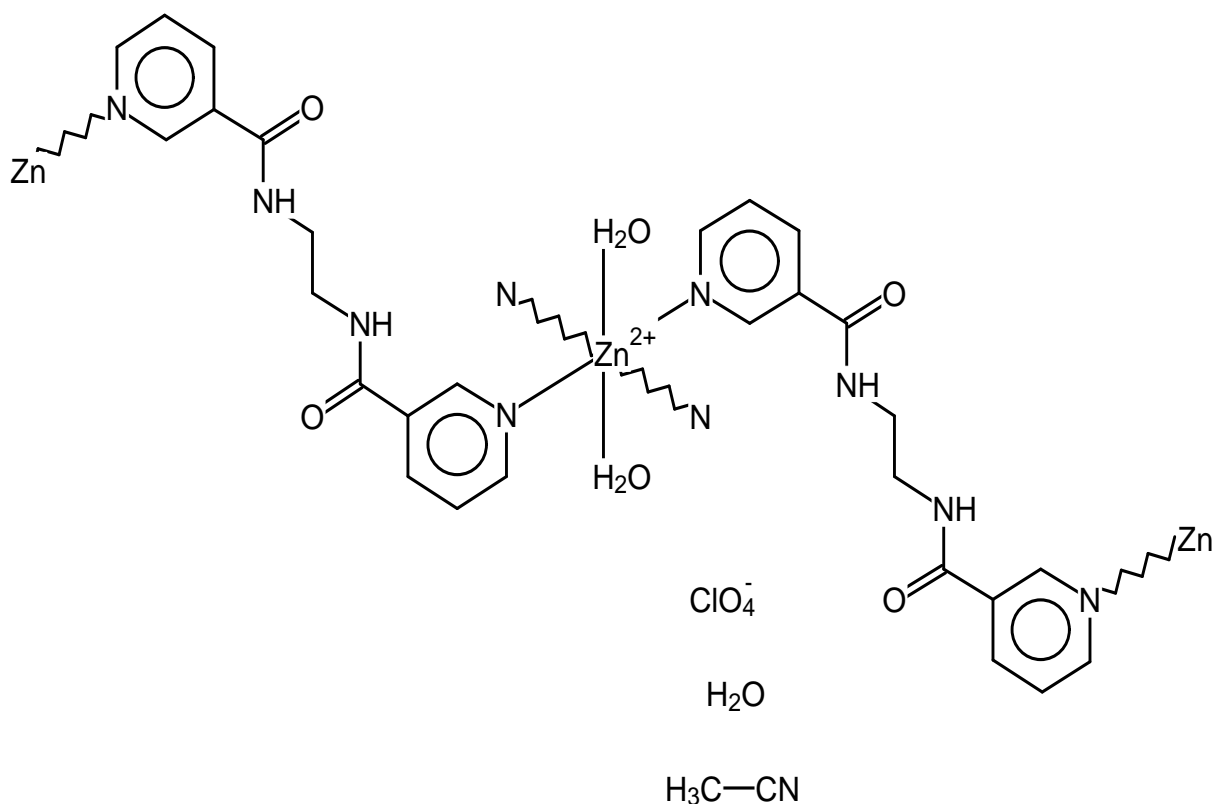
**Reference:** S.Muthu, J.H.K.Yip, J.J.Vittal (2001)  
*J.Chem.Soc.,Dalton Trans.* ,3577

**Formula:**  $(C_{28} H_{32} N_8 O_6 Zn_1^{2+})n, 2n(Cl_1 O_4^{1-}), n(C_2 H_3 N_1), 2n(H_2 O_1)$

**Compound Name:** catena-(trans-bis( $\mu_2$ -1,2-bis((Pyrid-3-yl)carbonylamino)ethane-N,N')-diaqua-zinc(ii) diperchlorate acetonitrile solvate dihydrate)

<b>Space Group:</b>	P-1	<b>Cell:</b>	<b>a</b> 7.854(0)	<b>b</b> 12.209(0)	<b>c</b> 12.386(0)
<b>Space Group No.:</b>	2	(Å, °)	$\alpha$ 64.59(0)	$\beta$ 77.10(0)	$\gamma$ 80.06(0)

<b>R-Factor (%):</b>	6.46	<b>Temperature(K):</b>	243	<b>Density(g/cm<sup>3</sup>):</b>	1.463
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## Search: search4 (Wed Jul 13 08:18:56 2011): Hit 6

### ACUROF

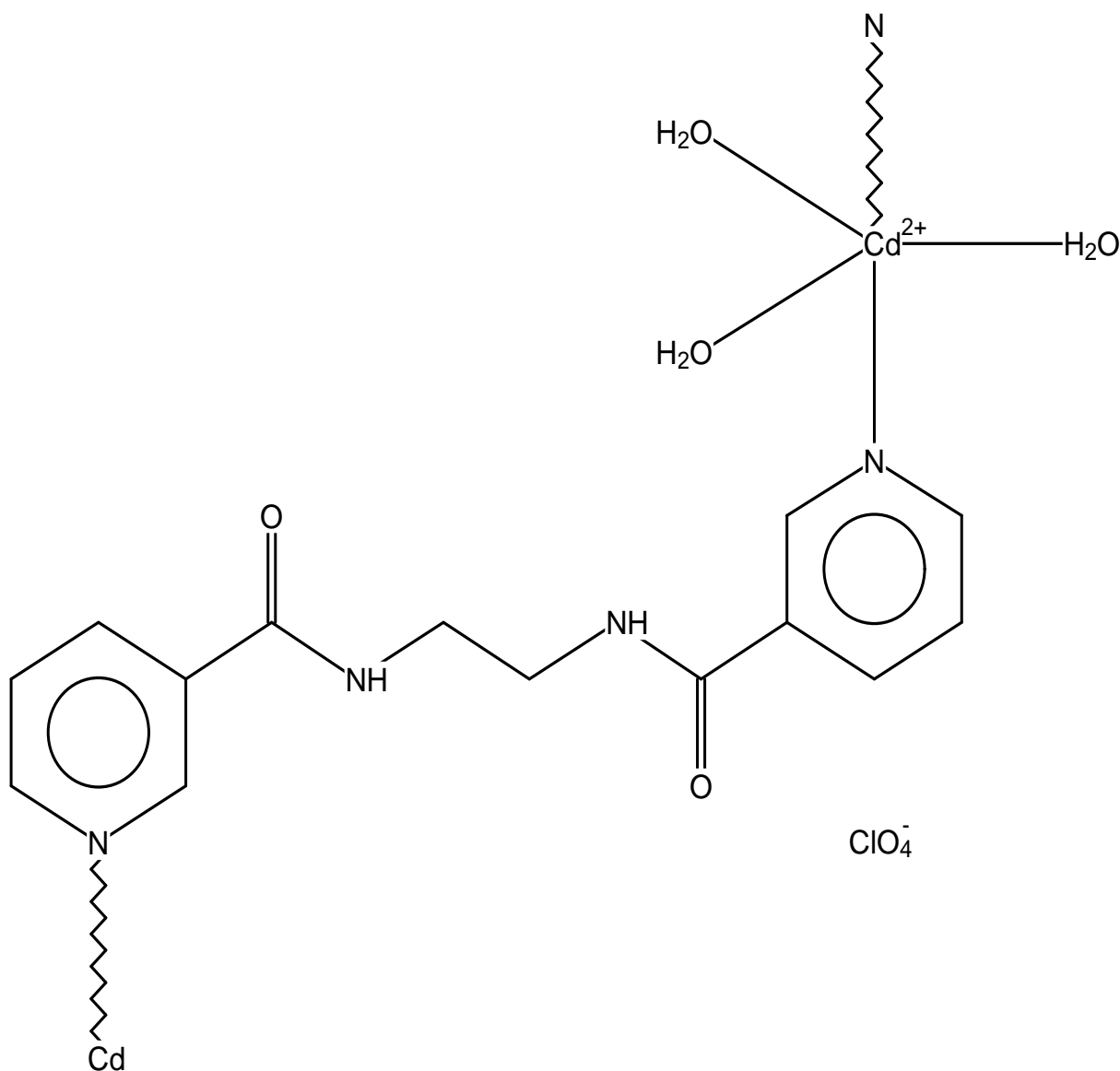
**Reference:** S.Muthu, J.H.K.Yip, J.J.Vittal (2001)  
*J.Chem.Soc.,Dalton Trans.* ,3577

**Formula:**  $(C_{14}H_{20}Cd_1N_4O_5^{2+})_n, 2n(Cl_1O_4^{1-})$

**Compound Name:** catena-(( $\mu_2$ -1,2-bis((Pyrid-3-yl)carbonylamino)ethane-N,N')-triaqua-cadmium(ii) diperchlorate)

**Space Group:** C2/c      **Cell:**    **a** 17.835(1)    **b** 7.537(0)    **c** 17.166(1)  
**Space Group No.:** 15      **(Å, °)**     $\alpha$  90.00       $\beta$  112.49(0)     $\gamma$  90.00

**R-Factor (%):** 4.89      **Temperature(K):** 223      **Density(g/cm<sup>3</sup>):** 1.980



## Search: search4 (Wed Jul 13 08:18:56 2011): Hit 7

### DIKHUB

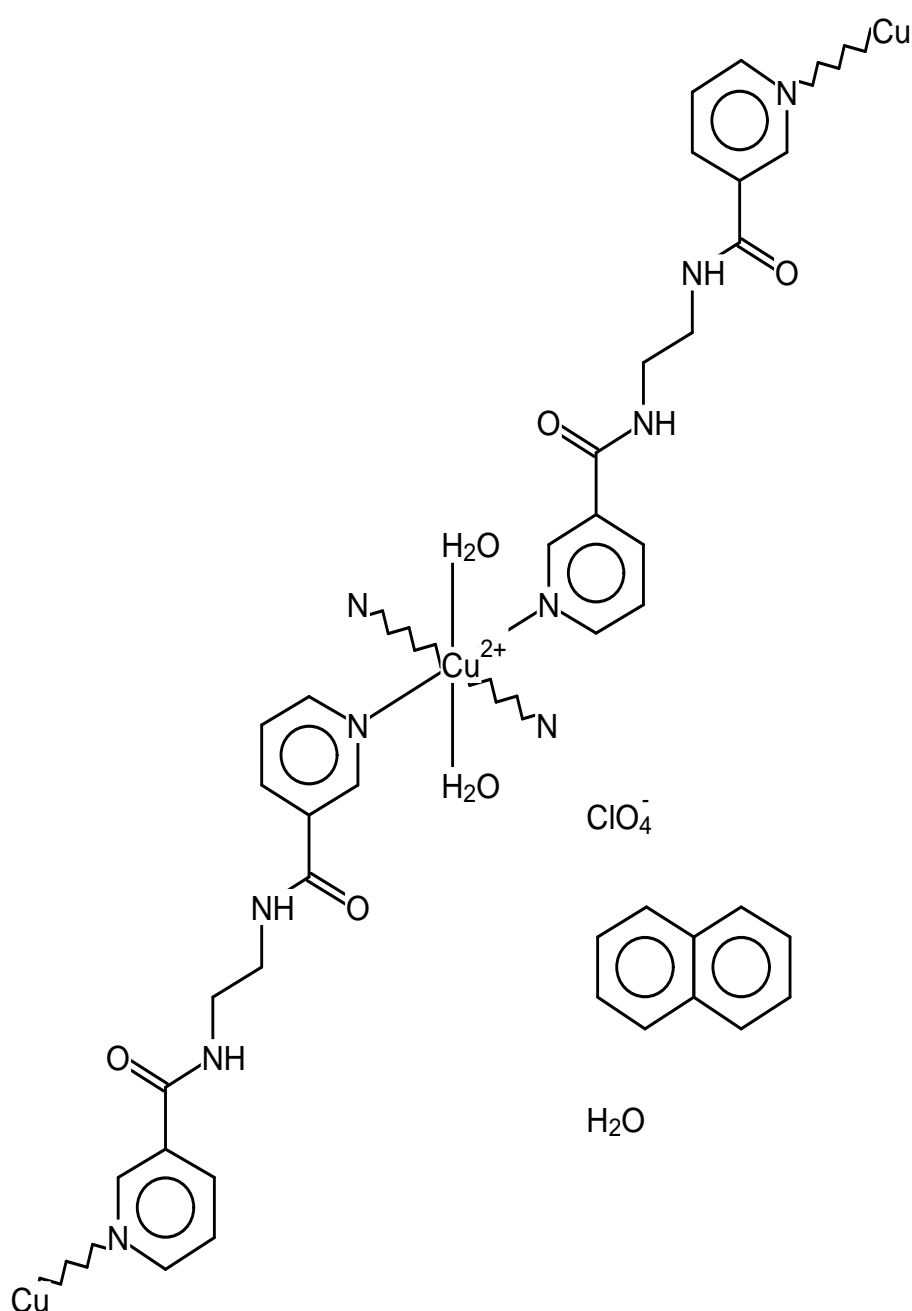
**Reference:** M.Sarkar, K.Biradha (2007) *Cryst.Growth Des.* ,7,1318

**Formula:**  $(C_{28} H_{32} Cu_1 N_8 O_6^{2+})_n, 2n(Cl_1 O_4^{1-}), n(C_{10} H_8), 2n(H_2 O_1)$

**Compound Name:** catena-(bis( $\mu_2$ -1,2-bis((3-Pyridyl)carbonylamino)ethane)-diaqua-copper(ii) doperchlorate naphthalene clathrate dihydrate)

**Space Group:** P-1      **Cell:**      **a** 8.019(1)      **b** 11.857(2)      **c** 12.088(2)  
**Space Group No.:** 2      **(Å, °)**       $\alpha$  70.49(3)       $\beta$  80.08(3)       $\gamma$  81.30(3)

**R-Factor (%):** 5.62      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.569



## Search: search4 (Wed Jul 13 08:18:56 2011): Hit 8

DIKJAJ

**Reference:** M.Sarkar, K.Biradha (2007) *Cryst.Growth Des.* ,7,1318

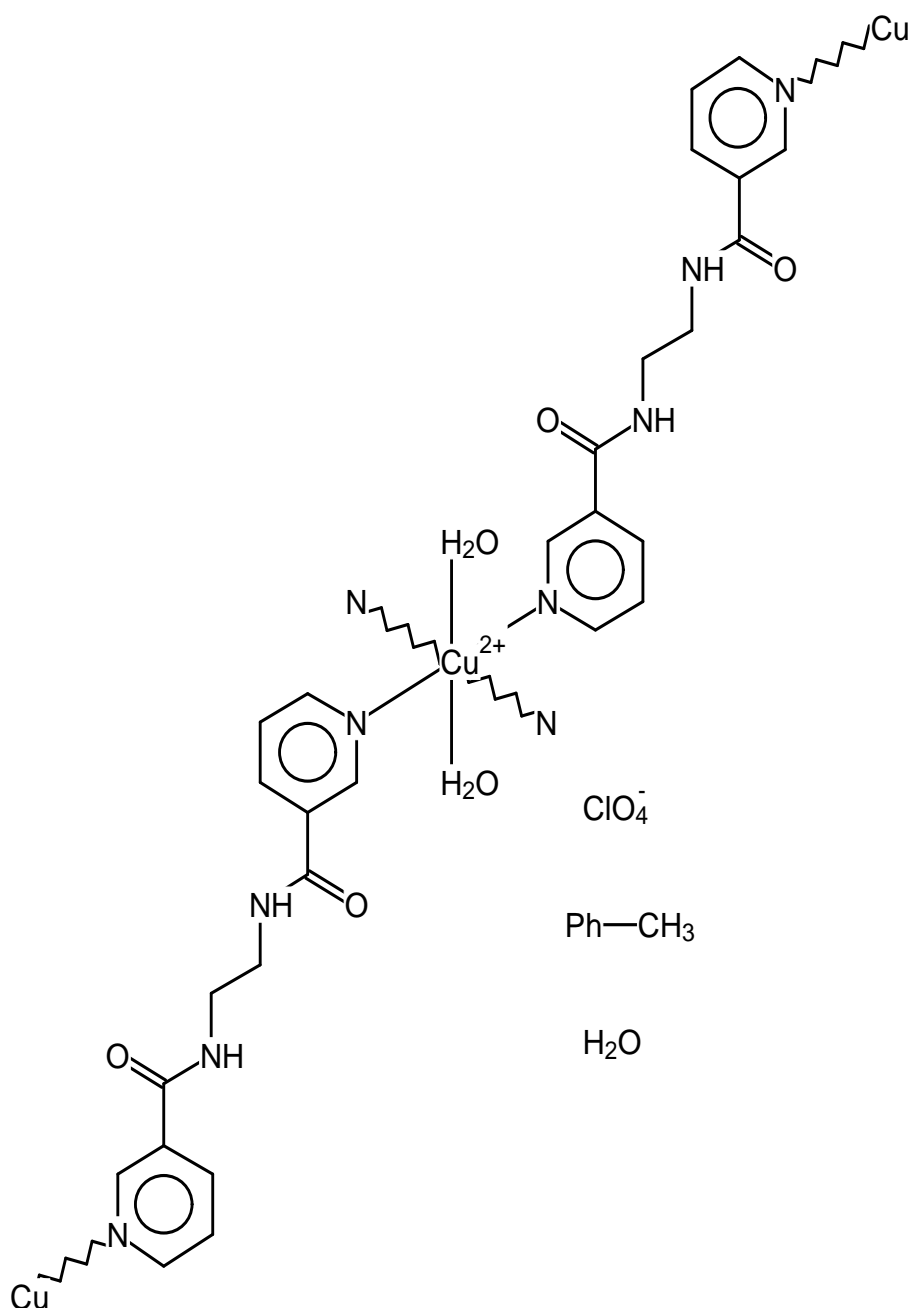
**Formula:**  $(C_{28} H_{32} Cu_1 N_8 O_6^{2+})_n, 2n(Cl_1 O_4^{1-}), n(C_7 H_8), 2n(H_2 O_1)$

**Compound Name:** catena-(bis( $\mu_2$ -1,2-bis((3-Pyridyl)carbonylamino)ethane)-diaqua-copper(ii) diperchlorate toluene clathrate dihydrate)

**Space Group:** P-1      **Cell:**      **a** 7.949(1)      **b** 12.001(2)      **c** 12.050(2)

**Space Group No.:** 2      **(Å, °)**       $\alpha$  68.69(3)       $\beta$  79.83(3)       $\gamma$  80.23(3)

**R-Factor (%):** 6.95      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.534



## Search: search4 (Wed Jul 13 08:18:56 2011): Hit 9

DIKJUD

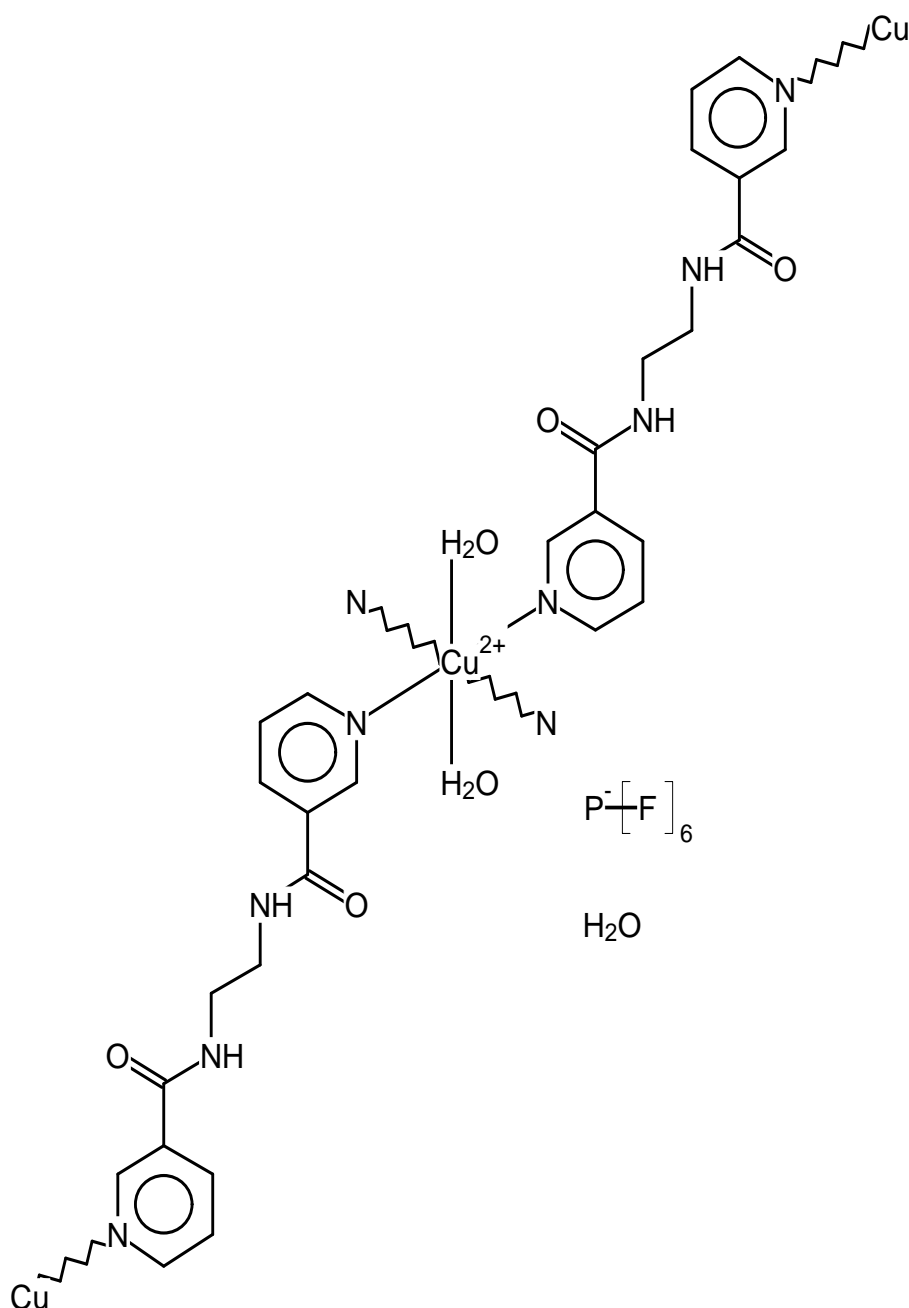
**Reference:** M.Sarkar, K.Biradha (2007) *Cryst.Growth Des.* ,7,1318

**Formula:**  $(C_{28} H_{32} Cu_1 N_8 O_6^{2+})_n, 2n(F_6 P_1^{-1}), n(H_2 O_1)$

**Compound Name:** catena-(bis( $\mu_2$ -1,2-bis((3-Pyridyl)carbonylamino)ethane)-diaqua-copper(ii) bis(hexafluorophosphate) monohydrate)

**Space Group:** Pca21      **Cell:**      **a** 21.296(4)      **b** 9.382(1)      **c** 18.803(4)  
**Space Group No.:** 29      **(Å, °)**       $\alpha$  90.00       $\beta$  90.00       $\gamma$  90.00

**R-Factor (%):** 8.27      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.676



## Search: search4 (Wed Jul 13 08:18:56 2011): Hit 10

### MIXMUC

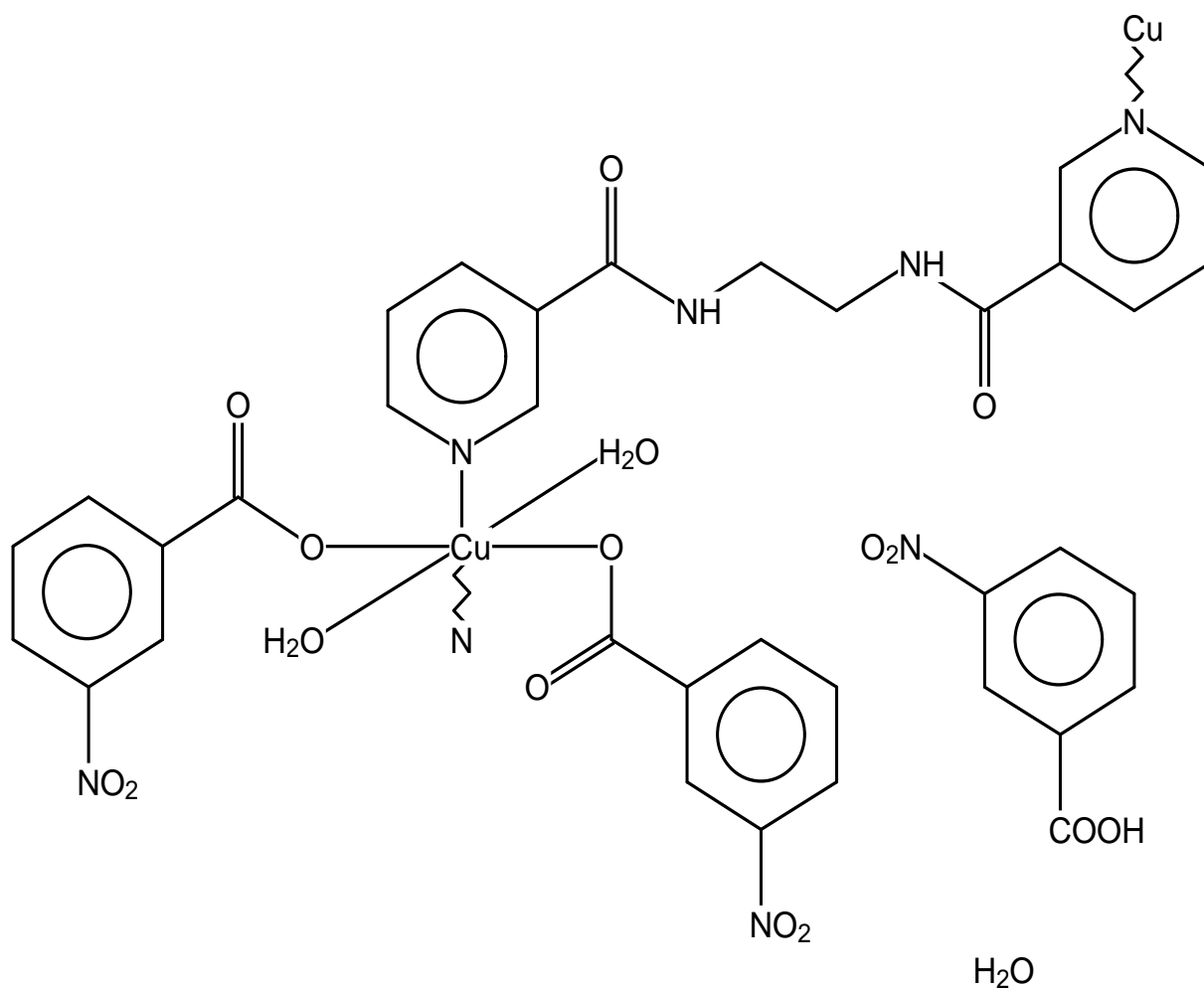
**Reference:** L.Rajput, K.Biradha (2008) *Polyhedron* ,**27**,1248

**Formula:** (C<sub>28</sub> H<sub>26</sub> Cu<sub>1</sub> N<sub>6</sub> O<sub>12</sub>)<sub>n</sub>,n(C<sub>7</sub> H<sub>5</sub> N<sub>1</sub> O<sub>4</sub>),2n(H<sub>2</sub> O<sub>1</sub>)

**Compound Name:** catena-((μ<sub>2</sub>-1,2-bis(3-Pyridinecarboxamido)ethane-N,N')-diaqua-bis(3-nitrobenzoato-O)-copper(ii) 3-nitrobenzoic acid dihydrate clathrate)

**Space Group:** P-1      **Cell:**      **a** 8.653(1)      **b** 11.355(2)      **c** 11.945(2)  
**Space Group No.:** 2      **(Å, °)**      α 111.36(3)      β 102.79(3)      γ 100.55(3)

**R-Factor (%):** 7.57      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.474



## Search: search4 (Wed Jul 13 08:18:56 2011): Hit 11

### MIXNIR

**Reference:** L.Rajput, K.Biradha (2008) *Polyhedron* ,**27**,1248

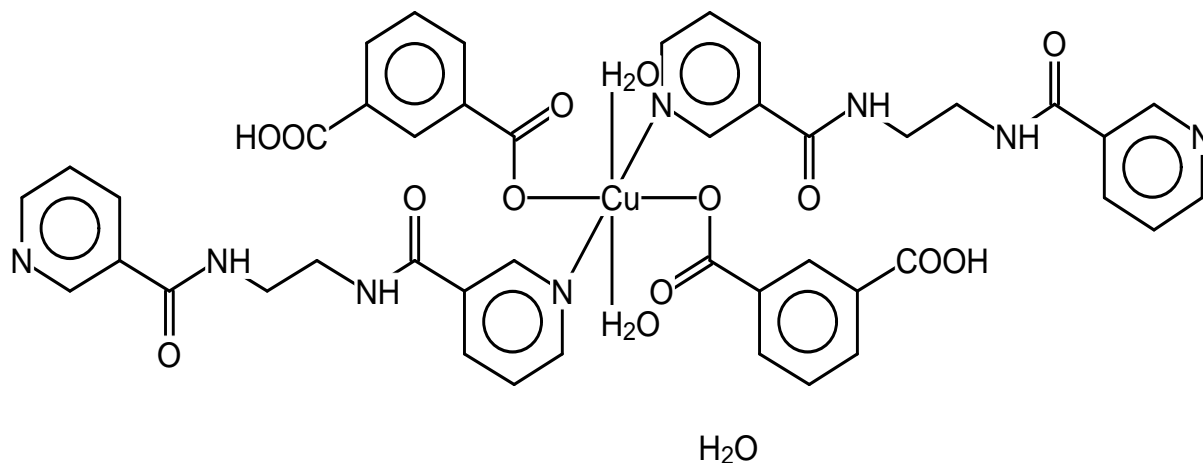
**Formula:** C<sub>44</sub> H<sub>42</sub> Cu<sub>1</sub> N<sub>8</sub> O<sub>14</sub>·4(H<sub>2</sub> O<sub>1</sub>)

**Compound Name:** Diaqua-bis(isophthalato-O)-bis(1,2-bis(3-pyridinecarboxamido)ethane-N)-copper(ii) tetrahydrate

**Space Group:** P-1      **Cell:**      **a** 7.013(1)      **b** 10.660(2)      **c** 16.628(3)

**Space Group No.:** 2      **(Å, °)**      **α** 98.21(3)      **β** 92.96(3)      **γ** 108.14(3)

**R-Factor (%):** 4.97      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.488



## Search: search4 (Wed Jul 13 08:18:56 2011): Hit 12

### MIXNOX

**Reference:** L.Rajput, K.Biradha (2008) *Polyhedron* ,**27**,1248

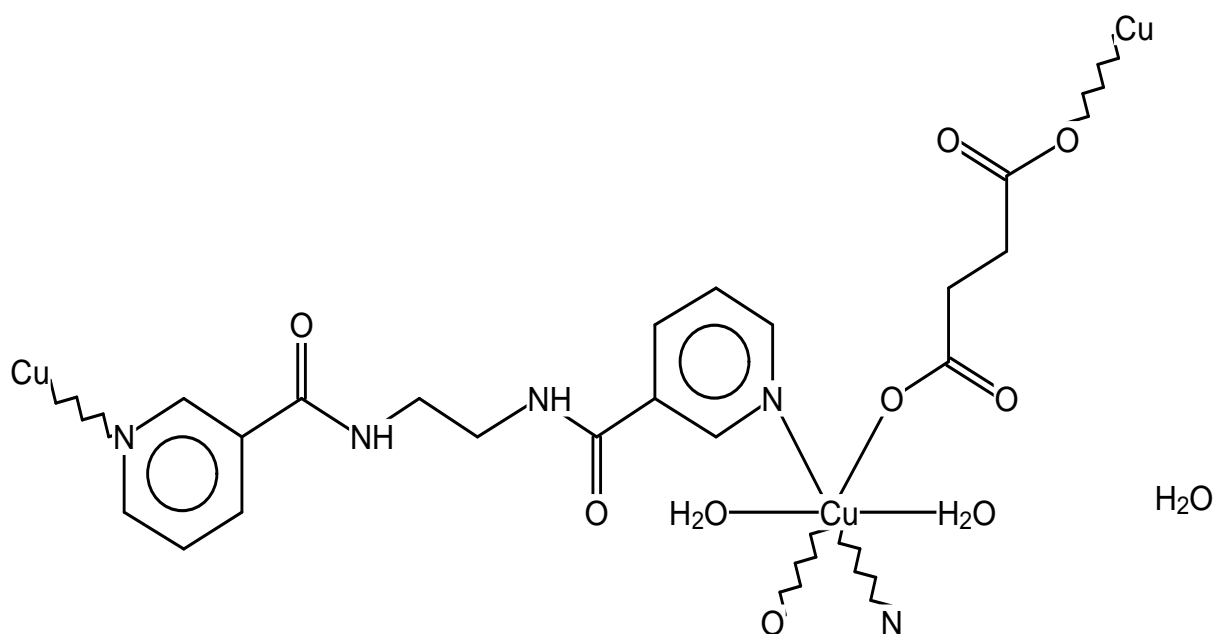
**Formula:** (C<sub>18</sub> H<sub>22</sub> Cu<sub>1</sub> N<sub>4</sub> O<sub>8</sub>)<sub>n</sub>,n(H<sub>2</sub> O<sub>1</sub>)

**Compound Name:** catena-((μ<sub>2</sub>-1,2-bis(3-Pyridinecarboxamido)ethane-N,N')-(μ<sub>2</sub>-succinato-O,O')-diaqua-copper(ii) monohydrate)

**Space Group:** C2/c      **Cell:**      **a** 10.196(2)      **b** 16.435(3)      **c** 12.705(3)

**Space Group No.:** 15      **(Å, °)**      **α** 90.00      **β** 97.14(3)      **γ** 90.00

**R-Factor (%):** 4.97      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.585



## Search: search4 (Wed Jul 13 08:18:56 2011): Hit 13

### SECPUM

**Reference:** M.Sarkar, K.Biradha (2006) *Eur.J.Inorg.Chem.* ,531

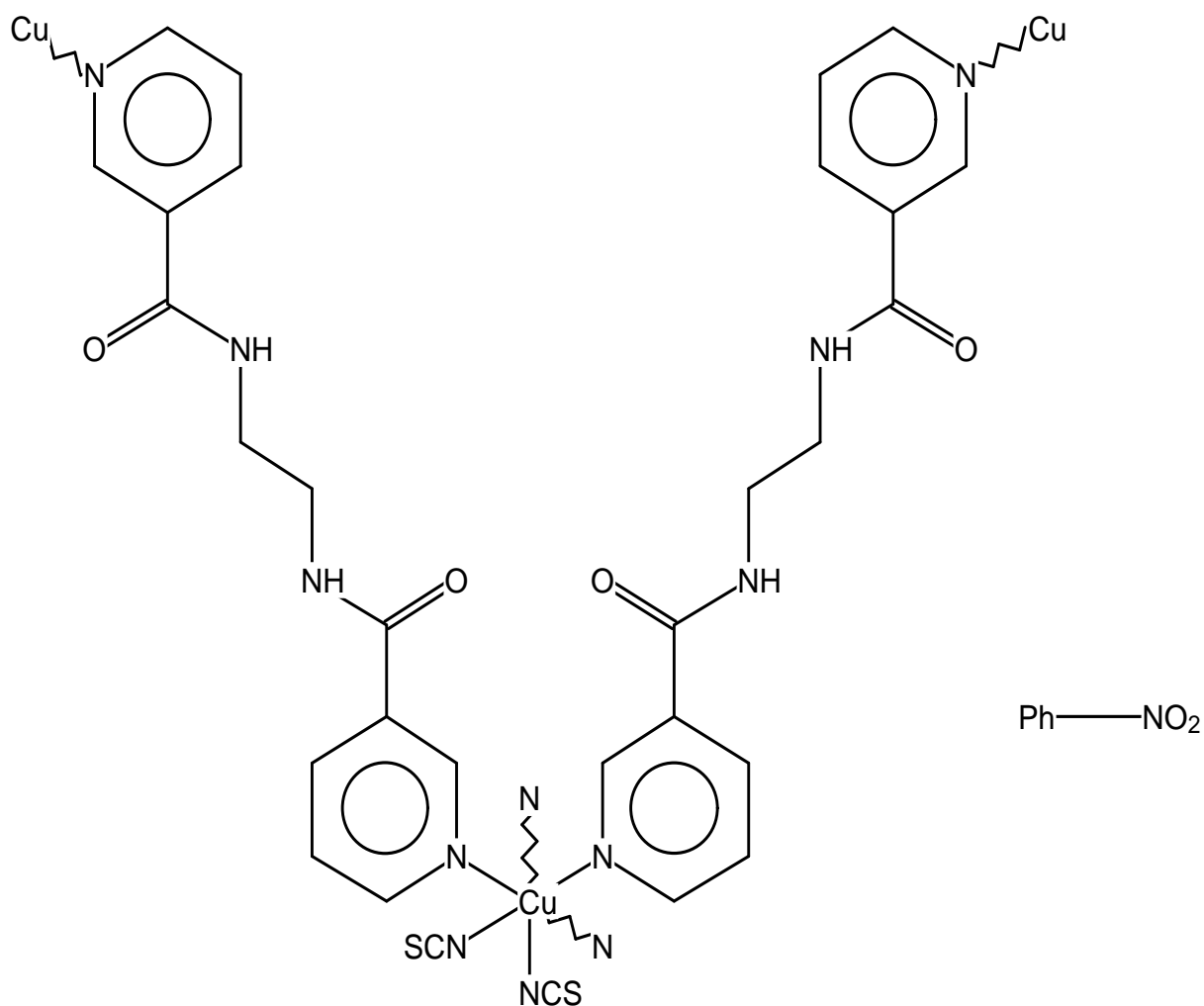
**Formula:**  $(C_{30} H_{28} Cu_1 N_{10} O_4 S_2)_n, 6n(C_6 H_5 N_1 O_2)$

**Compound Name:** catena-(bis(( $\mu_2$ -1,2-bis(3-Pyridinecarboxamido)ethane)-(isothiocyanato))-copper(ii) hexakis(nitrobenzene)clathrate)

**Space Group:** P-1      **Cell:**      **a** 9.967(2)      **b** 12.950(3)      **c** 14.945(3)

**Space Group No.:** 2      **(Å, °)**       $\alpha$  106.90(3)       $\beta$  102.94(3)       $\gamma$  102.11(3)

**R-Factor (%):** 7.78      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.409





## Search: search4 (Wed Jul 13 08:18:56 2011): Hit 14

WANSIO

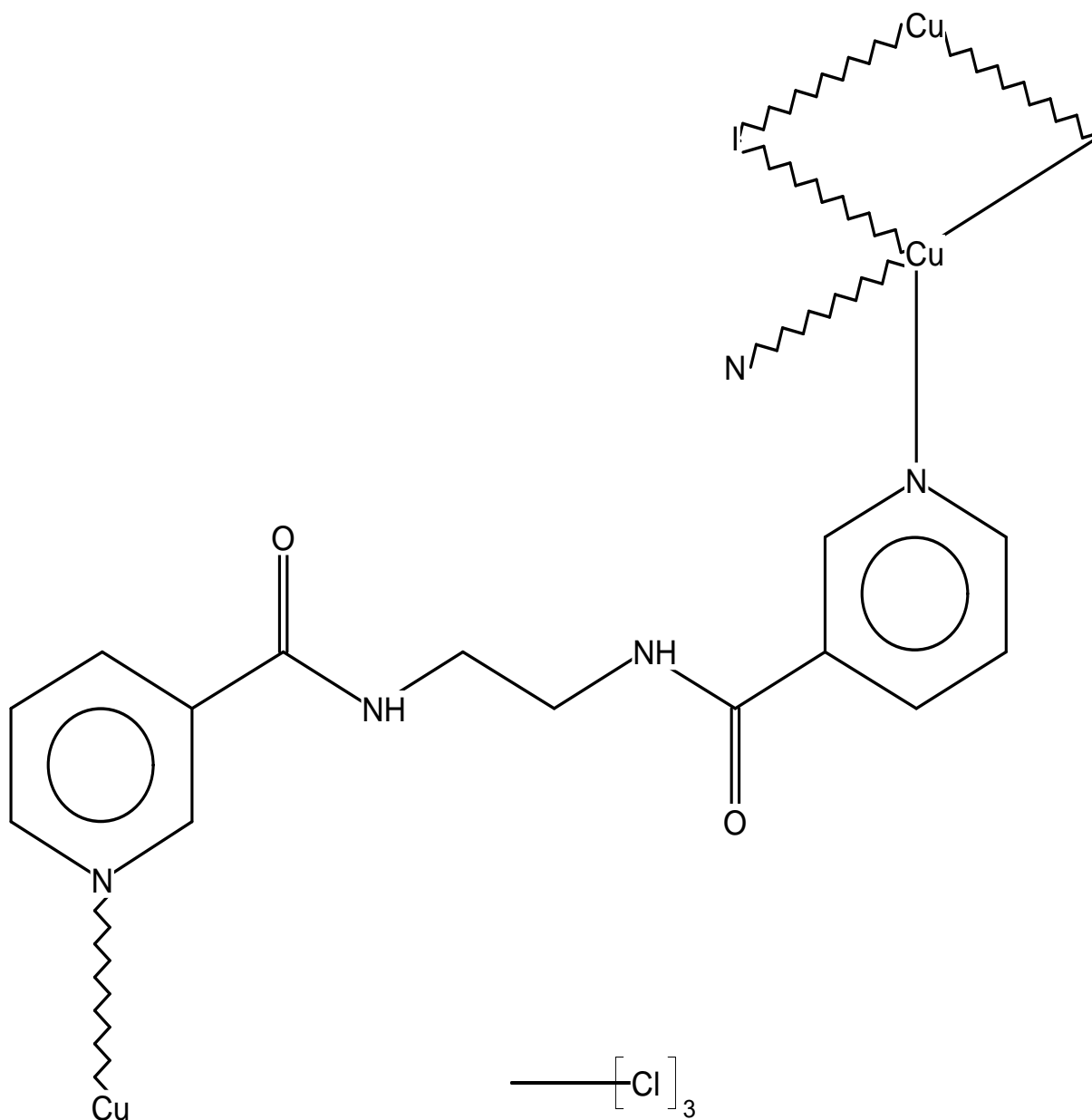
**Reference:** M.Sarkar, K.Biradha (2005) *Chem. Commun.* ,2229

**Formula:**  $(C_{14} H_{14} Cu_1 I_1 N_4 O_2)_n, 1.5n(C_1 H_1 Cl_3)$

**Compound Name:** catena-(( $\mu_2$ -1,2-bis(3-Pyridylcarbonylamino)ethane-N,N')-( $\mu_2$ -iodo)-copper chloroform solvate)

**Space Group:** C2/m      **Cell:**      **a** 9.649(1)      **b** 15.559(3)      **c** 15.163(3)  
**Space Group No.:** 12      **(Å, °)**       $\alpha$  90.00       $\beta$  91.96(3)       $\gamma$  90.00

**R-Factor (%):** 4.85      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.868



## Search: search4 (Wed Jul 13 08:18:56 2011): Hit 15

### WANSOU

**Reference:** M.Sarkar, K.Biradha (2005) *Chem. Commun.* ,2229

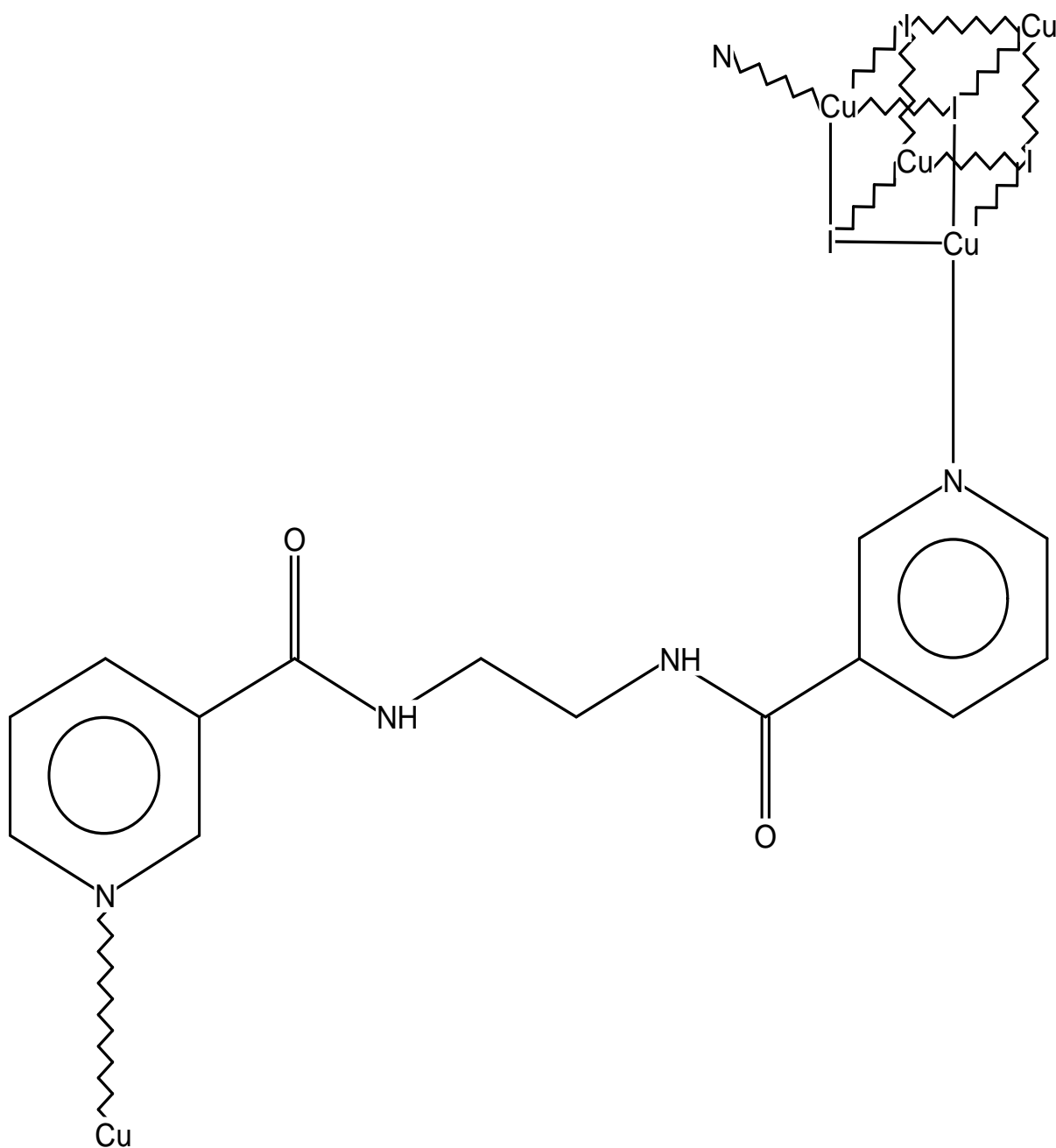
**Formula:**  $(C_{14} H_{14} Cu_2 I_2 N_4 O_2)_n$

**Compound Name:** catena-(bis( $\mu_3$ -Iodo)-( $\mu_2$ -1,2-bis(3-pyridylcarbonylamino)ethane-N,N')-di-copper)

**Space Group:** P2/c      **Cell:**      **a** 11.312(2)      **b** 10.012(2)      **c** 16.597(3)

**Space Group No.:** 13      **( $\text{\AA}$ , °)**       $\alpha$  90.00       $\beta$  97.25(3)       $\gamma$  90.00

**R-Factor (%):** 4.05      **Temperature(K):** 293      **Density( $\text{g/cm}^3$ ):** 2.320



## Search: search4 (Wed Jul 13 08:18:56 2011): Hit 16

### WANSUA

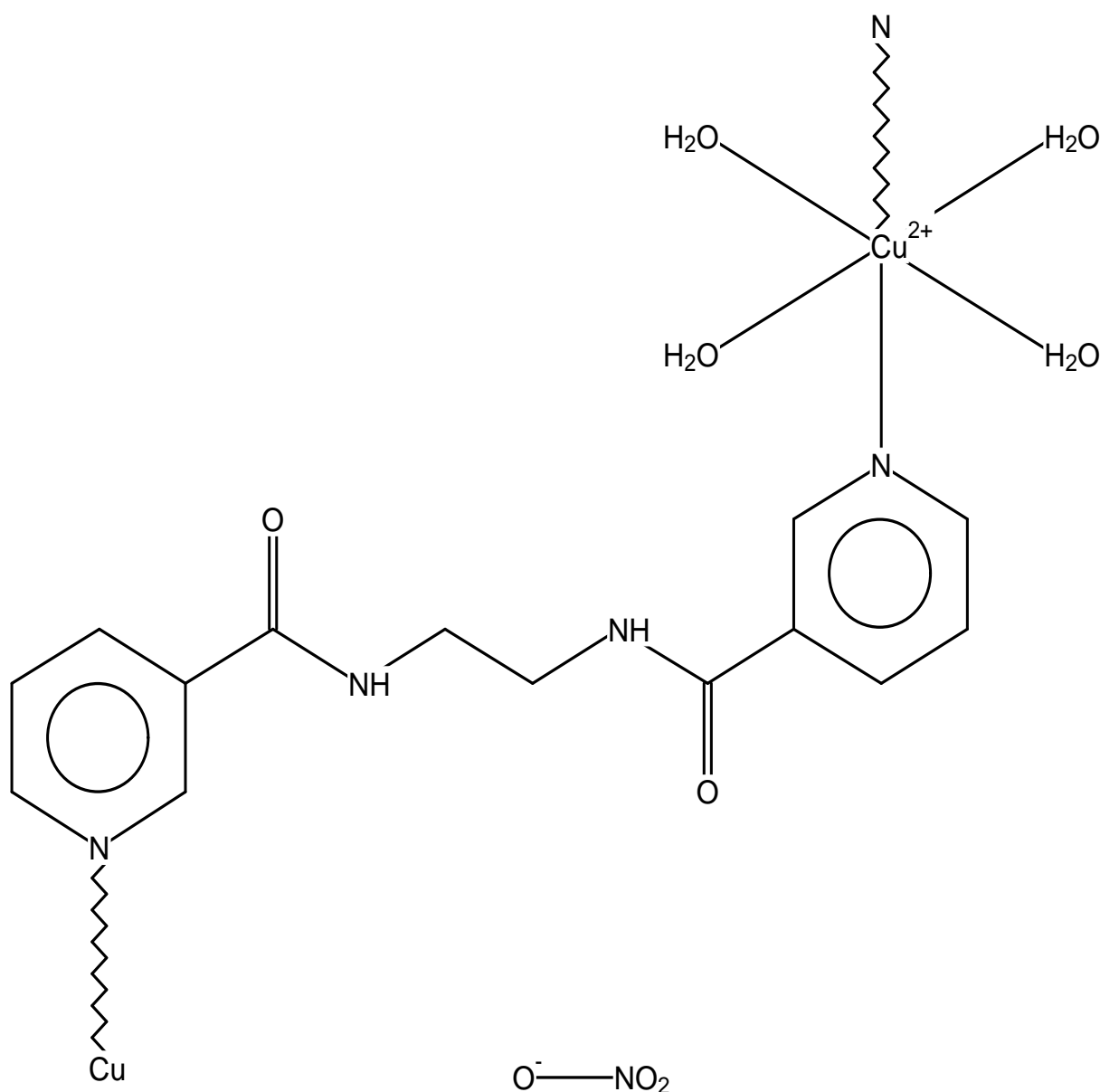
**Reference:** M.Sarkar, K.Biradha (2005) *Chem. Commun.* ,2229

**Formula:**  $(C_{14} H_{22} Cu_1 N_4 O_6^{2+})_n, 2n(N_1 O_3^{1-})$

**Compound Name:** catena-(( $\mu_2$ -1,2-bis(3-Pyridylcarbonylamino)ethane-N,N')-tetra-aqua-copper dinitrate)

**Space Group:** P21/n      **Cell:**      **a** 10.214(2)      **b** 7.125(1)      **c** 14.425(3)  
**Space Group No.:** 14      **(Å, °)**       $\alpha$  90.00       $\beta$  99.98(3)       $\gamma$  90.00

**R-Factor (%):** 4.44      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.702



## Search Overview

**Search:** search9  
**Date/Time done:** Wed Jul 13 08:31:33 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

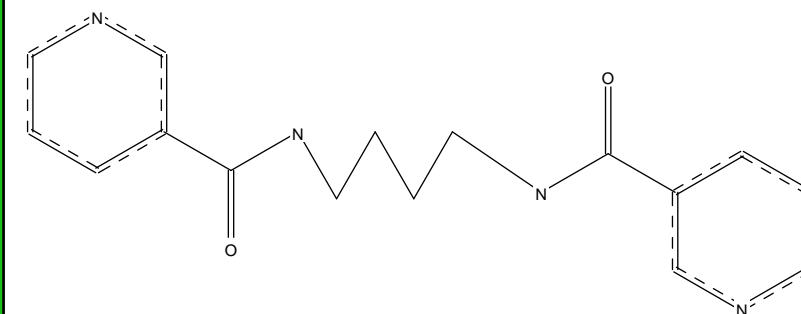
*Summary of queries used. Search found structures that:*

match

**Query 1**

**Query 2**

**Query 1**



**Query 2**

4M

## Search: search9 (Wed Jul 13 08:31:33 2011): Hit 1

### DIKHEL

**Reference:** M.Sarkar, K.Biradha (2007) *Cryst.Growth Des.* ,7,1318

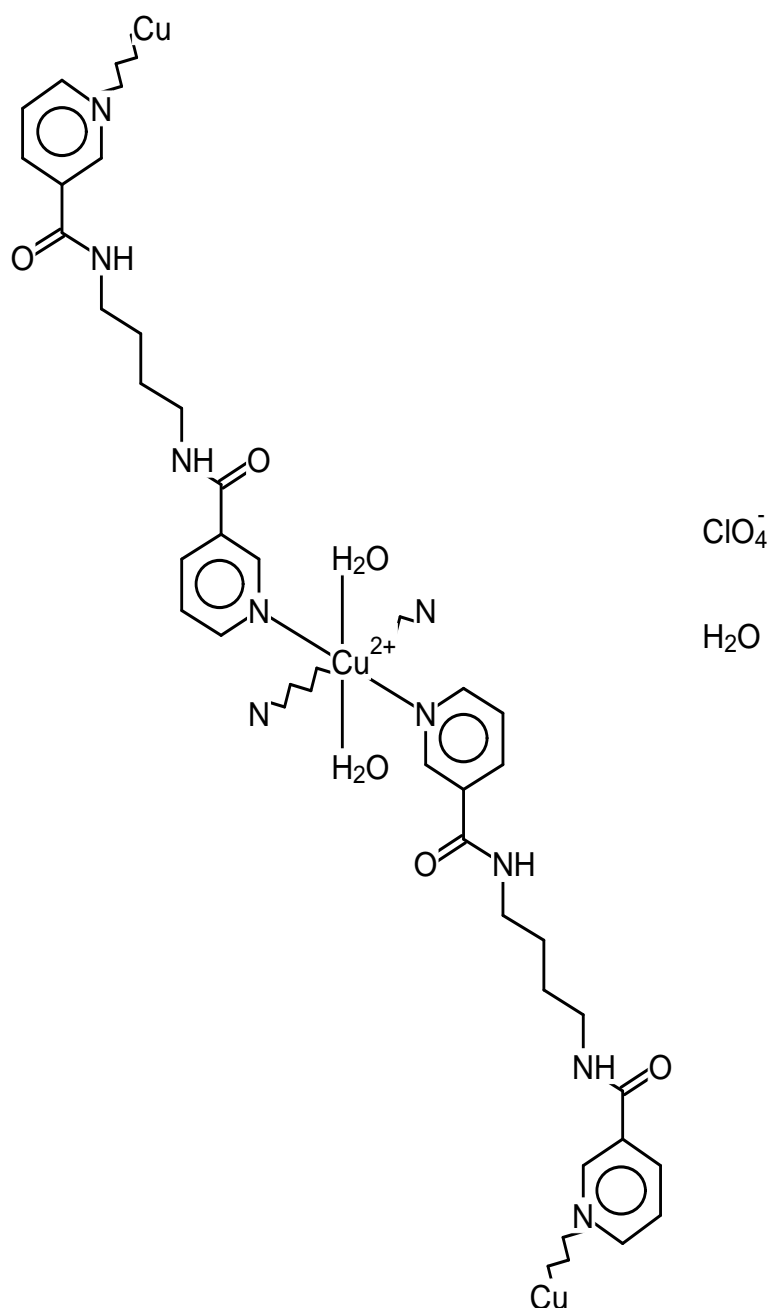
**Formula:**  $(C_{32}H_{40}Cu_1N_8O_6^{2+})_n, 2n(Cl_1O_4^{1-}), 2n(H_2O_1)$

**Compound Name:** catena-(bis( $\mu_2$ -1,4-bis((3-Pyridyl)carbonylamino)butane)-diaqua-copper(ii) diperchlorate dihydrate)

**Space Group:** C2      **Cell:**      **a** 20.770(4)      **b** 9.325(1)      **c** 11.425(2)

**Space Group No.:** 5      **(Å, °)**       $\alpha$  90.00       $\beta$  110.63(3)       $\gamma$  90.00

**R-Factor (%):** 4.94      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.493



## Search: search9 (Wed Jul 13 08:31:33 2011): Hit 2

### DIKHIP

**Reference:** M.Sarkar, K.Biradha (2007) *Cryst.Growth Des.* ,7,1318

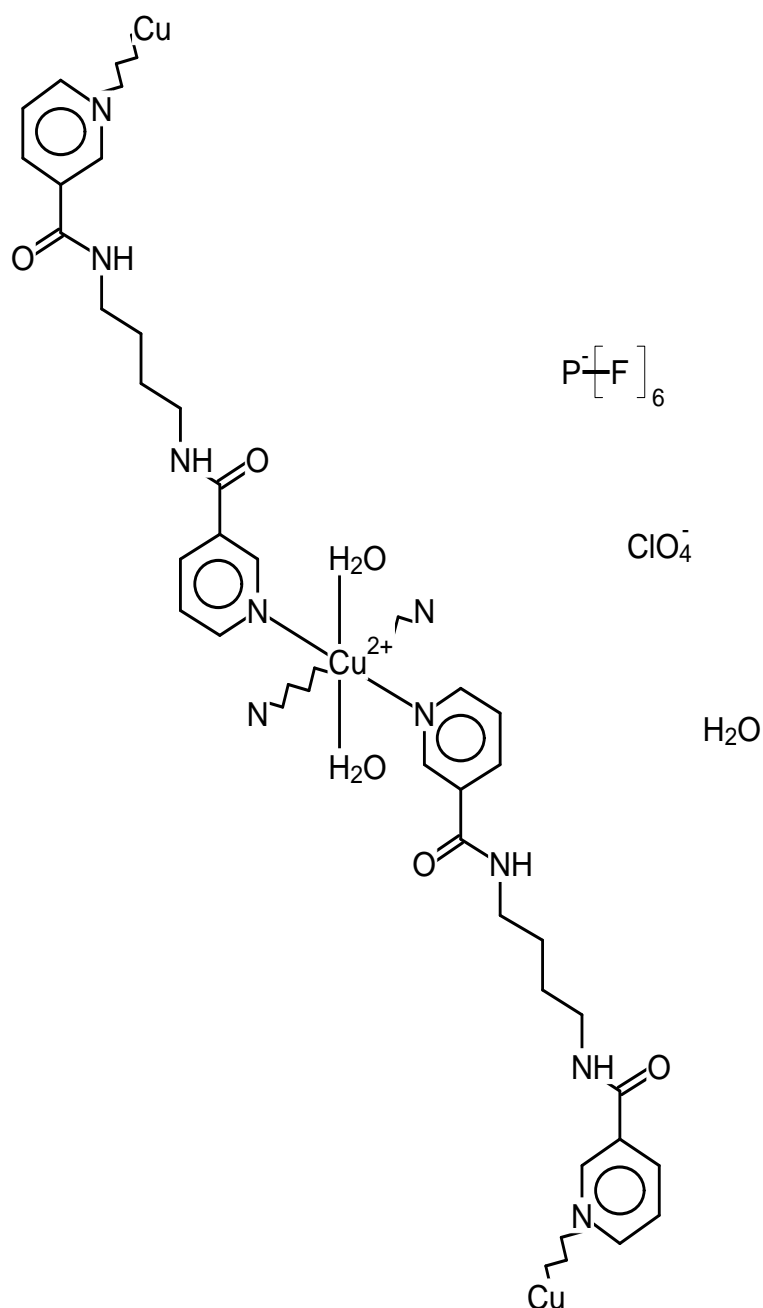
**Formula:**  $(C_{32}H_{40}Cu_1N_8O_6^{2+})_n, n(F_6P_1^{-1}), n(Cl_1O_4^{-1}), 2n(H_2O_1)$

**Compound Name:** catena-(bis( $\mu_2$ -1,4-bis((3-Pyridyl)carbonylamino)butane)-diaqua-copper(ii) hexafluorophosphate perchlorate dihydrate)

**Space Group:** C2      **Cell:**      **a** 20.687(4)      **b** 9.370(1)      **c** 11.422(2)

**Space Group No.:** 5      **(Å, °)**       $\alpha$  90.00       $\beta$  110.14(3)       $\gamma$  90.00

**R-Factor (%):** 7.40      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.561



## Search: search9 (Wed Jul 13 08:31:33 2011): Hit 3

DIKJIR

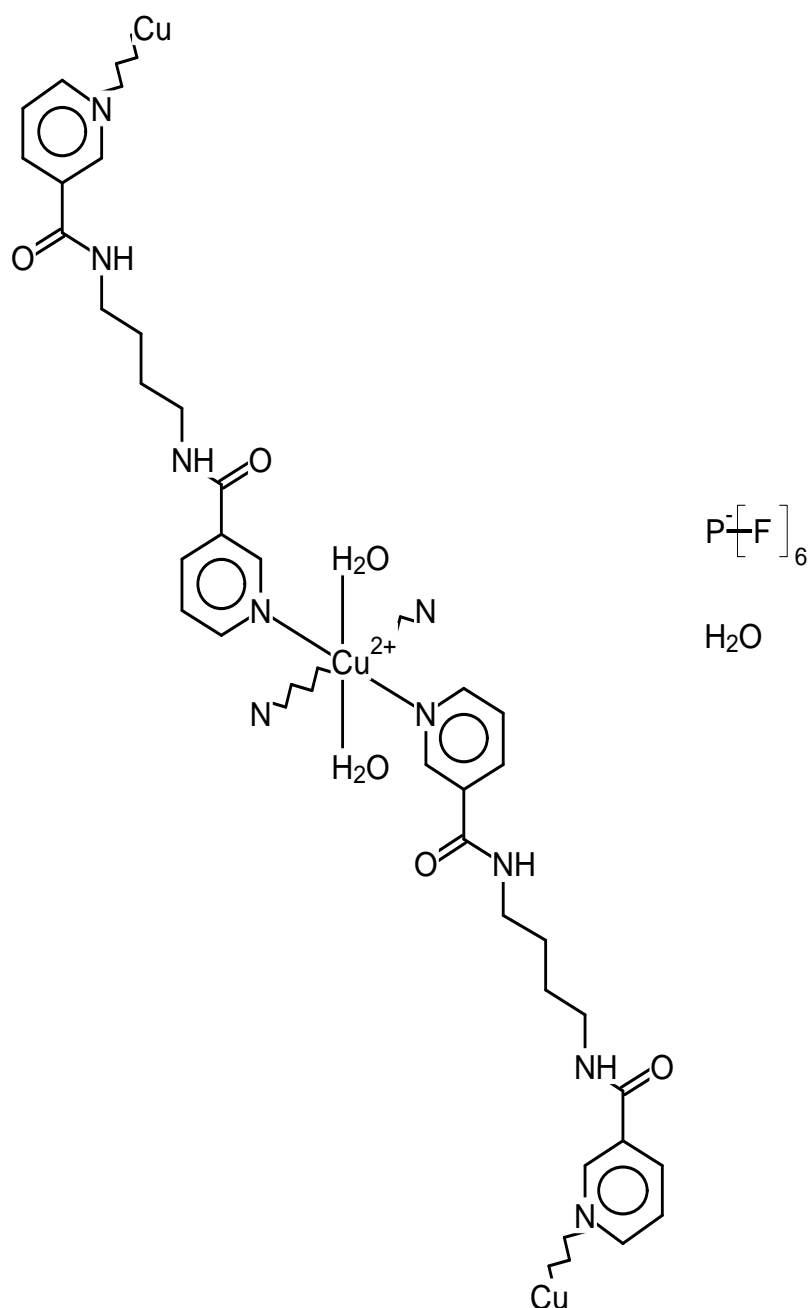
**Reference:** M.Sarkar, K.Biradha (2007) *Cryst.Growth Des.* ,7,1318

**Formula:**  $(C_{32}H_{40}Cu_1N_8O_6^{2+})_n, 2n(F_6P_1^{-1}), 4n(H_2O_1)$

**Compound Name:** catena-(bis( $\mu_2$ -1,4-bis((3-Pyridyl)carbonylamino)butane)-diaqua-copper(ii) bis(hexafluorophosphate) tetrahydrate)

**Space Group:** Ccca      **Cell:**      **a** 19.600(50)      **b** 22.020(50)      **c** 10.260(50)  
**Space Group No.:** 68      **(Å, °)**       $\alpha$  90.00       $\beta$  90.00       $\gamma$  90.00

**R-Factor (%):** 7.36      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.587



## Search: search9 (Wed Jul 13 08:31:33 2011): Hit 4

DIKJOX

**Reference:** M.Sarkar, K.Biradha (2007) *Cryst.Growth Des.* ,7,1318

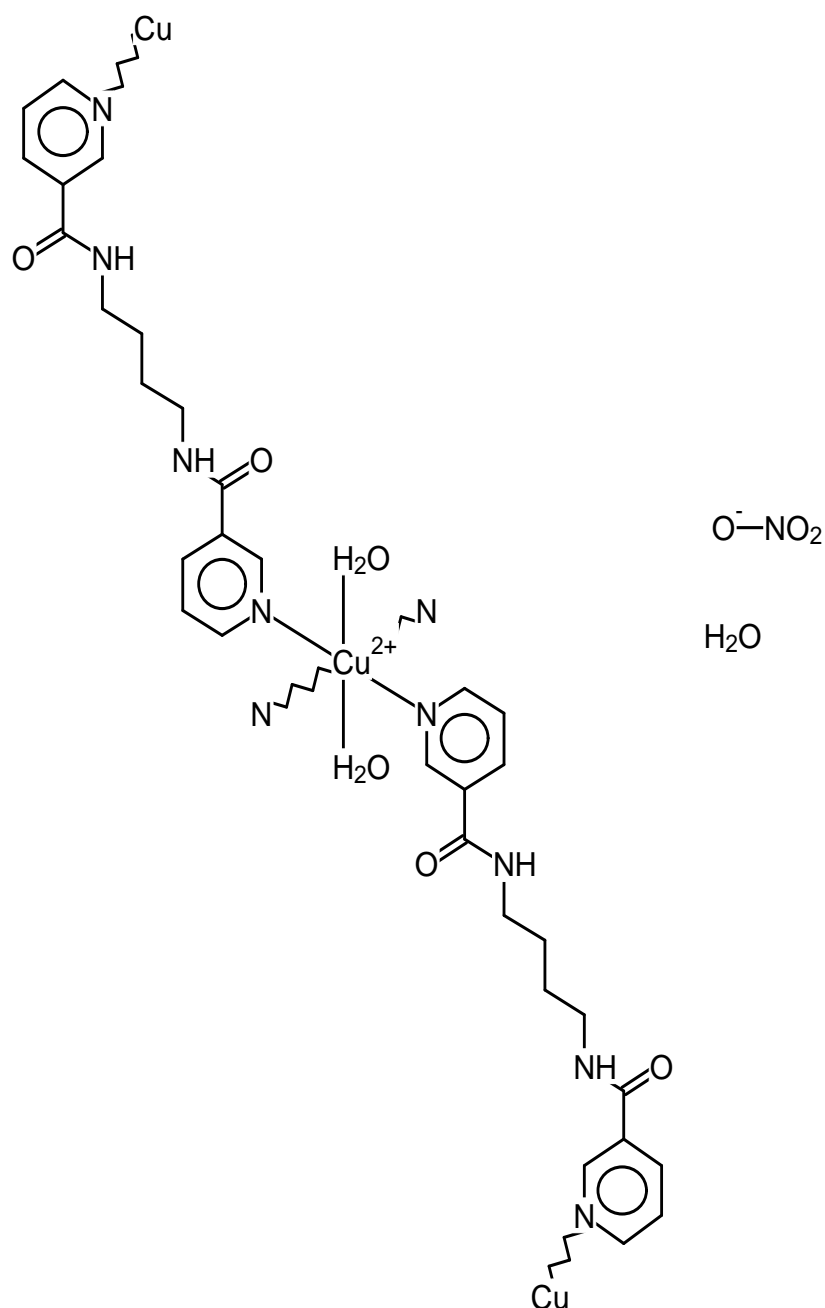
**Formula:**  $(C_{32}H_{40}Cu_1N_8O_6^{2+})_n, 2n(N_1O_3^{1-}), 3n(H_2O_1)$

**Compound Name:** catena-(bis( $\mu_2$ -1,4-bis((3-Pyridyl)carbonylamino)butane)-diaqua-copper(ii) dinitrate trihydrate)

**Space Group:** C2      **Cell:**      **a** 20.767(4)      **b** 9.295(1)      **c** 11.225(2)

**Space Group No.:** 5      **(Å, °)**       $\alpha$  90.00       $\beta$  112.09(3)       $\gamma$  90.00

**R-Factor (%):** 6.58      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.446





## Search: search9 (Wed Jul 13 08:31:33 2011): Hit 5

MIXNAJ

**Reference:** L.Rajput, K.Biradha (2008) *Polyhedron* ,**27**,1248

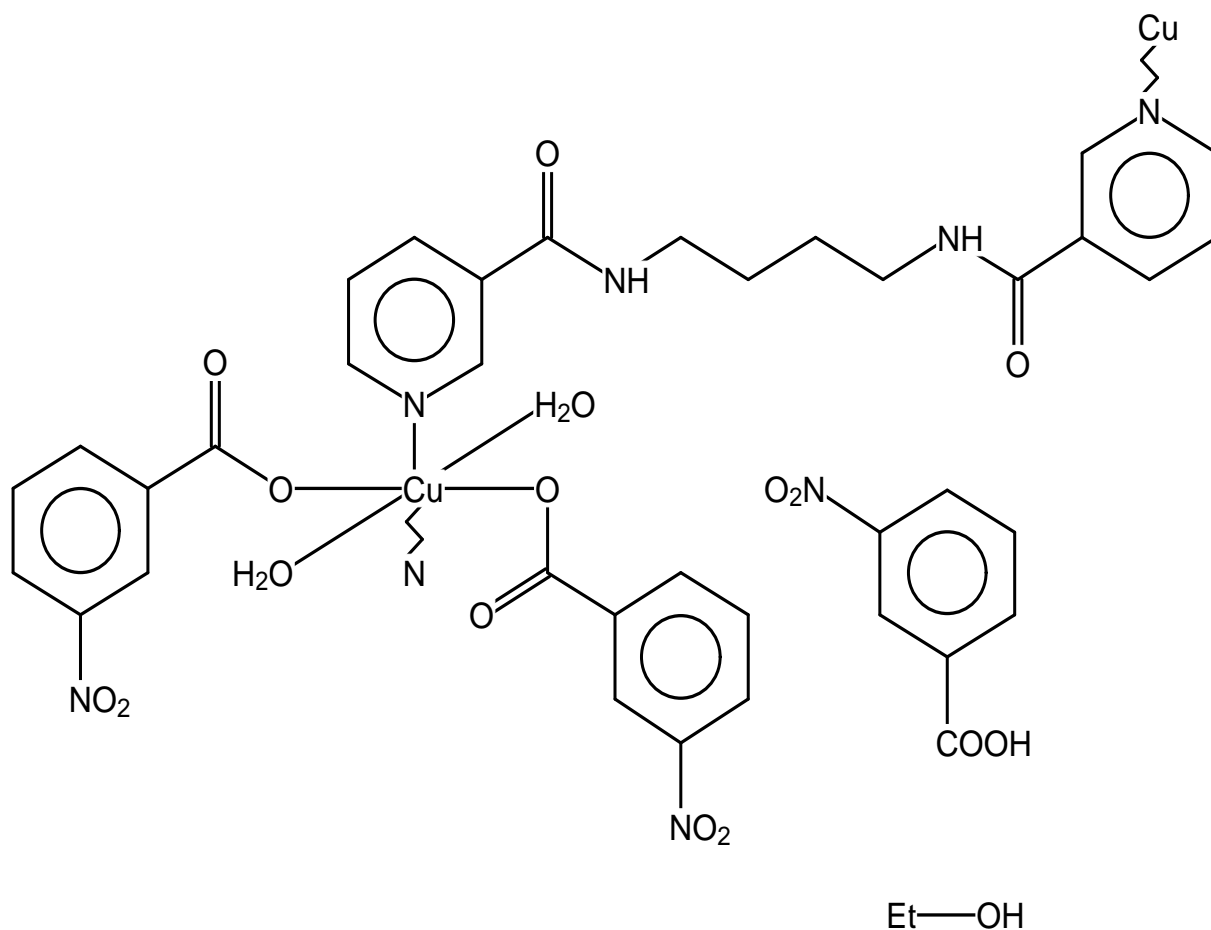
**Formula:** (C<sub>30</sub> H<sub>30</sub> Cu<sub>1</sub> N<sub>6</sub> O<sub>12</sub>)<sub>n</sub>,n(C<sub>7</sub> H<sub>5</sub> N<sub>1</sub> O<sub>4</sub>),n(C<sub>2</sub> H<sub>6</sub> O<sub>1</sub>)

**Compound Name:** catena-((μ<sub>2</sub>-1,4-bis(3-Pyridinecarboxamido)butane-N,N')-diaqua-bis(3-nitrobenzoato-O)-copper(ii) 3-nitrobenzoic acid ethanol clathrate)

**Space Group:** P-1      **Cell:**      **a** 8.731(1)      **b** 11.137(2)      **c** 12.603(3)

**Space Group No.:** 2      **(Å, °)**      **α** 106.51(3)      **β** 90.29(3)      **γ** 98.08(3)

**R-Factor (%):** 4.54      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.348



## Search Overview

**Search:** search13  
**Date/Time done:** Wed Jul 13 08:34:26 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: search13 (Wed Jul 13 08:34:26 2011): Hit 1

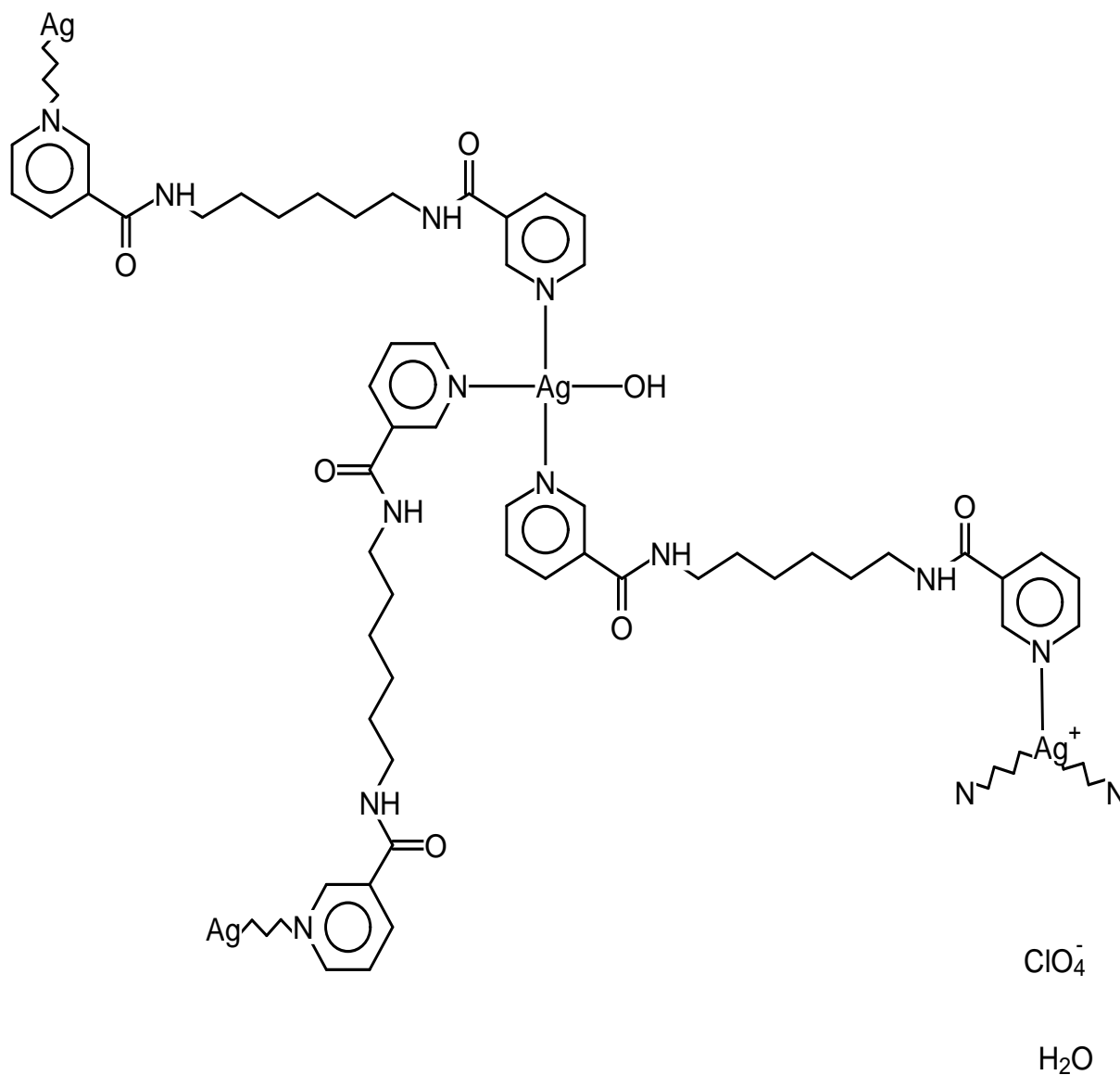
### AHIDEA

**Reference:** S.Muthu, J.H.K.Yip, J.J.Vittal (2002)  
*J.Chem.Soc.,Dalton Trans.* ,4561

**Formula:**  $(C_{54}H_{67}Ag_2N_{12}O_7^{1+})_n, n(Cl_1O_4^{1-}), 2.5n(H_2O_1)$

**Compound Name:** catena-(tris( $\mu_2$ -N,N'-Hexamethylene-bis(3-pyridinecarboxamide))-(hydroxy)-di-silver(i) perchlorate hydrate)

<b>Space Group:</b>	P32	<b>Cell:</b>	<b>a</b> 15.130(0)	<b>b</b> 15.130(0)	<b>c</b> 22.134(0)
<b>Space Group No.:</b>	145	(Å, °)	$\alpha$ 90.00	$\beta$ 90.00	$\gamma$ 120.00
<b>R-Factor (%):</b>	6.08	<b>Temperature(K):</b>	223	<b>Density(g/cm<sup>3</sup>):</b>	1.540



## Search: search13 (Wed Jul 13 08:34:26 2011): Hit 2

### AHIDIE

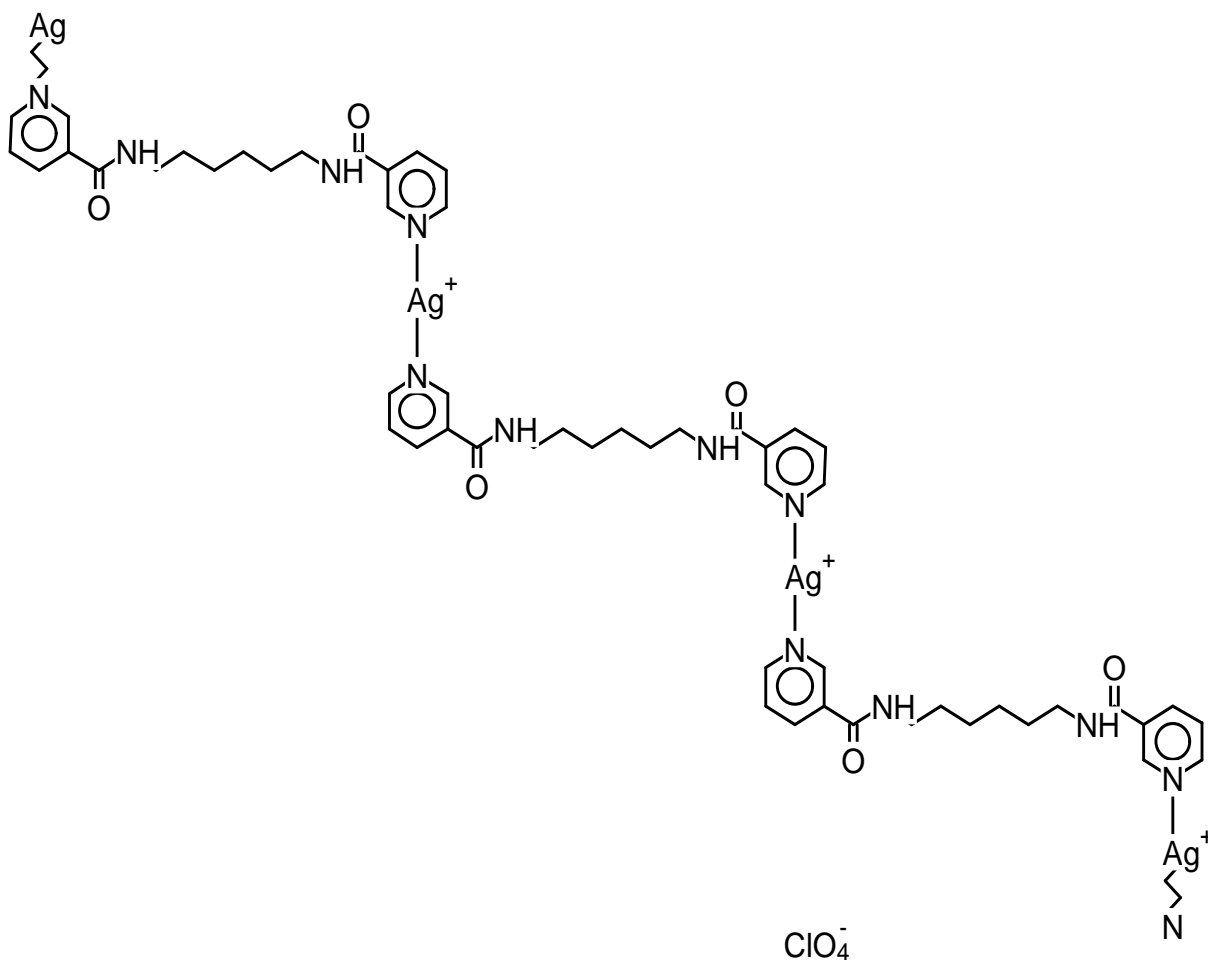
**Reference:** S.Muthu, J.H.K.Yip, J.J.Vittal (2002)  
*J.Chem.Soc.,Dalton Trans.*, 4561

**Formula:**  $(C_{54} H_{66} Ag_3 N_{12} O_6^{3+})_n, 3n(Cl_1 O_4^{1-})$

**Compound Name:** catena-(tris( $\mu_2$ -N,N'-Hexamethylene-bis(3-pyridinecarboxamide))-tri-silver(i) triperchlorate)

**Space Group:** C2/c      **Cell:**    **a** 26.502(2)    **b** 5.143(0)    **c** 44.366(3)  
**Space Group No.:** 15      **(Å, °)**     $\alpha$  90.00       $\beta$  94.35(0)     $\gamma$  90.00

**R-Factor (%):** 4.81      **Temperature(K):** 223      **Density(g/cm<sup>3</sup>):** 1.764



## Search: search13 (Wed Jul 13 08:34:26 2011): Hit 3

### AHIDOK

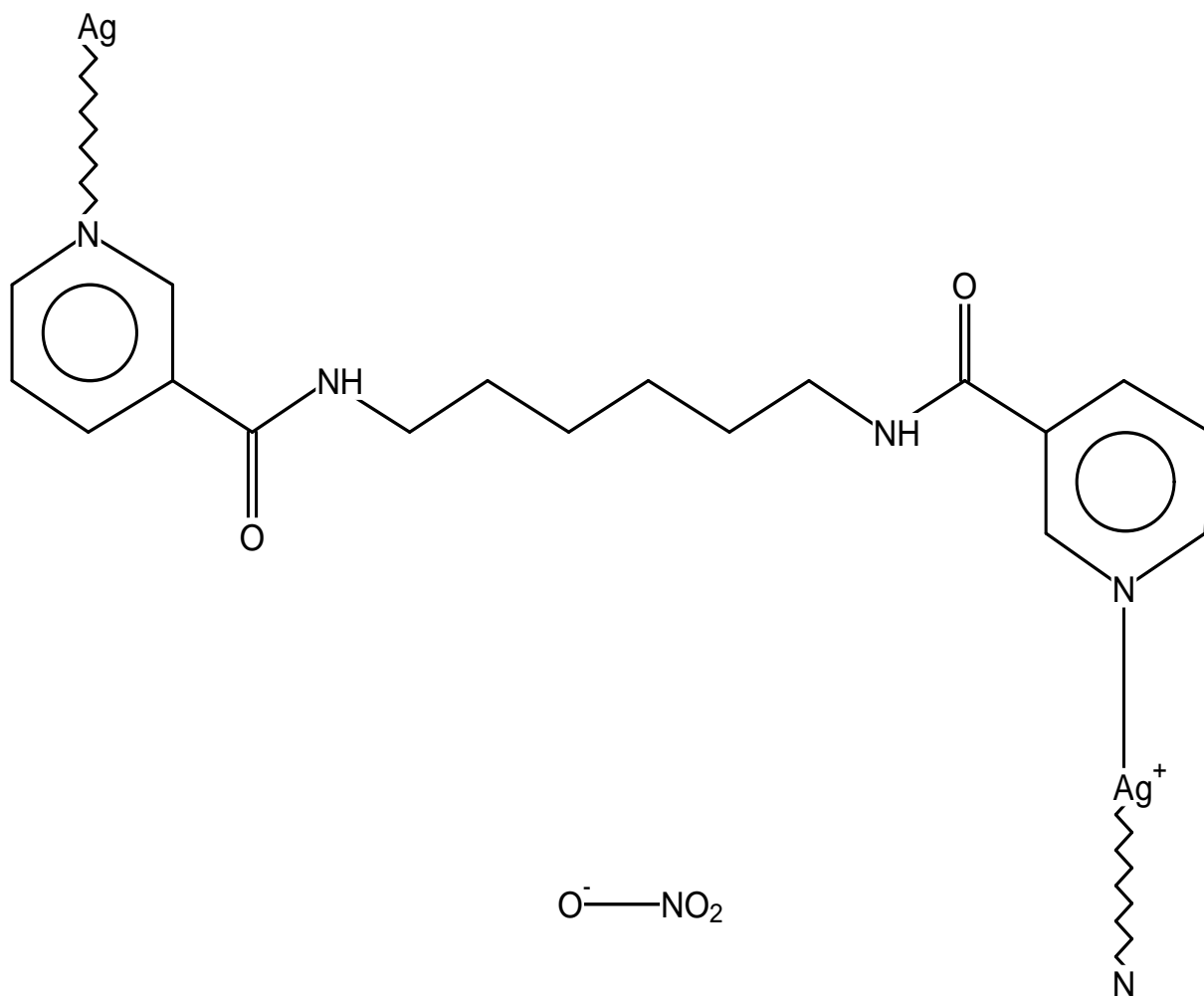
**Reference:** S.Muthu, J.H.K.Yip, J.J.Vittal (2002)  
*J.Chem.Soc.,Dalton Trans.* ,4561

**Formula:** (C<sub>18</sub> H<sub>22</sub> Ag<sub>1</sub> N<sub>4</sub> O<sub>2</sub><sup>1+</sup>)<sub>n</sub>,n(N<sub>1</sub> O<sub>3</sub><sup>1-</sup>)

**Compound Name:** catena-((μ<sub>2</sub>-N,N'-Hexamethylene-bis(3-pyridinecarboxamide))-silver(i) nitrate)

**Space Group:** P-1      **Cell:**    **a** 5.095(0)    **b** 6.993(0)    **c** 13.636(0)  
**Space Group No.:** 2      **(Å, °)**    **α** 93.51(0)    **β** 98.76(0)    **γ** 95.22(0)

**R-Factor (%):** 3.71      **Temperature(K):** 223      **Density(g/cm<sup>3</sup>):** 1.728



## Search: search13 (Wed Jul 13 08:34:26 2011): Hit 4

AHIDUQ

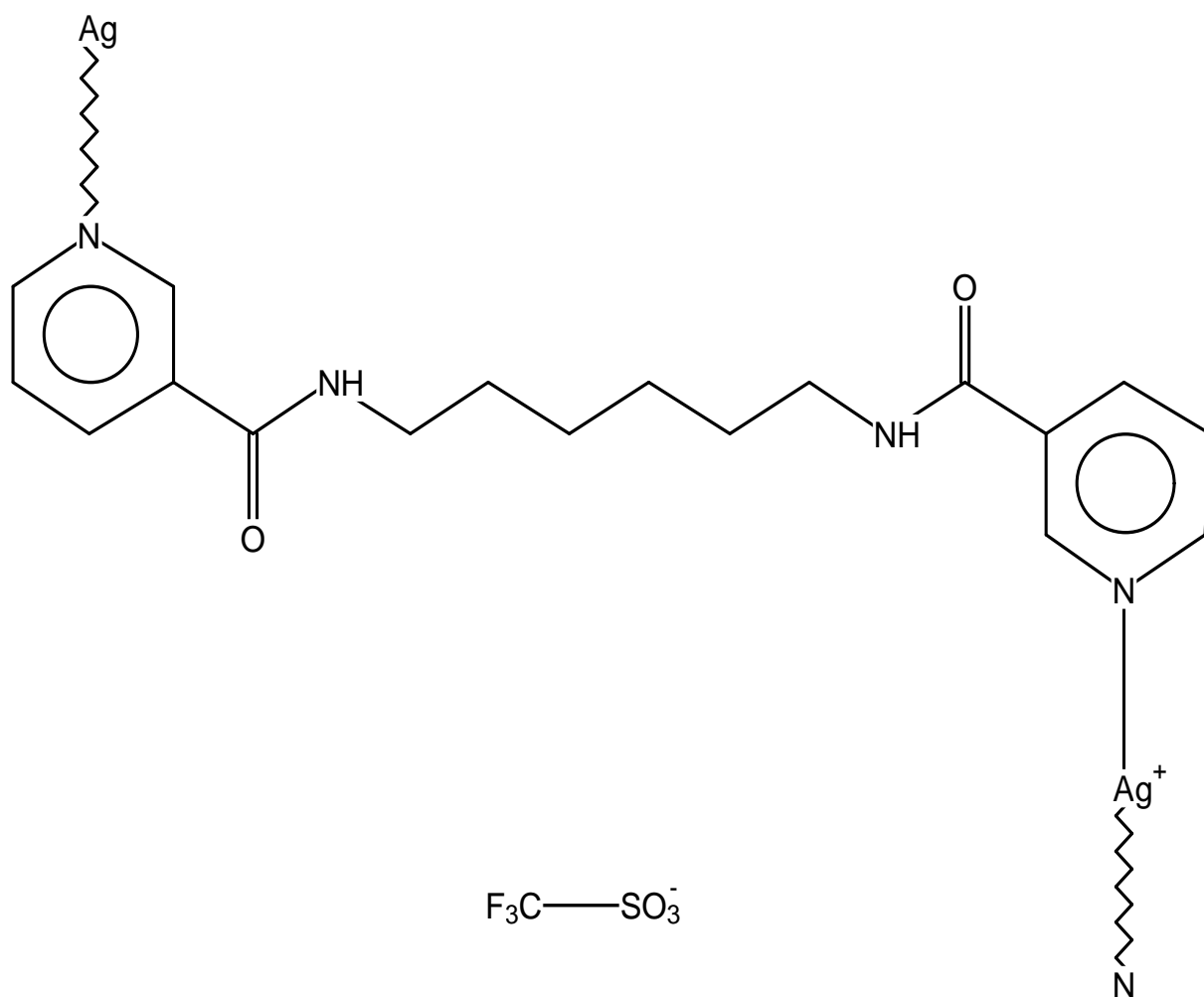
**Reference:** S.Muthu, J.H.K.Yip, J.J.Vittal (2002)  
*J.Chem.Soc.,Dalton Trans.* ,4561

**Formula:** (C<sub>18</sub> H<sub>22</sub> Ag<sub>1</sub> N<sub>4</sub> O<sub>2</sub><sup>1+</sup>)<sub>n</sub>,n(C<sub>1</sub> F<sub>3</sub> O<sub>3</sub> S<sub>1</sub><sup>1-</sup>)

**Compound Name:** catena-((μ<sub>2</sub>-N,N'-Hexamethylene-bis(3-pyridinecarboxamide))-silver(i) trifluoromethanesulfonate)

**Space Group:** P-1      **Cell:**    **a** 9.129(0)    **b** 10.051(0)    **c** 13.095(0)  
**Space Group No.:** 2      **(Å, °)**    α 108.61(0)    β 107.68(0)    γ 93.60(0)

**R-Factor (%):** 3.39      **Temperature(K):** 223      **Density(g/cm<sup>3</sup>):** 1.814



## Search: search13 (Wed Jul 13 08:34:26 2011): Hit 5

### MIXNEN

**Reference:** L.Rajput, K.Biradha (2008) *Polyhedron* ,**27**,1248

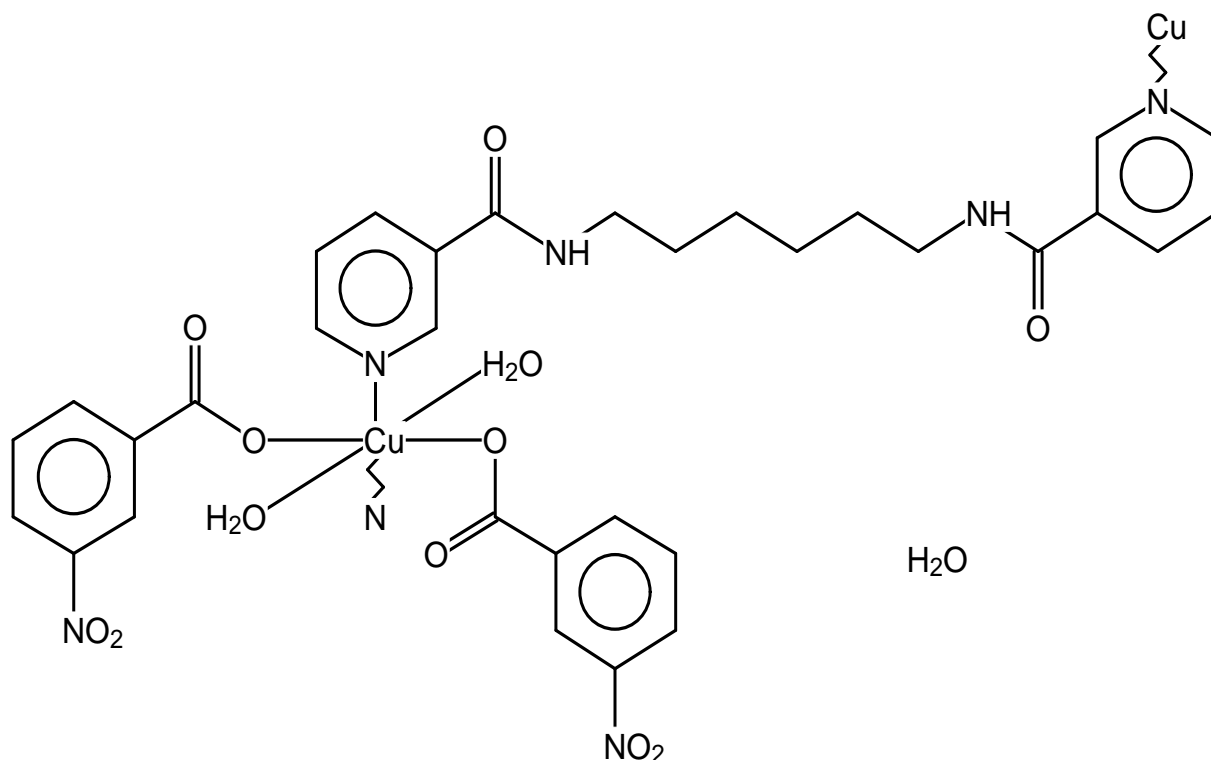
**Formula:** (C<sub>32</sub> H<sub>34</sub> Cu<sub>1</sub> N<sub>6</sub> O<sub>12</sub>)<sub>n</sub>,2n(H<sub>2</sub> O<sub>1</sub>)

**Compound Name:** catena-((μ<sub>2</sub>-1,6-bis(3-Pyridinecarboxamido)hexane-N,N')-diaqua-bis(3-nitrobenzoato-O)-copper(ii) dihydrate clathrate)

**Space Group:** P-1      **Cell:**      **a** 8.630(1)      **b** 8.967(1)      **c** 12.467(3)

**Space Group No.:** 2      **(Å, °)**      **α** 93.51(3)      **β** 106.47(3)      **γ** 96.74(3)

**R-Factor (%):** 6.48      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.443



## Search: search13 (Wed Jul 13 08:34:26 2011): Hit 6

### UHIYAM

**Reference:** L.Rajput, K.Biradha (2009) *CrystEngComm* ,11,1220

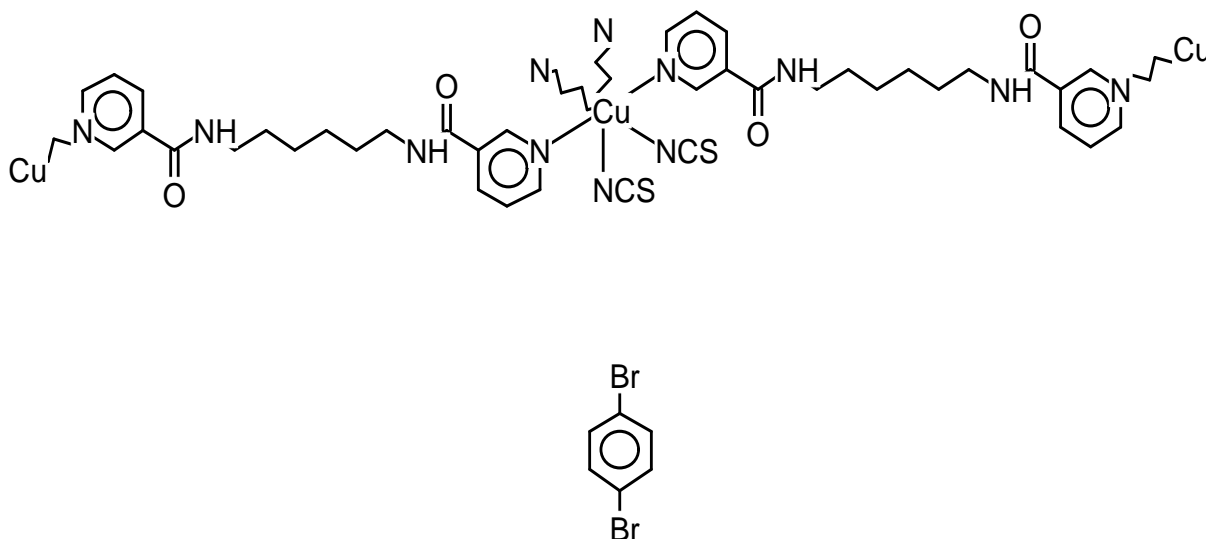
**Formula:**  $(C_{38} H_{44} Cu_1 N_{10} O_4 S_2)_n, 2n(C_6 H_4 Br_2)$

**Compound Name:** catena-(bis( $\mu_2$ -N,N'-(Hexane-1,6-diyl)pyridine-3-carboxamide-N,N')-bis(isothiocyanato)-copper(ii) bis(1,4-dibromobenzene) clathrate)

**Space Group:** P-1      **Cell:**      **a** 9.210(6)      **b** 10.155(7)      **c** 15.921(11)

**Space Group No.:** 2      **(Å, °)**       $\alpha$  93.77(2)       $\beta$  104.08(2)       $\gamma$  109.20(2)

**R-Factor (%):** 5.15      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.608





## Search: search13 (Wed Jul 13 08:34:26 2011): Hit 7

UHIYEQ

**Reference:** L.Rajput, K.Biradha (2009) *CrystEngComm* ,11,1220

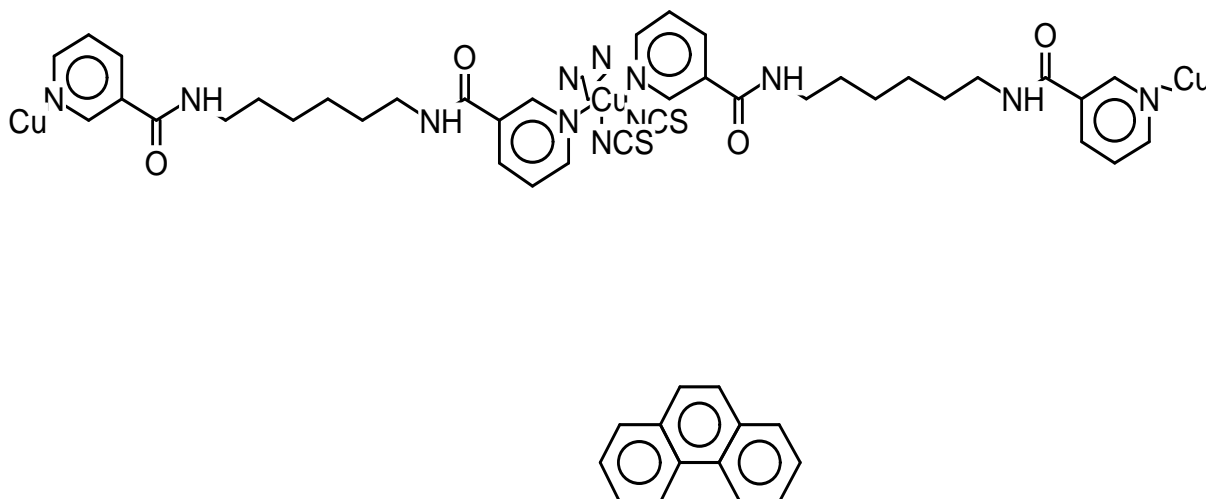
**Formula:** (C<sub>38</sub> H<sub>44</sub> Cu<sub>1</sub> N<sub>10</sub> O<sub>4</sub> S<sub>2</sub>)<sub>n</sub>,2n(C<sub>14</sub> H<sub>10</sub>)

**Compound Name:** catena-(bis(μ<sub>2</sub>-N,N'-(Hexane-1,6-diyl)pyridine-3-carboxamide-N,N')-bis(isothiocyanato)-copper(ii) bis(phenanthrene) clathrate)

**Space Group:** P21/n      **Cell:**      **a** 10.161(1)      **b** 15.061(1)      **c** 20.010(2)

**Space Group No.:** 14      **(Å, °)**      α 90.00      β 100.34(0)      γ 90.00

**R-Factor (%):** 6.18      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.311

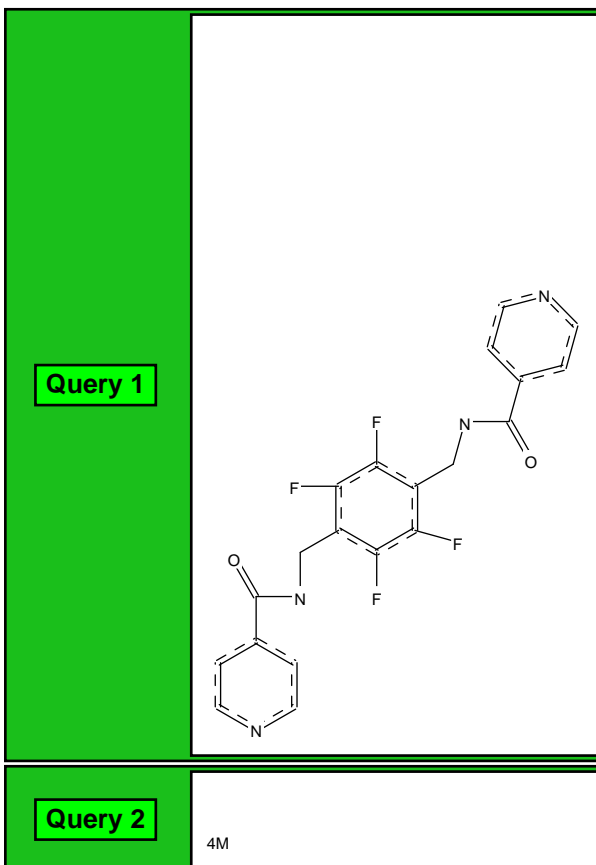


## Search Overview

**Search:** search17  
**Date/Time done:** Thu May 26 15:25:18 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:** 3

### Summary of queries used. Search found structures that:

Query 1 <sup>match</sup> Query 2



## Search: search17 (Thu May 26 15:25:18 2011): Hit 1

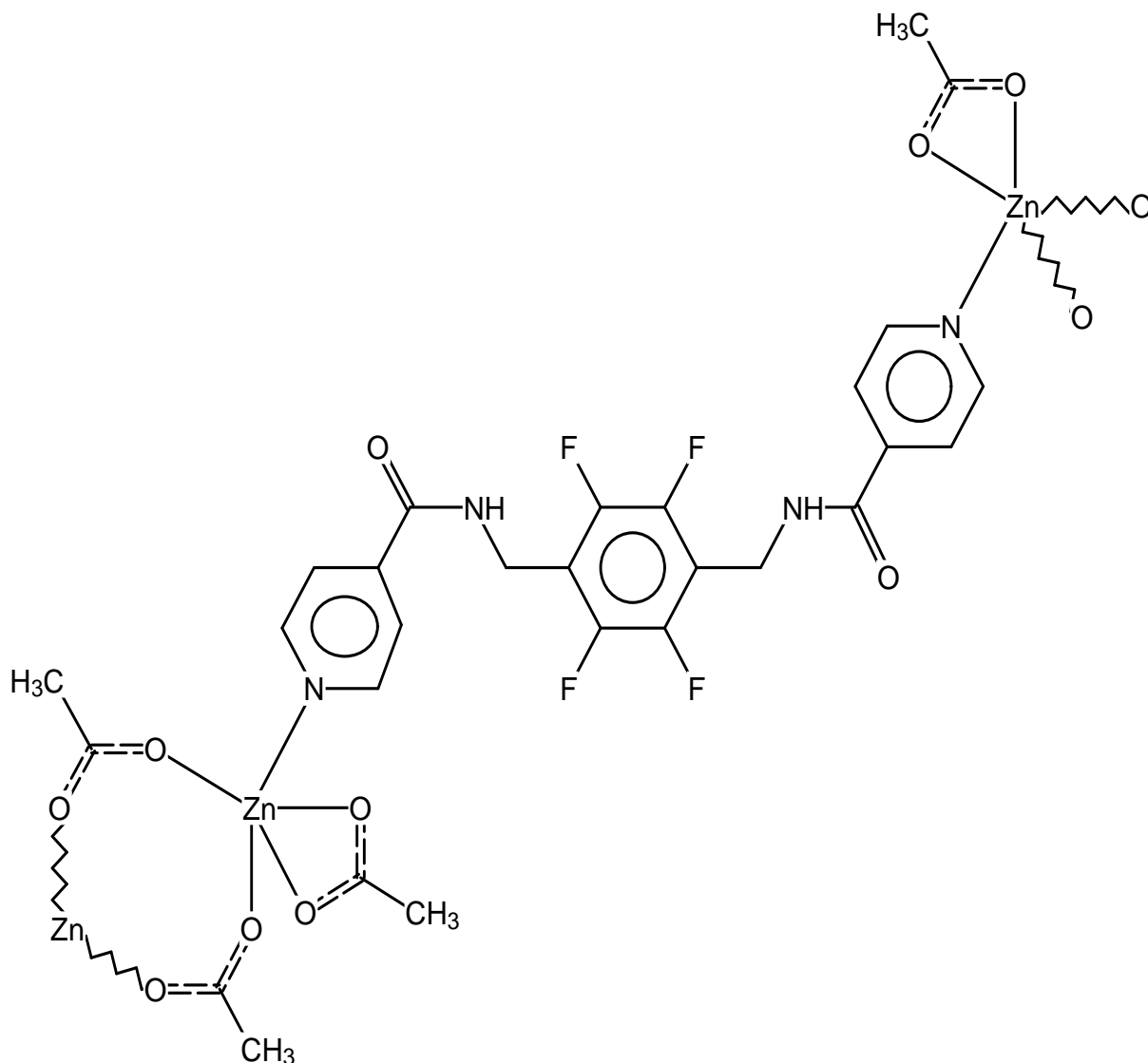
### CIBYAO

**Reference:** Shengchun Chen, Mingyang He, Kang Yan, Qun Chen, Yi Guo, Yifeng Zhang (2007) *Inorg.Chem.Commun.* ,**10**,451

**Formula:** (C<sub>28</sub> H<sub>26</sub> F<sub>4</sub> N<sub>4</sub> O<sub>10</sub> Zn<sub>2</sub>)<sub>n</sub>

**Compound Name:** catena-(bis(μ<sub>2</sub>-Acetato-O,O')-(μ<sub>2</sub>-N,N'-((2,3,5,6-tetrafluoro-1,4-phenylene)-bis(methylene))-bis(pyridine-4-carboxamide)-N'',N''')-bis(acetato-O,O')-di-zinc(ii))

<b>Space Group:</b>	C2/c	<b>Cell:</b>	<b>a</b> 27.312(5)	<b>b</b> 8.094(1)	<b>c</b> 14.201(3)
<b>Space Group No.:</b>	15	<b>(Å, °)</b>	<b>α</b> 90.00	<b>β</b> 96.70(2)	<b>γ</b> 90.00
<b>R-Factor (%):</b>	5.84	<b>Temperature(K):</b>	298	<b>Density(g/cm<sup>3</sup>):</b>	1.673



## Search: search17 (Thu May 26 15:25:18 2011): Hit 2

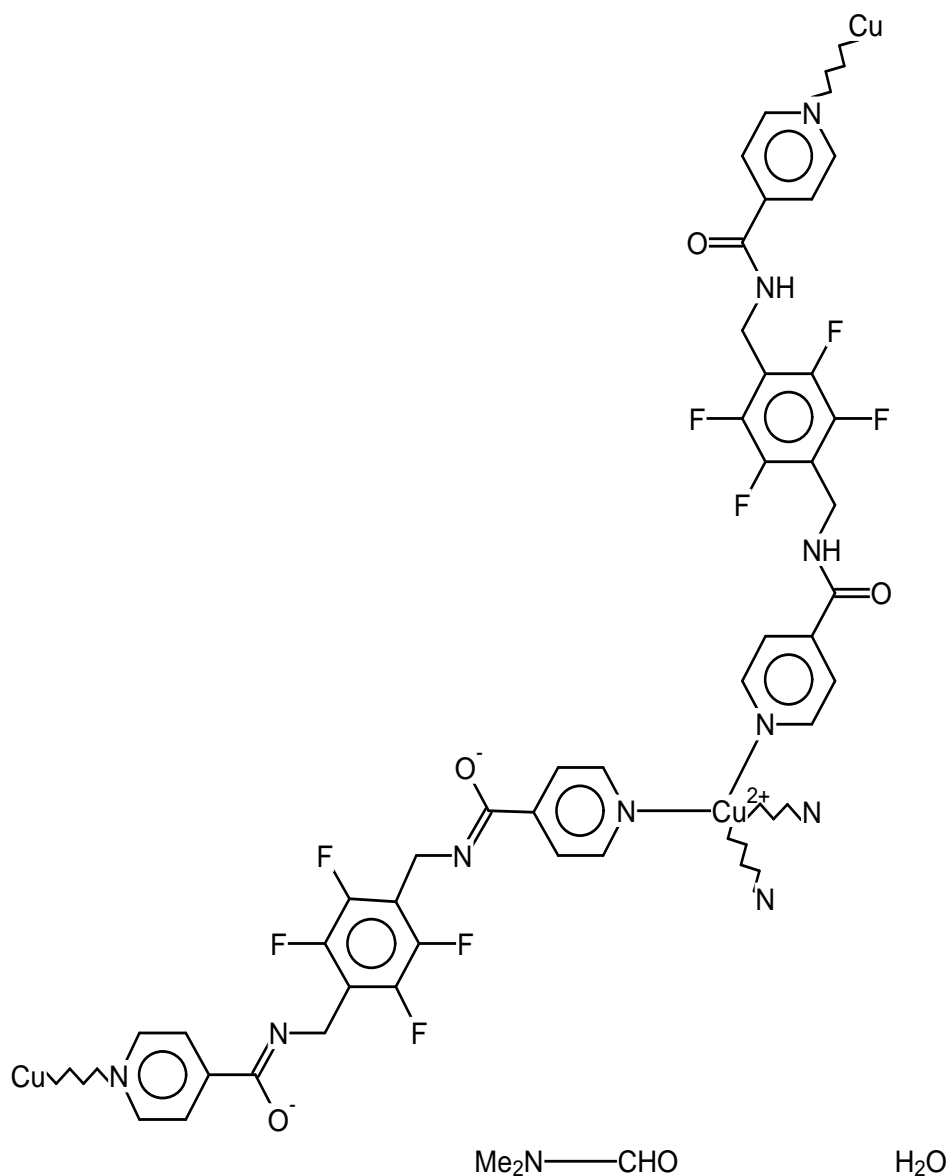
NOMVER

**Reference:** Qun Chen, Sheng-Chun Chen, Bo Xiao, Zhi-Hui Zhang, Ming-Yang He, Fang-Hua Yin, Miao Du (2008) *Inorg.Chem.Commun.* , 11,1371

**Formula:**  $(C_{40} H_{26} Cu_1 F_8 N_8 O_4)_n, 2n(C_3 H_7 N_1 O_1), 5n(H_2 O_1)$

**Compound Name:** catena-(( $\mu_2$ -N,N'-((2,3,5,6-tetrafluoro-1,4-phenylene) bis(methylene)) bis(pyridine-4-carboxamide))-( $\mu_2$ -N,N'-((2,3,5,6-tetrafluoro-1,4-phenylene)bis(methylene))bis(pyridine-4-carboxamido))-copper(ii) N,N-dimethylformamide solvate pentahydrate)

<b>Space Group:</b>	P-1	<b>Cell:</b>	<b>a</b> 9.103(1)	<b>b</b> 11.595(2)	<b>c</b> 15.349(3)
<b>Space Group No.:</b>	2	<b>(Å, °)</b>	$\alpha$ 78.35(0)	$\beta$ 72.75(0)	$\gamma$ 73.77(0)
<b>R-Factor (%):</b>	5.58	<b>Temperature(K):</b>	291	<b>Density(g/cm<sup>3</sup>):</b>	1.279



## Search: search17 (Thu May 26 15:25:18 2011): Hit 3

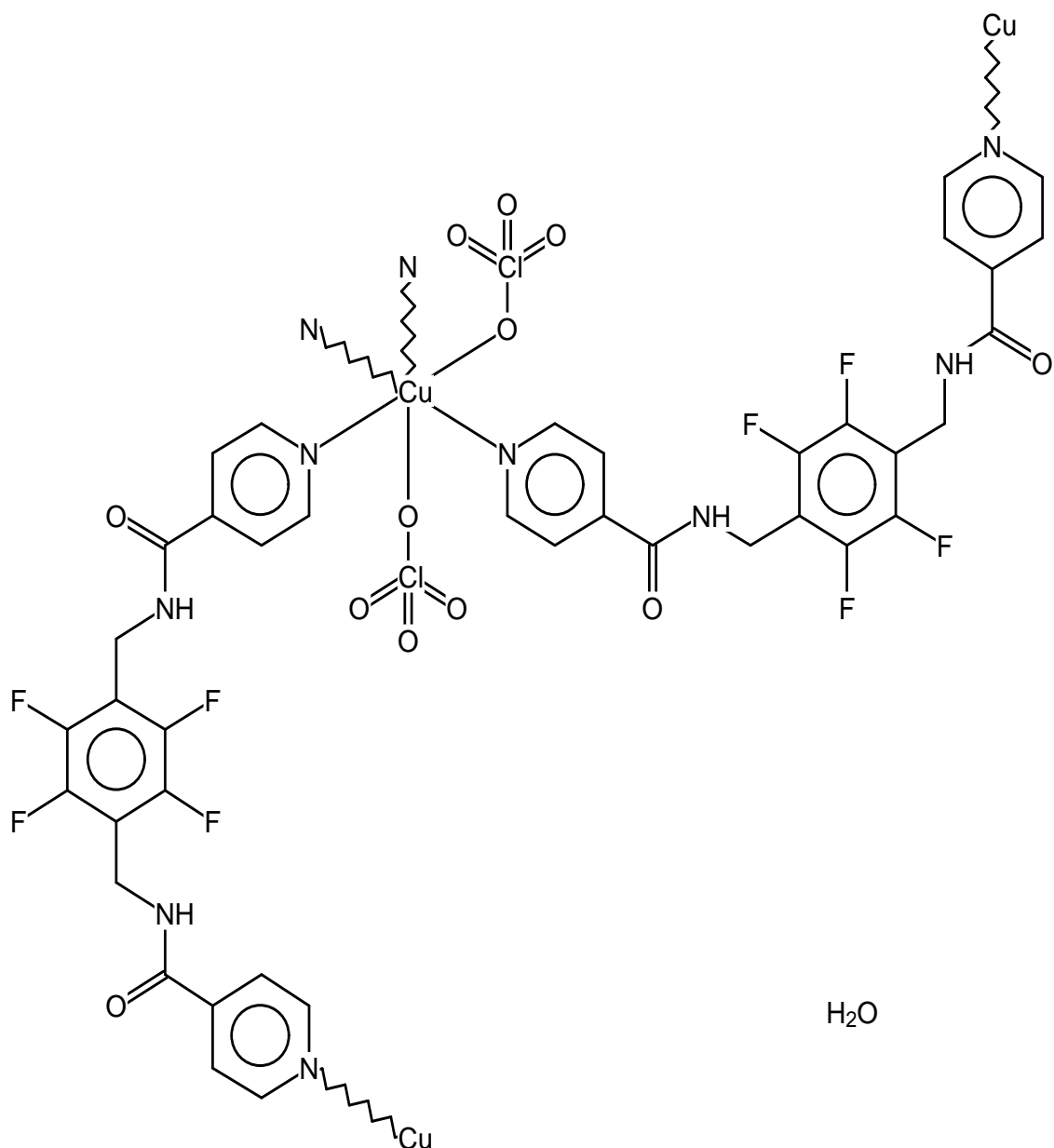
### NOMVIV

**Reference:** Qun Chen, Sheng-Chun Chen, Bo Xiao, Zhi-Hui Zhang, Ming-Yang He, Fang-Hua Yin, Miao Du (2008) *Inorg.Chem.Commun.* , 11,1371

**Formula:** (C<sub>40</sub> H<sub>28</sub> Cl<sub>2</sub> Cu<sub>1</sub> F<sub>8</sub> N<sub>8</sub> O<sub>12</sub>)<sub>n</sub>,3n(H<sub>2</sub> O<sub>1</sub>)

**Compound Name:** catena-(bis(μ<sub>2</sub>-N,N'-((2,3,5,6-tetrafluoro-1,4-phenylene) bis(methylene)) bis(pyridine-4-carboxamide))-diperchlorato-copper(ii) trihydrate)

<b>Space Group:</b>	P21/n	<b>Cell:</b>	<b>a</b> 19.217(2)	<b>b</b> 17.184(1)	<b>c</b> 19.528(2)
<b>Space Group No.:</b>	14	<b>(Å, °)</b>	<b>α</b> 90.00	<b>β</b> 115.67(0)	<b>γ</b> 90.00
<b>R-Factor (%):</b>	5.56	<b>Temperature(K):</b>	291	<b>Density(g/cm<sup>3</sup>):</b>	1.318



## Search Overview

**Search:** search19  
**Date/Time done:** Thu May 26 18:22:58 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

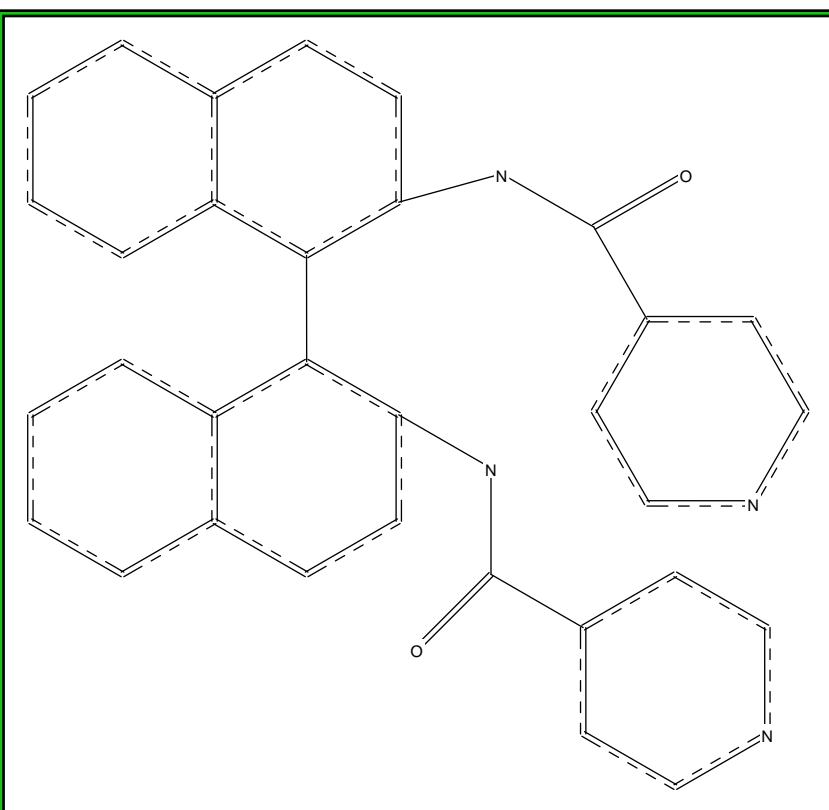
*Summary of queries used. Search found structures that:*

match

**Query 1**

**Query 2**

**Query 1**



**Query 2**

4M

## Search: search19 (Thu May 26 18:22:58 2011): Hit 1

### JAPJAM

**Reference:** T.J.Burchell, R.J.Puddephatt (2005) *Inorg.Chem.* ,**44**,3718

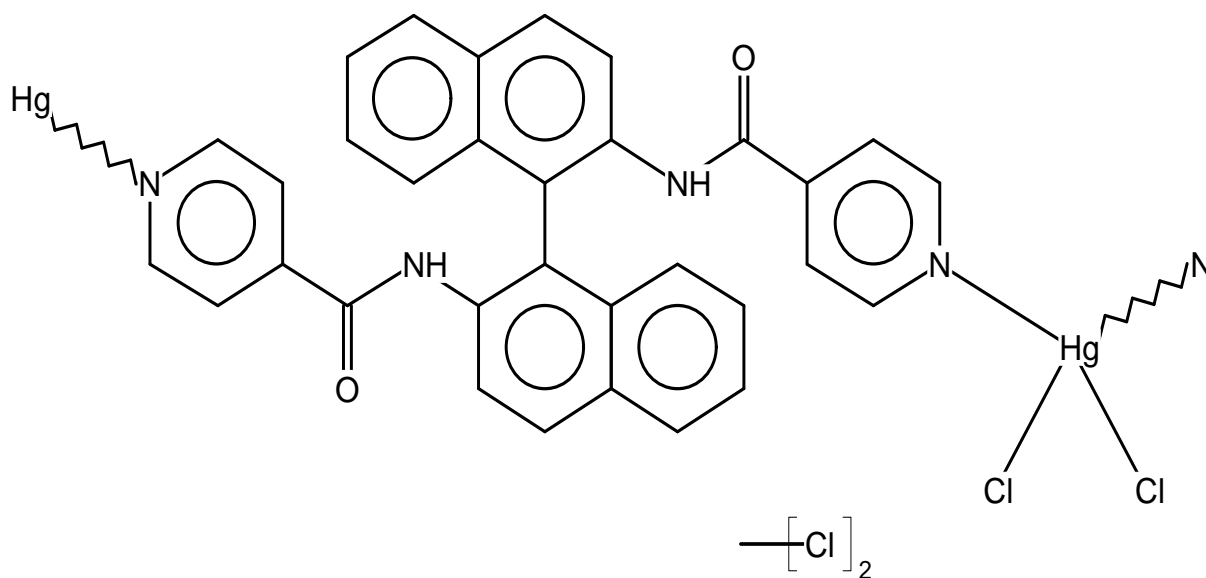
**Formula:** (C<sub>32</sub> H<sub>22</sub> Cl<sub>2</sub> Hg<sub>1</sub> N<sub>4</sub> O<sub>2</sub>)<sub>n</sub>,n(C<sub>1</sub> H<sub>2</sub> Cl<sub>2</sub>)

**Compound Name:** catena-((μ<sub>2</sub>-rac-2,2'-bis((4-Pyridyl)carbonylamino)-1,1'-binaphthyl-N,N')-dichloro-mercury(ii) dichloromethane solvate)

**Space Group:** P21/n      **Cell:**      **a** 10.188(2)      **b** 22.928(5)      **c** 13.624(3)

**Space Group No.:** 14      **(Å, °)**      **α** 90.00      **β** 93.11(3)      **γ** 90.00

**R-Factor (%):** 4.13      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.779



## Search: search19 (Thu May 26 18:22:58 2011): Hit 2

JAPJAM01

**Reference:** T.J.Burchell, R.J.Puddephatt (2005) *Inorg.Chem.* ,**44**,3718

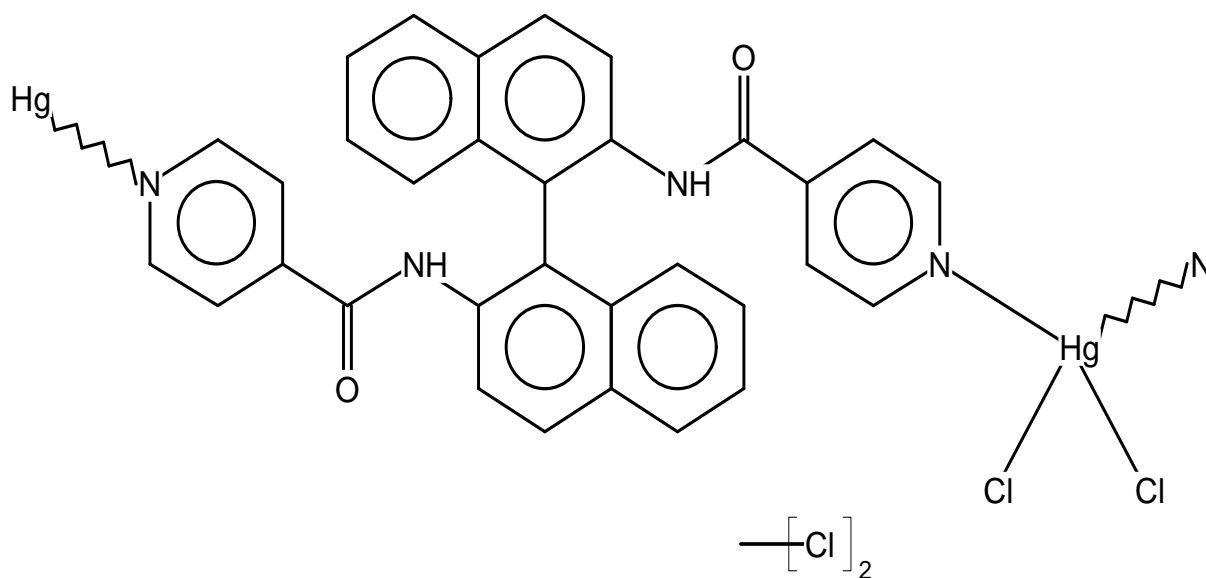
**Formula:** (C<sub>32</sub> H<sub>22</sub> Cl<sub>2</sub> Hg<sub>1</sub> N<sub>4</sub> O<sub>2</sub>)<sub>n</sub>,n(C<sub>1</sub> H<sub>2</sub> Cl<sub>2</sub>)

**Compound Name:** catena-((μ<sub>2</sub>-rac-2,2'-bis((4-Pyridyl)carbonylamino)-1,1'-binaphthyl-N,N')-dichloro-mercury(ii) dichloromethane clathrate)

**Space Group:** P21/c      **Cell:**      **a** 17.124(3)      **b** 11.727(2)      **c** 16.249(3)

**Space Group No.:** 14      **(Å, °)**      **α** 90.00      **β** 103.84(3)      **γ** 90.00

**R-Factor (%):** 4.32      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.784





## Search: search19 (Thu May 26 18:22:58 2011): Hit 3

JAPJEQ

**Reference:** T.J.Burchell, R.J.Puddephatt (2005) *Inorg.Chem.* ,**44**,3718

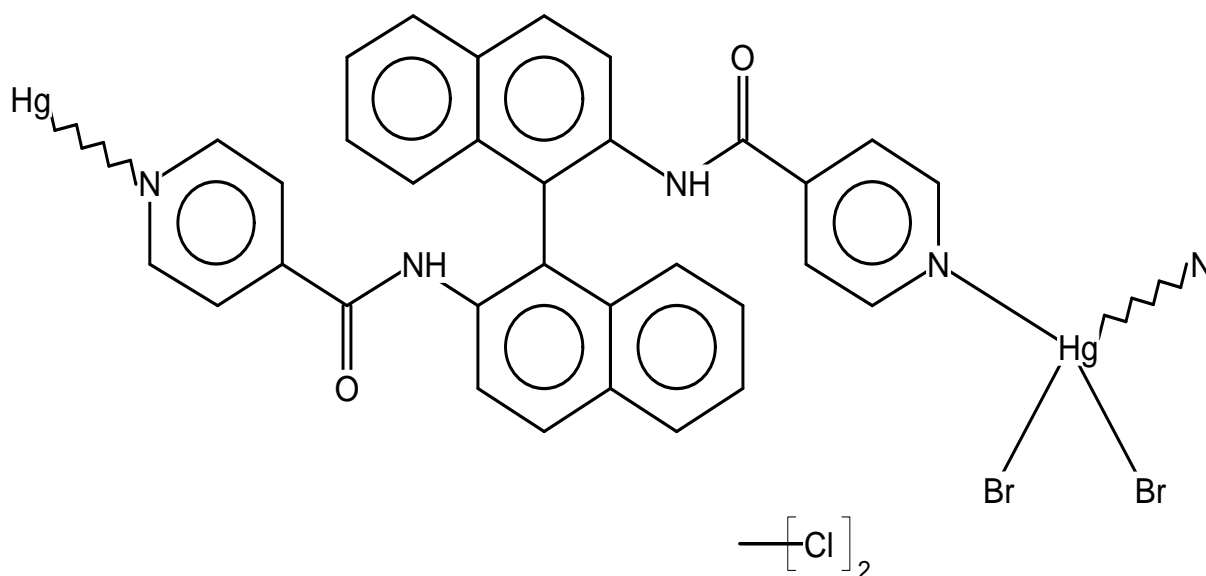
**Formula:** (C<sub>32</sub> H<sub>22</sub> Br<sub>2</sub> Hg<sub>1</sub> N<sub>4</sub> O<sub>2</sub>)<sub>n</sub>,n(C<sub>1</sub> H<sub>2</sub> Cl<sub>2</sub>)

**Compound Name:** catena-((μ<sub>2</sub>-rac-2,2'-bis((4-Pyridyl)carbonylamino)-1,1'-binaphthyl-N,N')-dibromo-mercury(ii) dichloromethane clathrate)

**Space Group:** P21/c      **Cell:**      **a** 17.239(3)      **b** 11.940(2)      **c** 16.268(3)

**Space Group No.:** 14      **(Å, °)**      **α** 90.00      **β** 103.34(3)      **γ** 90.00

**R-Factor (%):** 4.26      **Temperature(K):** 123      **Density(g/cm<sup>3</sup>):** 1.916



## Search: search19 (Thu May 26 18:22:58 2011): Hit 4

JAPJIU

**Reference:** T.J.Burchell, R.J.Puddephatt (2005) *Inorg.Chem.* ,**44**,3718

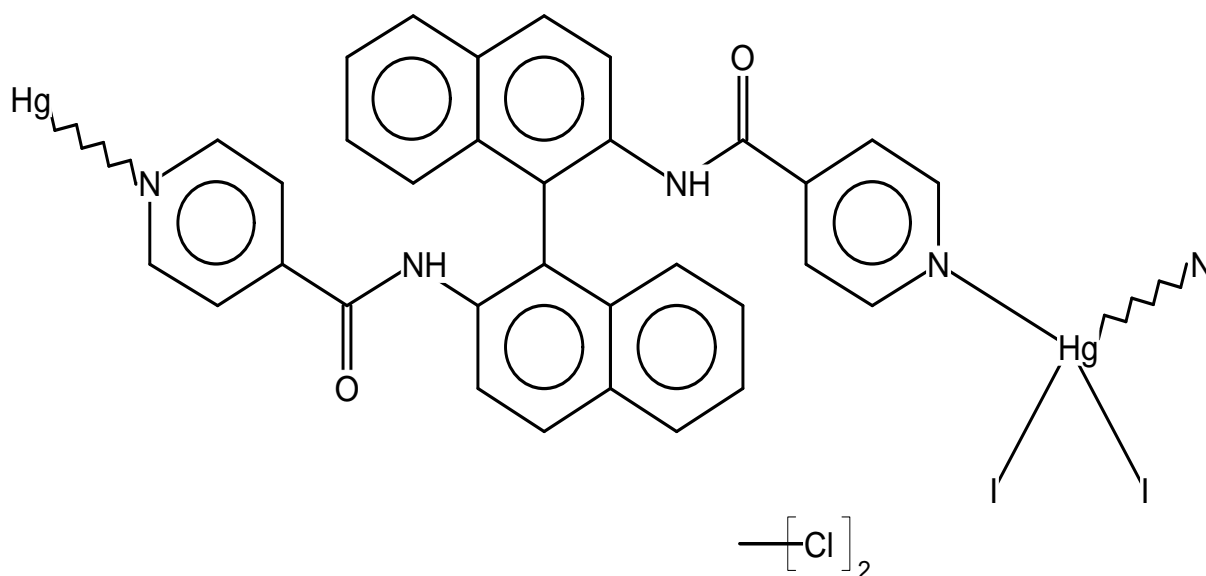
**Formula:** (C<sub>32</sub> H<sub>22</sub> Hg<sub>1</sub> I<sub>2</sub> N<sub>4</sub> O<sub>2</sub>)<sub>n</sub>.2.25n(C<sub>1</sub> H<sub>2</sub> Cl<sub>2</sub>)

**Compound Name:** catena-((μ<sub>2</sub>-rac-2,2'-bis((4-Pyridyl)carbonylamino)-1,1'-binaphthyl-N,N')-di-iodo-mercury(ii) dichloromethane clathrate)

**Space Group:** C2/c      **Cell:**      **a** 20.856(4)      **b** 15.847(3)      **c** 23.865(5)

**Space Group No.:** 15      **(Å, °)**      **α** 90.00      **β** 96.91(3)      **γ** 90.00

**R-Factor (%):** 7.40      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.934



## Search: search19 (Thu May 26 18:22:58 2011): Hit 5

JAPJOA

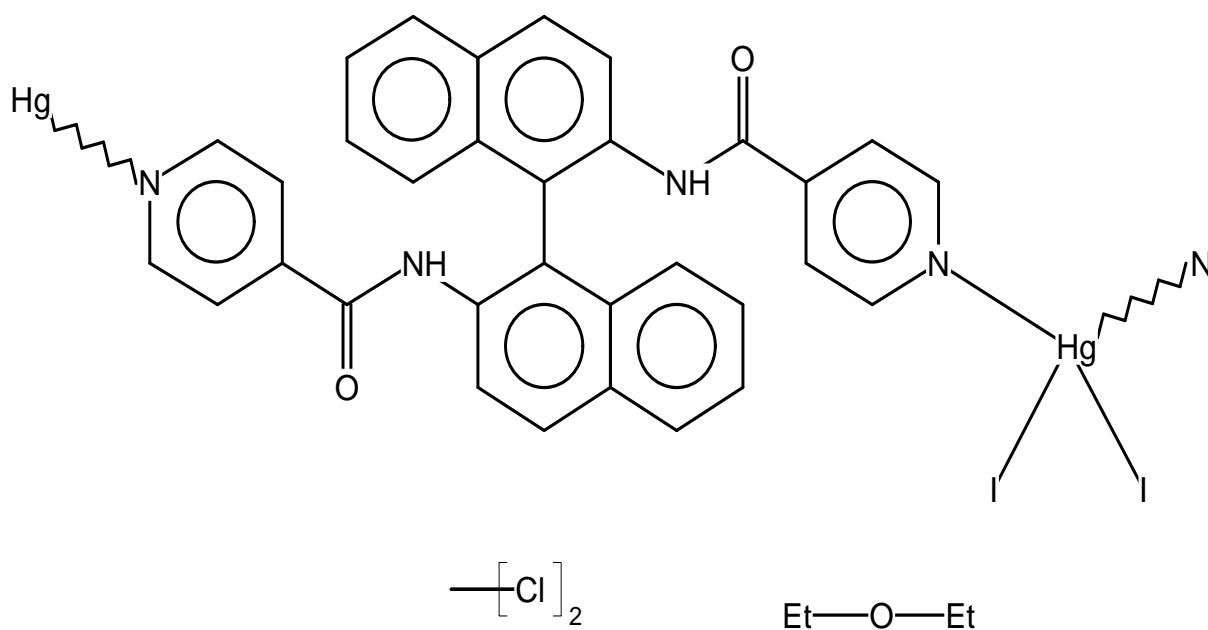
**Reference:** T.J.Burchell, R.J.Puddephatt (2005) *Inorg.Chem.* ,**44**,3718

**Formula:** (C<sub>32</sub> H<sub>22</sub> Hg<sub>1</sub> I<sub>2</sub> N<sub>4</sub> O<sub>2</sub>)<sub>n</sub>,n(C<sub>1</sub> H<sub>2</sub> Cl<sub>2</sub>),n(C<sub>4</sub> H<sub>10</sub> O<sub>1</sub>)

**Compound Name:** catena-((μ<sub>2</sub>-(R)-2,2'-bis((4-Pyridyl)carbonylamino)-1,1'-binaphthyl-N,N')-di-iodo-mercury(ii) dichloromethane diethyl ether solvate)

**Space Group:** P212121    **Cell:**    **a** 15.023(3)    **b** 15.582(3)    **c** 16.554(3)  
**Space Group No.:** 19    **(Å, °)**    **α** 90.00    **β** 90.00    **γ** 90.00

**R-Factor (%):** 4.65    **Temperature(K):** 150    **Density(g/cm<sup>3</sup>):** 1.899



## Search: search19 (Thu May 26 18:22:58 2011): Hit 6

### JAPKER

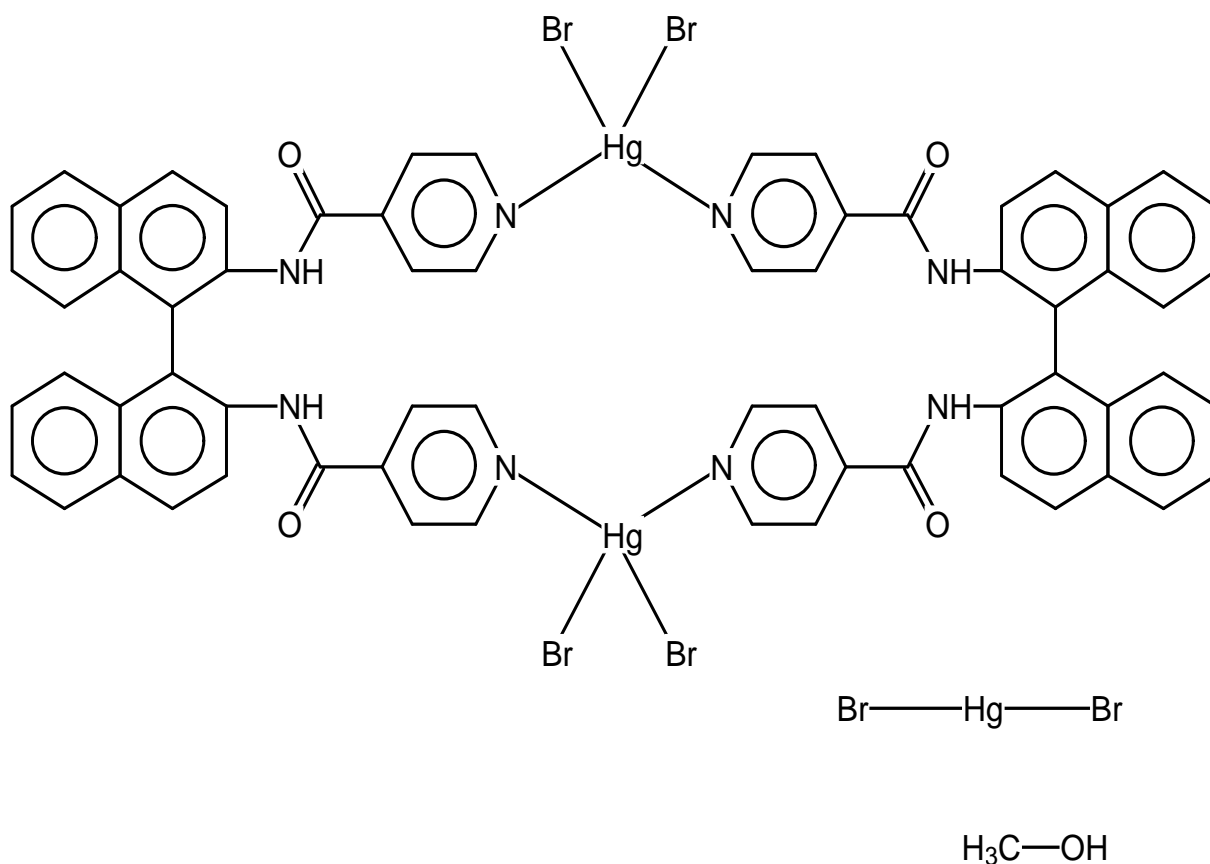
**Reference:** T.J.Burchell, R.J.Puddephatt (2005) *Inorg.Chem.* ,**44**,3718

**Formula:** C<sub>64</sub> H<sub>44</sub> Br<sub>4</sub> Hg<sub>2</sub> N<sub>8</sub> O<sub>4</sub>,Br<sub>2</sub> Hg<sub>1</sub>,C<sub>1</sub> H<sub>4</sub> O<sub>1</sub>

**Compound Name:** meso-bis(μ<sub>2</sub>-2,2'-bis((4-Pyridyl)carbonylamino)-1,1'-binaphthyl-N,N')-tetrabromo-di-mercury(ii) dibromo-mercury(ii) clathrate methanol solvate

**Space Group:** P21/c      **Cell:**      **a** 16.652(3)      **b** 12.318(3)      **c** 16.223(3)  
**Space Group No.:** 14      **(Å, °)**      **α** 90.00      **β** 102.03(3)      **γ** 90.00

**R-Factor (%):** 6.25      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 2.145



## Search: search19 (Thu May 26 18:22:58 2011): Hit 7

### JAPKIV

**Reference:** T.J.Burchell, R.J.Puddephatt (2005) *Inorg.Chem.* ,**44**,3718

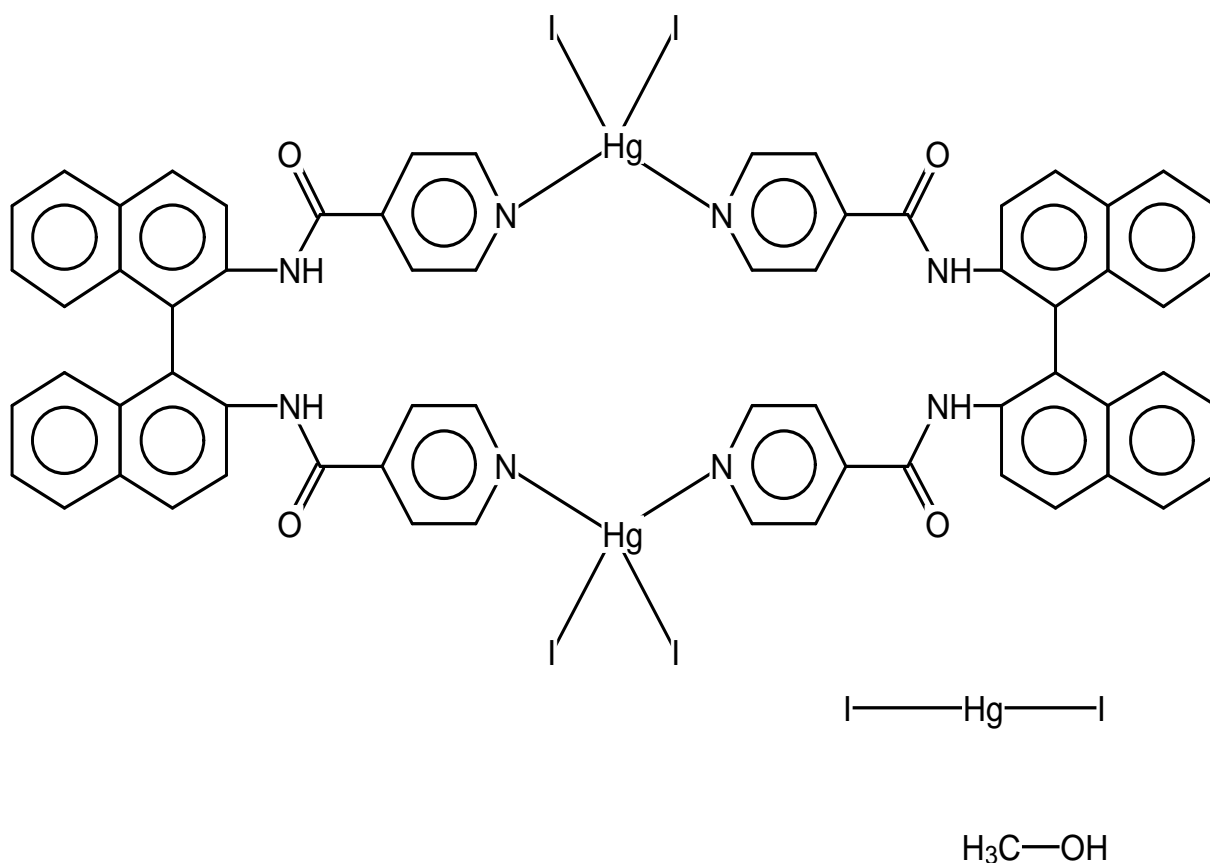
**Formula:** C<sub>64</sub> H<sub>44</sub> Hg<sub>2</sub> I<sub>4</sub> N<sub>8</sub> O<sub>4</sub>.Hg<sub>1</sub> I<sub>2</sub>.4(C<sub>1</sub> H<sub>4</sub> O<sub>1</sub>)

**Compound Name:** meso-bis(μ<sub>2</sub>-2,2'-bis((4-Pyridyl)carbonylamino)-1,1'-binaphthyl-N,N')-tetra-iodo-di-mercury(ii) di-iodo-mercury(ii) clathrate methanol solvate

**Space Group:** C2/c      **Cell:**    **a** 34.840(7)    **b** 13.241(3)    **c** 16.423(3)

**Space Group No.:** 15      **(Å, °)**    **α** 90.00      **β** 103.28(3)    **γ** 90.00

**R-Factor (%):** 9.57      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 2.234



## Search: search19 (Thu May 26 18:22:58 2011): Hit 8

### JAPKOB

**Reference:** T.J.Burchell, R.J.Puddephatt (2005) *Inorg.Chem.* ,**44**,3718

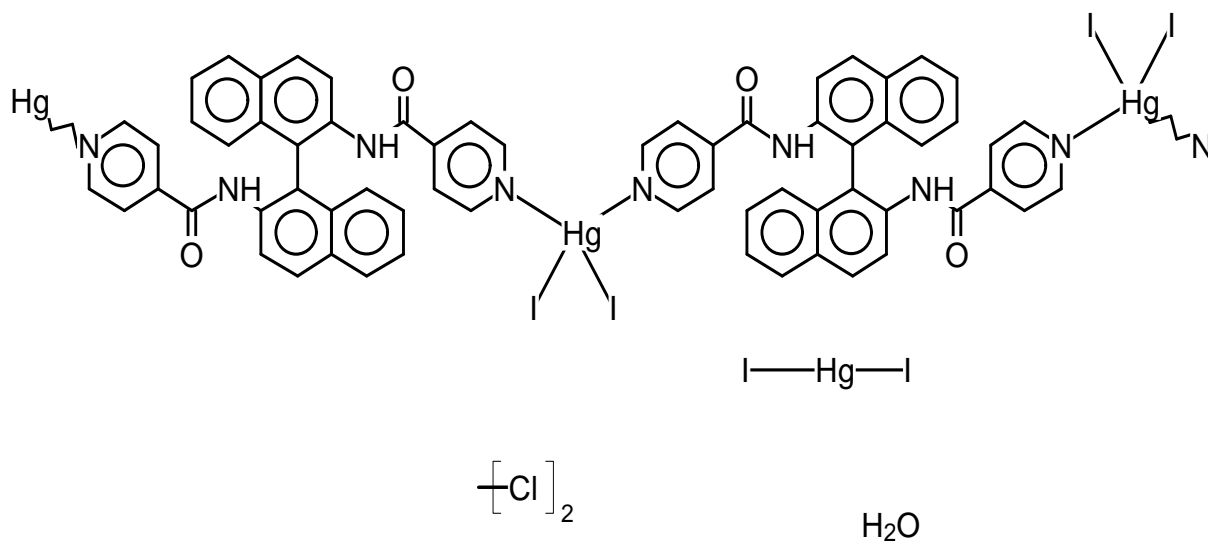
**Formula:**  $(C_{64} H_{44} Hg_2 I_4 N_8 O_4)_n, 0.17n(Hg_1 I_2), n(C_1 H_2 Cl_2), 0.17n(H_2 O_1)$

**Compound Name:** catena-(bis( $\mu_2$ -rac-2,2'-bis((4-Pyridyl)carbonylamino)-1,1'-binaphthyl-N, N')-tetraiodo-di-mercury(ii) di-iodo-mercury clathrate dichloromethane solvate hydrate)

**Space Group:** R-3      **Cell:**      **a** 26.836(4)      **b** 26.836(4)      **c** 53.305(11)

**Space Group No.:** 148      **(Å, °)**       $\alpha$  90.00       $\beta$  90.00       $\gamma$  120.00

**R-Factor (%):** 9.54      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.855



## Search: search19 (Thu May 26 18:22:58 2011): Hit 9

### YECTAC

**Reference:** T.J.Burchell, R.J.Puddephatt (2006) *Inorg.Chem.* ,**45**,650

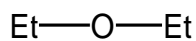
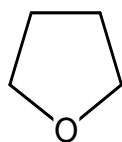
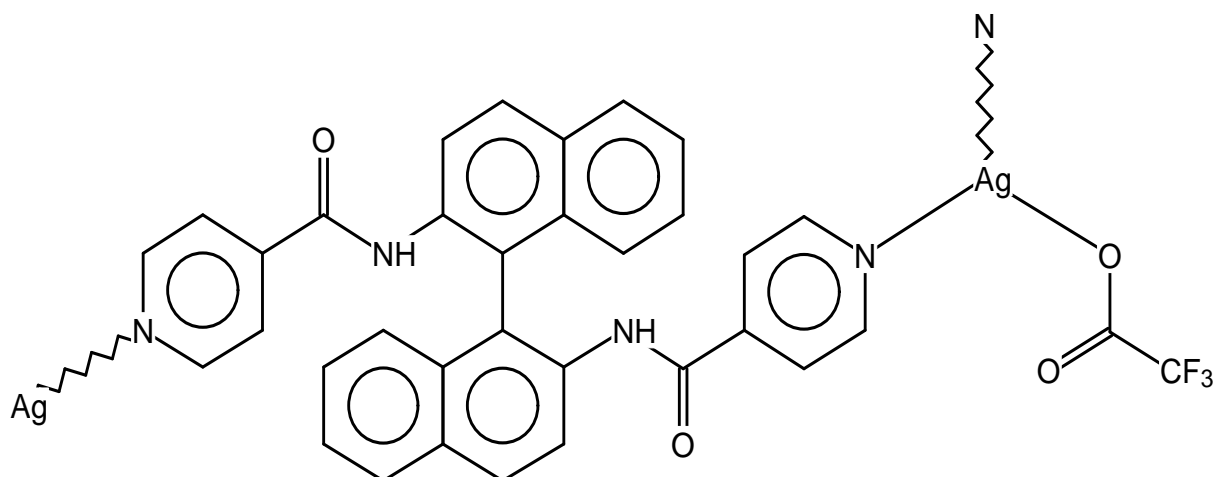
**Formula:**  $(C_{34} H_{22} Ag_1 F_3 N_4 O_4)_n, 0.7n(C_4 H_8 O_1), 0.3n(C_4 H_{10} O_1)$

**Compound Name:** catena-(( $\mu_2$ -rac-2,2'-bis(4-Pyridylcarbonylamino)-1,1'-binaphthalene-N, N')-(trifluoroacetato-O)-silver(i) tetrahydrofuran diethyl ether solvate)

**Space Group:** C2/c      **Cell:**      **a** 30.263(6)      **b** 13.942(3)      **c** 16.903(3)

**Space Group No.:** 15      **(Å, °)**       $\alpha$  90.00       $\beta$  109.96(3)       $\gamma$  90.00

**R-Factor (%):** 6.22      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.562



## Search: search19 (Thu May 26 18:22:58 2011): Hit 10

YECTUW

**Reference:** T.J.Burchell, R.J.Puddephatt (2006) *Inorg.Chem.* ,**45**,650

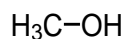
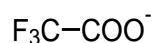
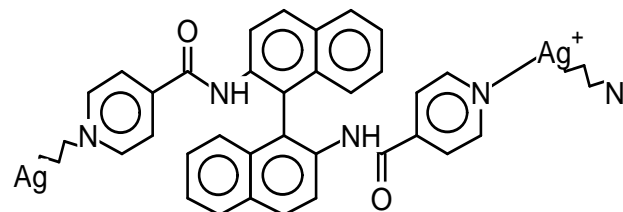
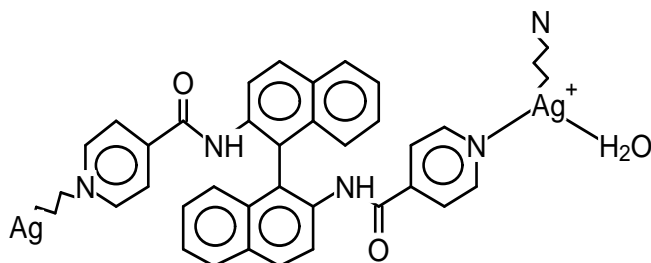
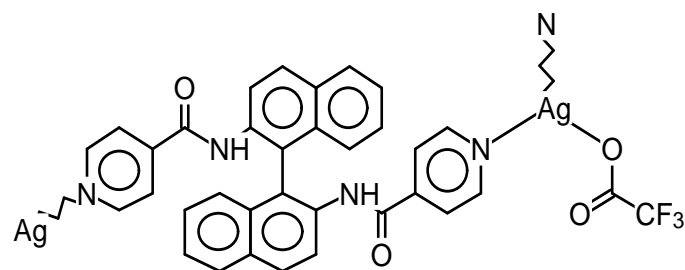
**Formula:**  $(C_{34} H_{22} Ag_1 F_3 N_4 O_4)_2n, n(C_{32} H_{24} Ag_1 N_4 O_3^{1+}), n(C_{32} H_{22} Ag_1 N_4 O_2^{1+}), 2n(C_2 F_3)$

**Compound Name:** catena-(bis(( $\mu_2$ -(R)-2,2'-bis(4-Pyridylcarbonylamino)-1,1'-binaphthalene-N,N')-(trifluoroacetato-O)-silver(i)) ( $\mu_2$ -(R)-2,2'-bis(4-pyridylcarbonylamino)-1,1'-binaphthalene-N,N')-aqua-silver(i) ( $\mu_2$ -(R)-2,2'-bis(4-pyridylcarbonylamino)-1,1'-binaphthalene-N,N')-silver(i) bis(trifluoroacetate) tetrahydrofuran methanol solvate monohydrate)

**Space Group:** P212121 **Cell:** **a** 23.500(5) **b** 23.828(5) **c** 26.897(5)

**Space Group No.:** 19 **(Å, °)**  **$\alpha$**  90.00  **$\beta$**  90.00  **$\gamma$**  90.00

**R-Factor (%):** 6.36 **Temperature(K):** 150 **Density(g/cm<sup>3</sup>):** 1.479





## Search Overview

**Search:** search20  
**Date/Time done:** Thu May 26 18:24:48 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:** 6

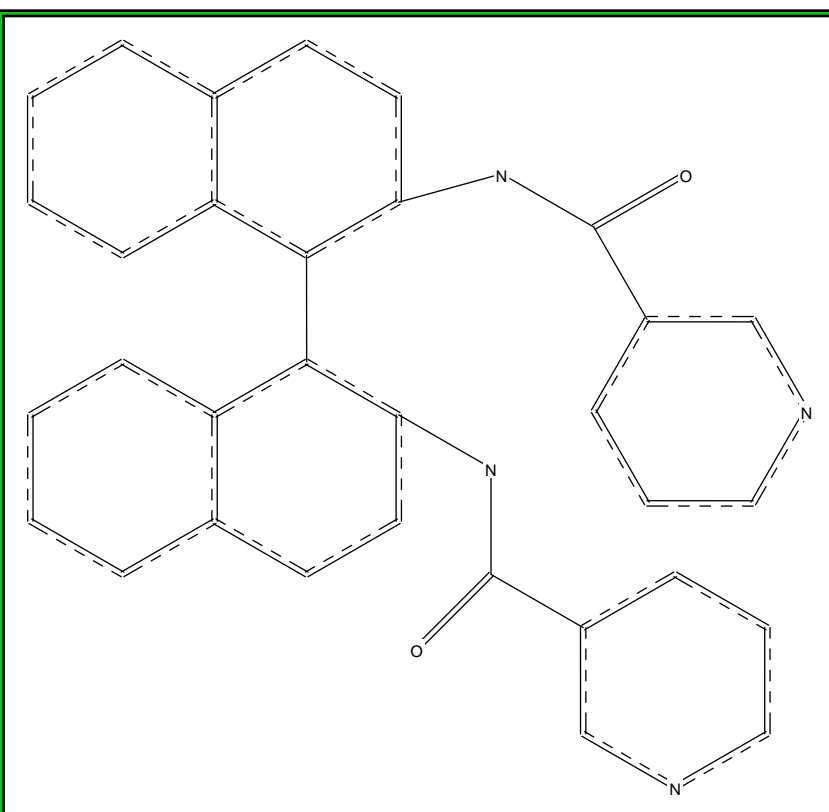
*Summary of queries used. Search found structures that:*

match

**Query 1**

**Query 2**

**Query 1**



**Query 2**

4M

# Search: search20 (Thu May 26 18:24:48 2011): Hit 1

FEJVAS

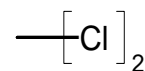
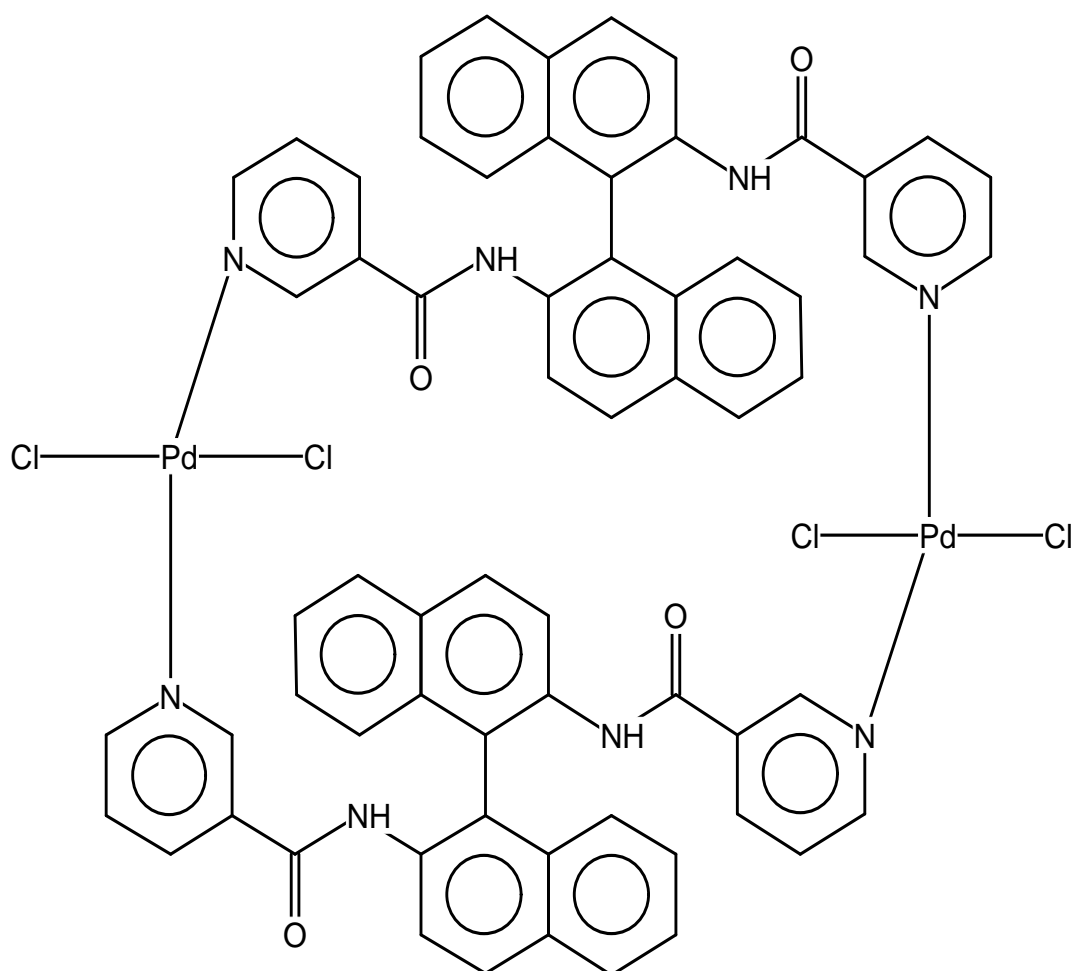
**Reference:** T.J.Burchell, D.J.Eisler, R.J.Puddephatt (2005)  
*Dalton Trans.* ,268

**Formula:** C<sub>64</sub> H<sub>44</sub> Cl<sub>4</sub> N<sub>8</sub> O<sub>4</sub> Pd<sub>2</sub>·5.05(C<sub>1</sub> H<sub>2</sub> Cl<sub>2</sub>)

**Compound Name:** trans-(bis(μ<sub>2</sub>-rac-(2,2'-bis(3-Pyridylcarbonylamino)-1,1'-binaphthyl))-tetrachloro-di-palladium(ii)) dichloromethane solvate

**Space Group:** C2/c      **Cell:**    **a** 33.094(7)    **b** 14.712(3)    **c** 35.077(7)  
**Space Group No.:** 15      **(Å, °)**    **α** 90.00      **β** 107.77(3)    **γ** 90.00

**R-Factor (%):** 8.71      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.448



## Search: search20 (Thu May 26 18:24:48 2011): Hit 2

### JAPJUG

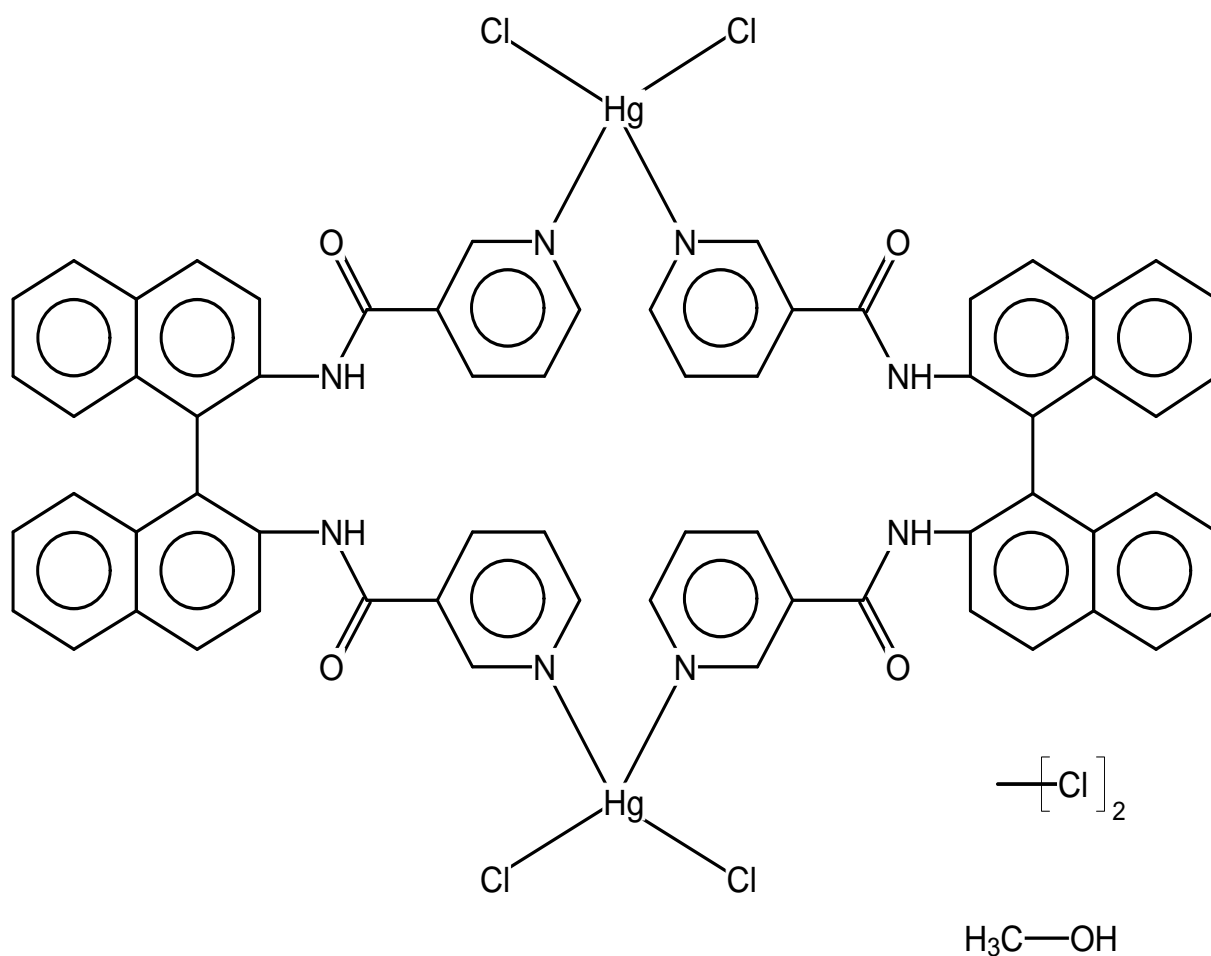
**Reference:** T.J.Burchell, R.J.Puddephatt (2005) *Inorg.Chem.* ,**44**,3718

**Formula:** C<sub>64</sub> H<sub>44</sub> Cl<sub>4</sub> Hg<sub>2</sub> N<sub>8</sub> O<sub>4</sub>,0.8(C<sub>1</sub> H<sub>2</sub> Cl<sub>2</sub>),1.2(C<sub>1</sub> H<sub>4</sub> O<sub>1</sub>)

**Compound Name:** meso-bis(μ<sub>2</sub>-2,2'-bis((3-Pyridyl)carbonylamino)-1,1'-binaphthyl-N,N')-tetrachloro-di-mercury(ii) dichloromethane methanol solvate

**Space Group:** P21/c      **Cell:**      **a** 18.204(4)      **b** 10.865(2)      **c** 16.030(3)  
**Space Group No.:** 14      **(Å, °)**      α 90.00      β 91.91(3)      γ 90.00

**R-Factor (%):** 7.09      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.717



## Search: search20 (Thu May 26 18:24:48 2011): Hit 3

### JAPKAN

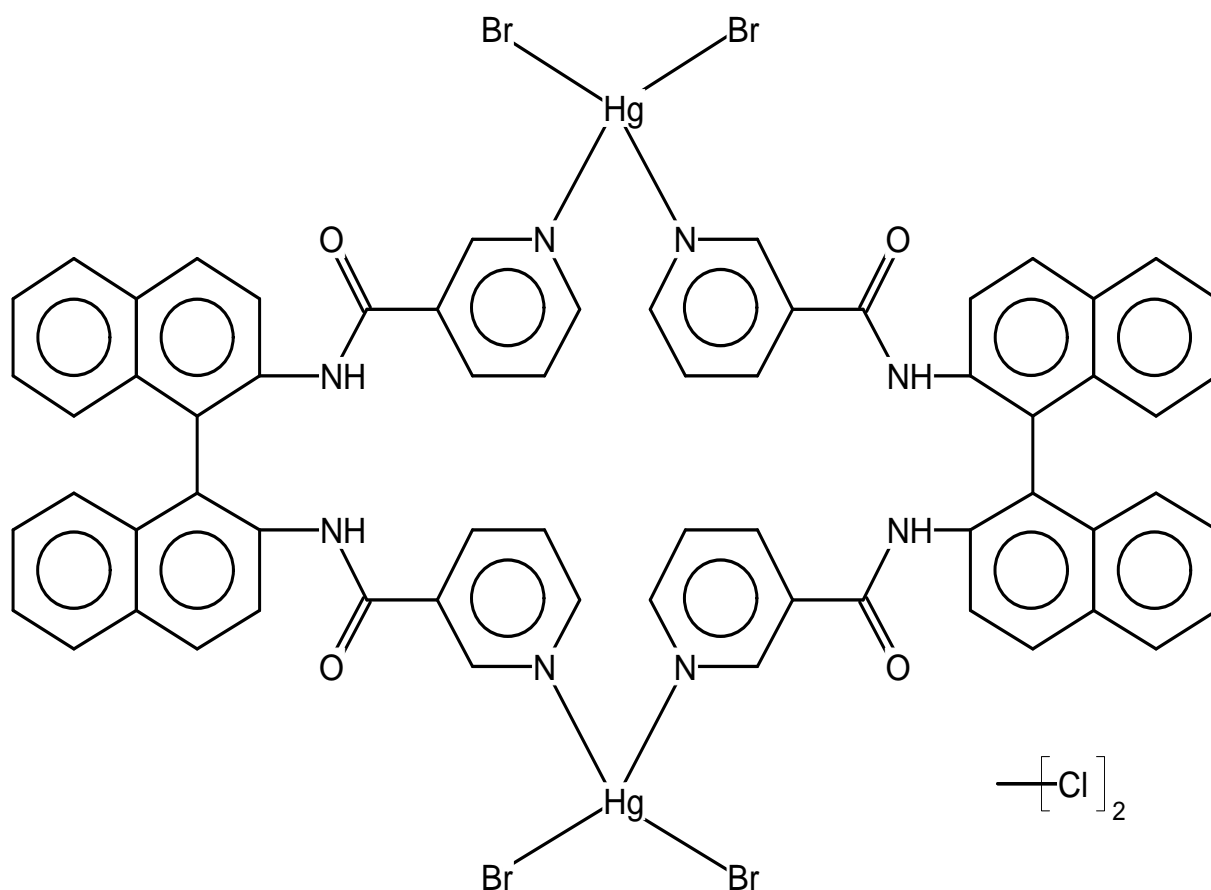
**Reference:** T.J.Burchell, R.J.Puddephatt (2005) *Inorg.Chem.* ,**44**,3718

**Formula:** C<sub>64</sub> H<sub>44</sub> Br<sub>4</sub> Hg<sub>2</sub> N<sub>8</sub> O<sub>4</sub>·2(C<sub>1</sub> H<sub>2</sub> Cl<sub>2</sub>)

**Compound Name:** meso-bis(μ<sub>2</sub>-2,2'-bis((3-Pyridyl)carbonylamino)-1,1'-binaphthyl-N,N')-tetrabromo-di-mercury(ii) dichloromethane solvate

**Space Group:** P21/c      **Cell:**      **a** 18.187(4)      **b** 11.165(2)      **c** 16.286(3)  
**Space Group No.:** 14      **(Å, °)**      **α** 90.00      **β** 92.50(3)      **γ** 90.00

**R-Factor (%):** 5.14      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.890



## Search: search20 (Thu May 26 18:24:48 2011): Hit 4

### YECTEG

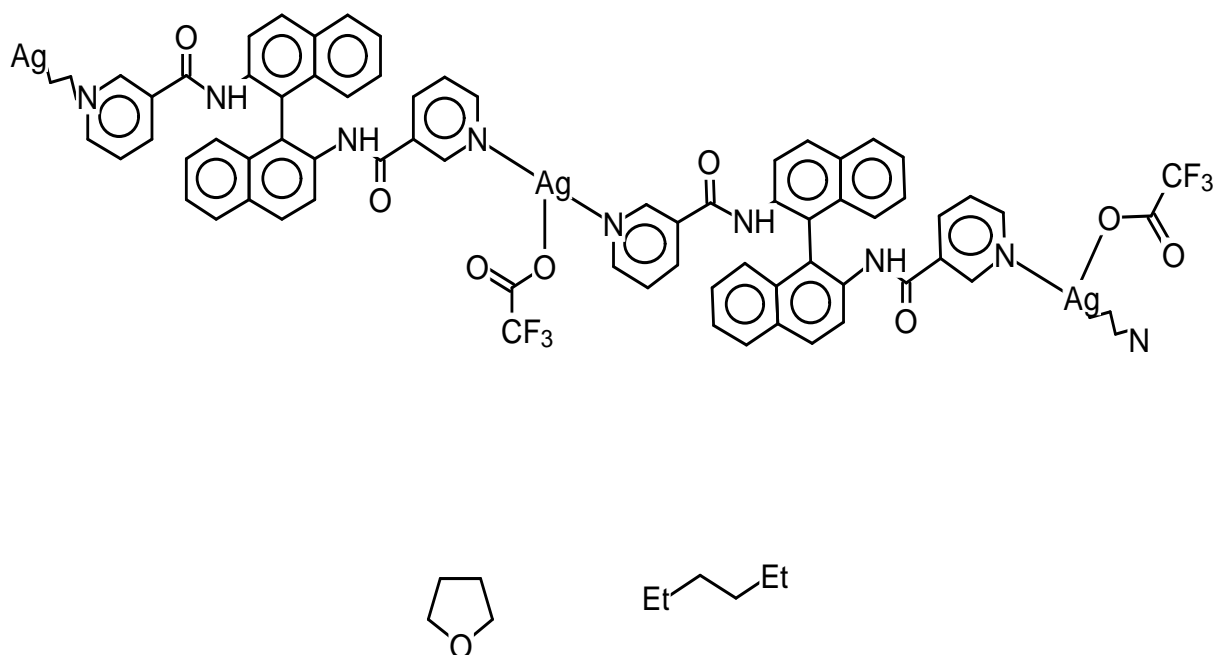
**Reference:** T.J.Burchell, R.J.Puddephatt (2006) *Inorg.Chem.* ,**45**,650

**Formula:** (C<sub>68</sub> H<sub>44</sub> Ag<sub>2</sub> F<sub>6</sub> N<sub>8</sub> O<sub>8</sub>)<sub>n</sub>,n(C<sub>4</sub> H<sub>8</sub> O<sub>1</sub>),1.5n(C<sub>6</sub> H<sub>14</sub>)

**Compound Name:** catena-(bis(μ<sub>2</sub>-rac-2,2'-bis(3-Pyridylcarbonylamino)-1,1'-binaphthalene-N,N')-bis(trifluoroacetato-O)-di-silver(i) tetrahydrofuran n-hexane solvate)

**Space Group:** P21/n      **Cell:**      **a** 14.291(3)      **b** 10.937(2)      **c** 24.711(5)  
**Space Group No.:** 14      **(Å, °)**      α 90.00      β 92.77(3)      γ 90.00

**R-Factor (%):** 8.38      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.405



## Search: search20 (Thu May 26 18:24:48 2011): Hit 5

### YECTIK

**Reference:** T.J.Burchell, R.J.Puddephatt (2006) *Inorg.Chem.* ,**45**,650

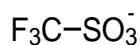
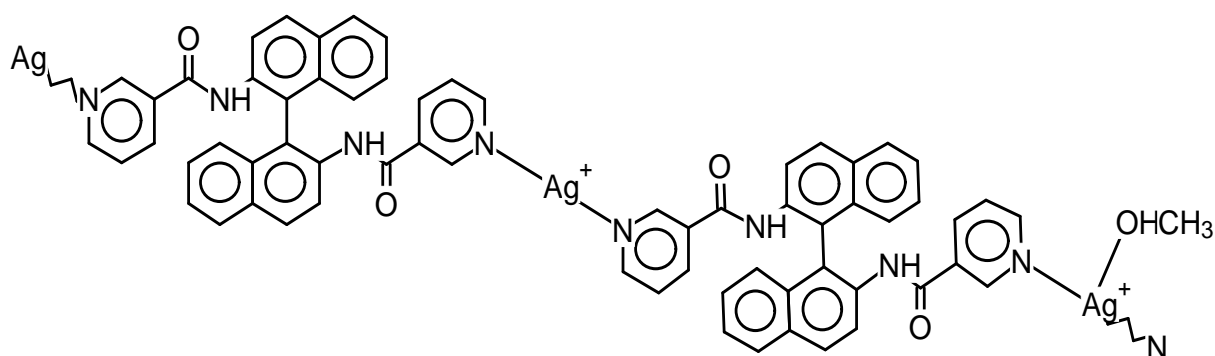
**Formula:**  $(C_{65} H_{48} Ag_2 N_8 O_5^{2+})_n, 2n(C_1 F_3 O_3 S_1^{-1}), n(C_4 H_8 O_1)$

**Compound Name:** catena-(bis( $\mu_2$ -rac-2,2'-bis(3-Pyridylcarbonylamino)-1,1'-binaphthalene-N,N')-methanol-di-silver(i) bis(trifluoromethanesulfonate) tetrahydrofuran solvate)

**Space Group:** P-1      **Cell:**      **a** 13.882(3)      **b** 13.959(3)      **c** 19.119(4)

**Space Group No.:** 2      **(Å, °)**       $\alpha$  99.13(3)       $\beta$  103.92(3)       $\gamma$  105.97(3)

**R-Factor (%):** 5.28      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.591



## Search: search20 (Thu May 26 18:24:48 2011): Hit 6

YECTOQ

**Reference:** T.J.Burchell, R.J.Puddephatt (2006) *Inorg.Chem.* ,**45**,650

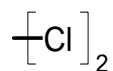
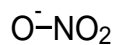
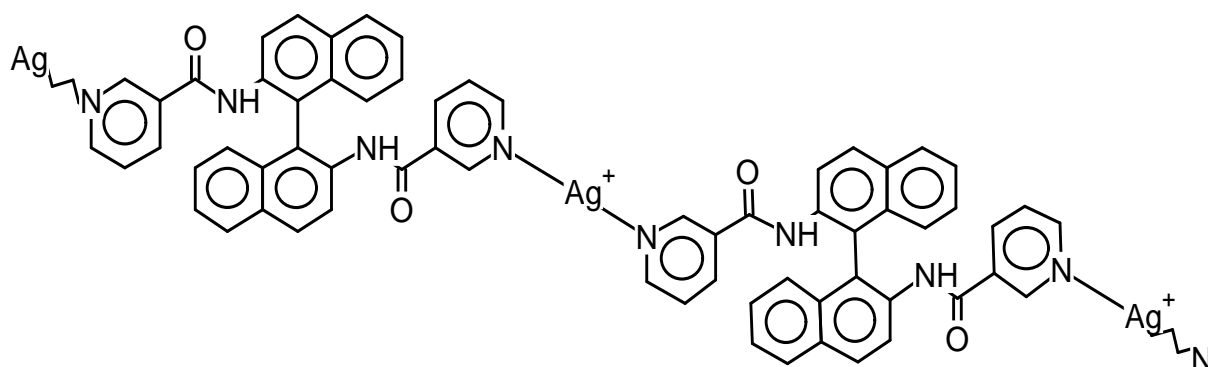
**Formula:**  $(C_{64} H_{44} Ag_2 N_8 O_4^{2+})_n, 2n(N_1 O_3^{1-}), 4n(C_1 H_2 Cl_2)$

**Compound Name:** catena-(bis( $\mu_2$ -rac-2,2'-bis(3-Pyridylcarbonylamino)-1,1'-binaphthalene-N,N')-di-silver(i) dinitrate dichloromethane solvate)

**Space Group:** P-1      **Cell:**      **a** 13.459(3)      **b** 13.672(3)      **c** 19.467(4)

**Space Group No.:** 2      **(Å, °)**       $\alpha$  97.74(3)       $\beta$  106.86(3)       $\gamma$  94.18(3)

**R-Factor (%):** 6.82      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.643

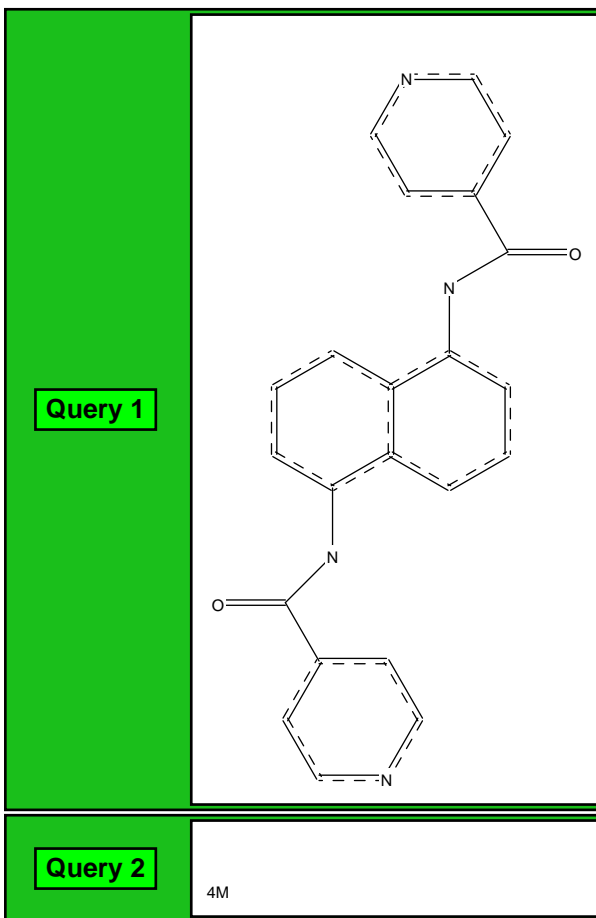


## Search Overview

**Search:** search23  
**Date/Time done:** Thu May 26 18:33:03 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:** 3

Summary of queries used. Search found structures that:

Query 1 <sup>match</sup> Query 2





## Search: search23 (Thu May 26 18:33:03 2011): Hit 1

### YOFTET

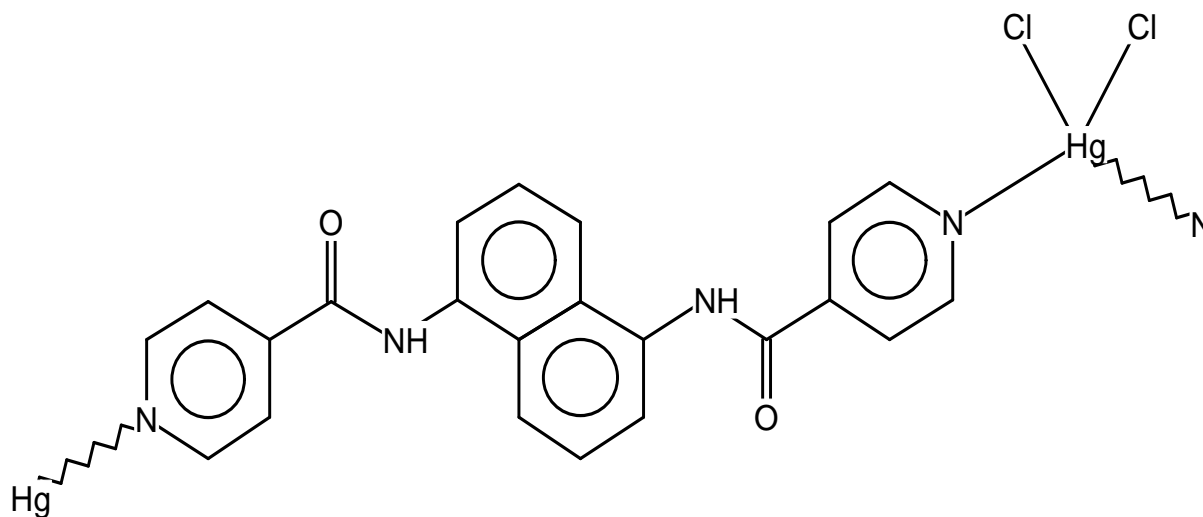
**Reference:** S.A.Cardile, T.J.Burchell, M.C.Jennings, R.J.Puddephatt  
(2007) *J.Inorg.Organomet.Polym.Mater.* ,17,235

**Formula:** (C<sub>22</sub> H<sub>16</sub> Cl<sub>2</sub> Hg<sub>1</sub> N<sub>4</sub> O<sub>2</sub>)<sub>n</sub>

**Compound Name:** catena-((μ<sub>2</sub>-1,5-bis(isonicotinamido)naphthalene)-dichloro-mercury(ii))

**Space Group:** P-1      **Cell:**    **a** 4.813(0)    **b** 15.264(0)    **c** 15.774(0)  
**Space Group No.:** 2      **(Å, °)**    α 112.03      β 95.81(0)      γ 98.61(0)

**R-Factor (%):** 7.55      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 2.031



## Search: search23 (Thu May 26 18:33:03 2011): Hit 2

### YOFTIX

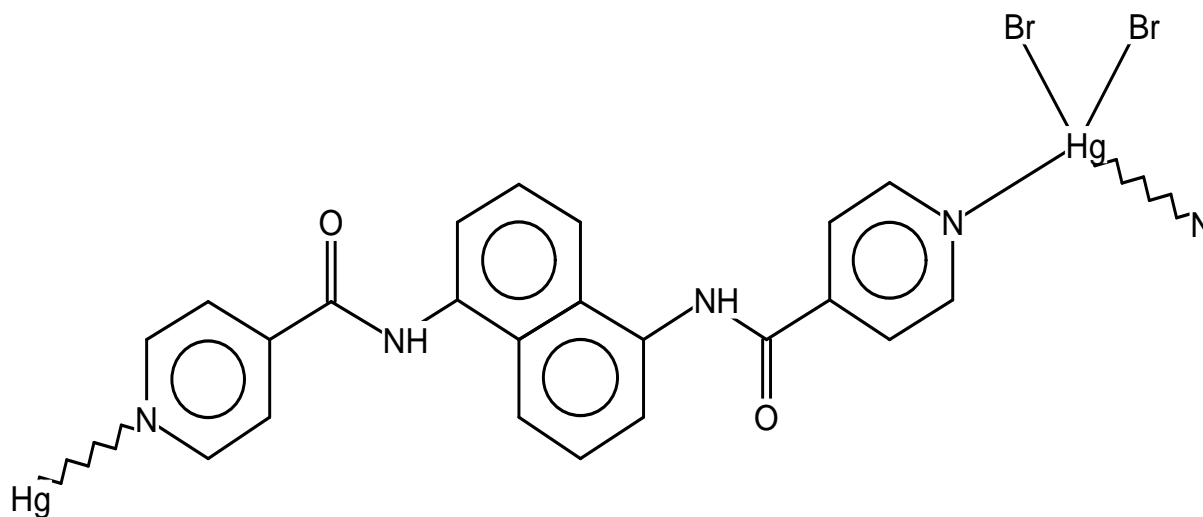
**Reference:** S.A.Cardile, T.J.Burchell, M.C.Jennings, R.J.Puddephatt  
(2007) *J.Inorg.Organomet.Polym.Mater.* ,17,235

**Formula:** (C<sub>22</sub> H<sub>16</sub> Br<sub>2</sub> Hg<sub>1</sub> N<sub>4</sub> O<sub>2</sub>)<sub>n</sub>

**Compound Name:** catena-((μ<sub>2</sub>-1,5-bis(isonicotinamido)naphthalene)-dibromo-mercury(ii))

**Space Group:** P-1      **Cell:**    **a** 4.816(0)    **b** 15.646(1)    **c** 15.752(1)  
**Space Group No.:** 2      **(Å, °)**    α 111.26(0)    β 95.49(0)    γ 98.68(0)

**R-Factor (%):** 3.92      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 2.244



## Search: search23 (Thu May 26 18:33:03 2011): Hit 3

### YOFTOD

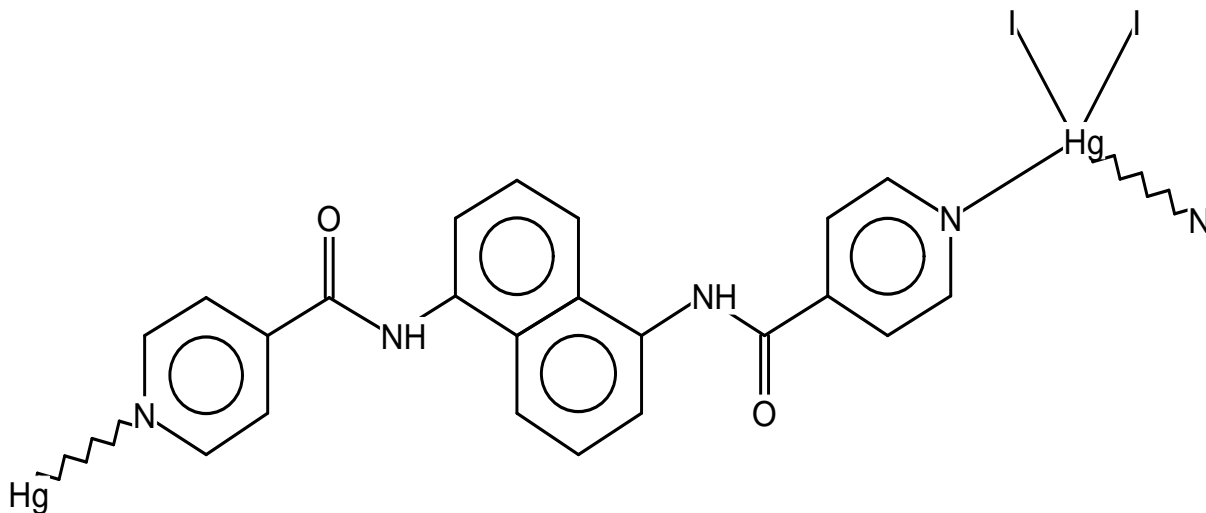
**Reference:** S.A.Cardile, T.J.Burchell, M.C.Jennings, R.J.Puddephatt  
(2007) *J.Inorg.Organomet.Polym.Mater.* ,17,235

**Formula:** (C<sub>22</sub> H<sub>16</sub> Hg<sub>1</sub> I<sub>2</sub> N<sub>4</sub> O<sub>2</sub>)<sub>n</sub>

**Compound Name:** catena-((μ<sub>2</sub>-1,5-bis(isonicotinamido)naphthalene)-diiodo-mercury(ii))

**Space Group:** Pbcn      **Cell:**      **a** 9.624(0)      **b** 14.447(0)      **c** 16.150(0)  
**Space Group No.:** 60      **(Å, °)**      α 90.00      β 90.00      γ 90.00

**R-Factor (%):** 4.58      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 2.434



## Search Overview

**Search:** search24  
**Date/Time done:** Thu May 26 18:36:16 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

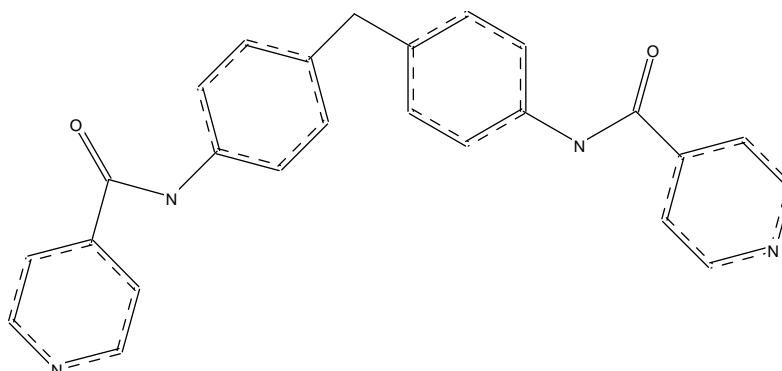
*Summary of queries used. Search found structures that:*

match

**Query 1**

**Query 2**

**Query 1**



**Query 2**

4M

## Search: search24 (Thu May 26 18:36:16 2011): Hit 1

### LOKGEY

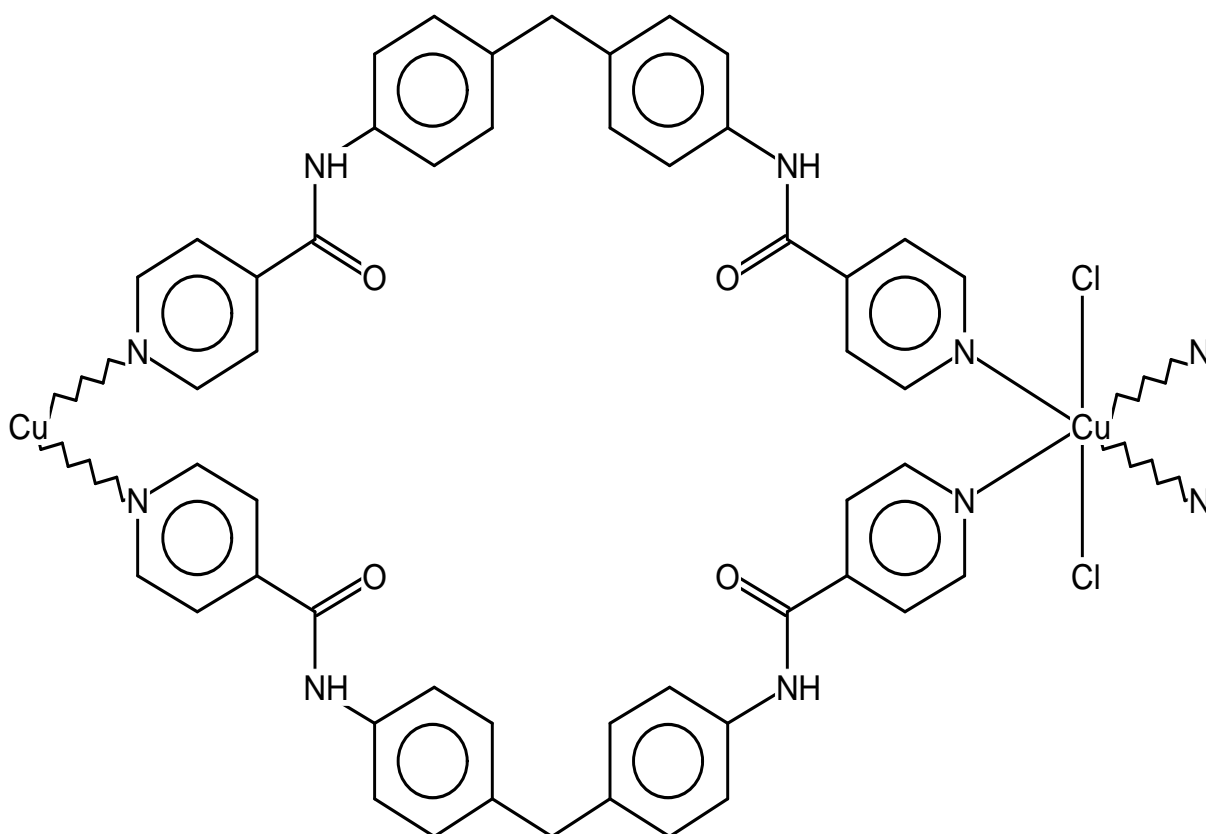
**Reference:** Chun-Wei Yeh, Jhy-Der Chen, Ju-Chun Wang (2008)  
*Polyhedron* ,27,3611

**Formula:** (C<sub>50</sub> H<sub>40</sub> Cl<sub>2</sub> Cu<sub>1</sub> N<sub>8</sub> O<sub>4</sub>)<sub>n</sub>

**Compound Name:** catena-[bis(μ<sub>2</sub>-N,N'-(Methylenedi-p-phenylene)bis(pyridine-4-carboxamide))-dichloro-copper(ii) unknown solvate]

**Space Group:** C2/c      **Cell:**    **a** 25.987(3)    **b** 19.128(3)    **c** 15.500(2)  
**Space Group No.:** 15      **(Å, °)**    **α** 90.00      **β** 121.35(0)    **γ** 90.00

**R-Factor (%):** 6.61      **Temperature(K):** 295      **Density(g/cm<sup>3</sup>):** 0.960



## Search: search24 (Thu May 26 18:36:16 2011): Hit 2

### LOKGIC

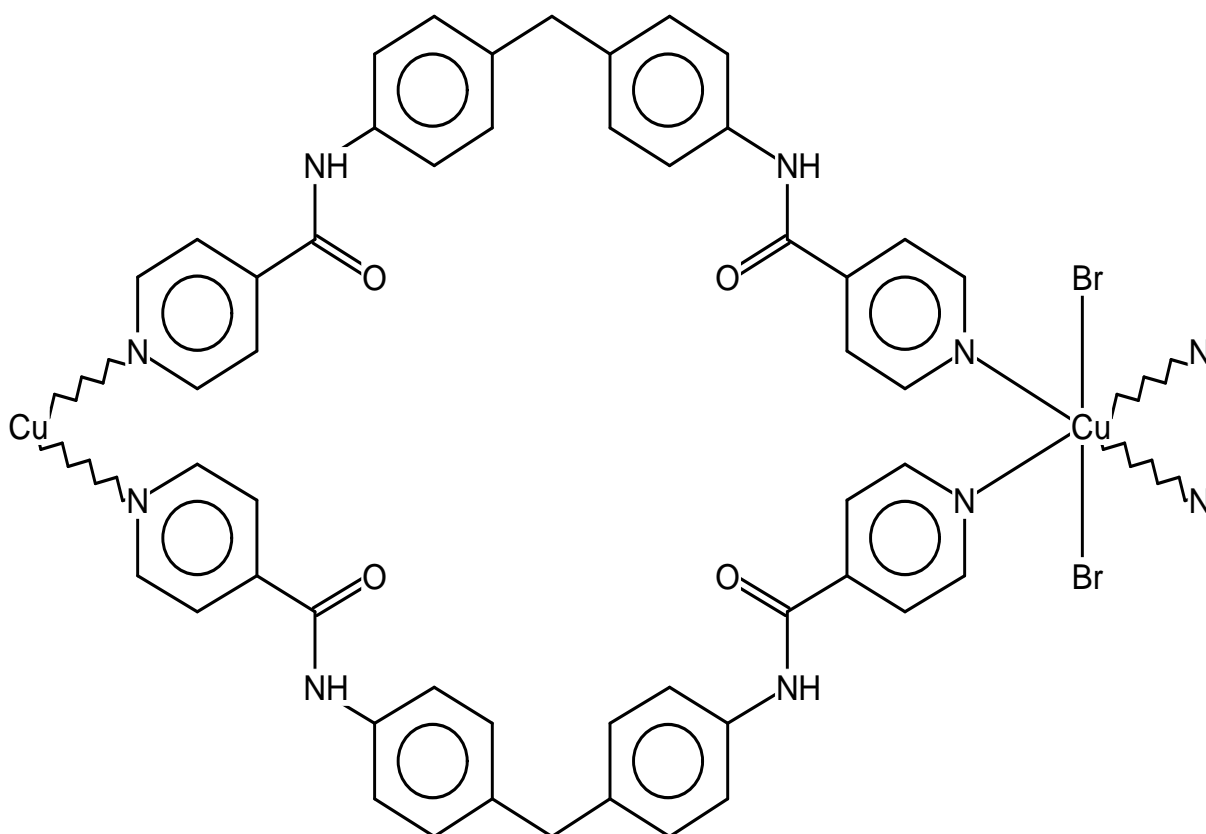
**Reference:** Chun-Wei Yeh, Jhy-Der Chen, Ju-Chun Wang (2008)  
*Polyhedron* ,27,3611

**Formula:** (C<sub>50</sub> H<sub>40</sub> Br<sub>2</sub> Cu<sub>1</sub> N<sub>8</sub> O<sub>4</sub>)<sub>n</sub>

**Compound Name:** catena-[bis(μ<sub>2</sub>-N,N'-(Methylenedi-p-phenylene)bis(pyridine-4-carboxamide))-dibromo-copper(ii) unknown solvate]

**Space Group:** C2/c      **Cell:**      **a** 26.737(4)      **b** 19.056(4)      **c** 15.746(3)  
**Space Group No.:** 15      **(Å, °)**      **α** 90.00      **β** 122.04(1)      **γ** 90.00

**R-Factor (%):** 7.56      **Temperature(K):** 295      **Density(g/cm<sup>3</sup>):** 1.016



## Search: search24 (Thu May 26 18:36:16 2011): Hit 3

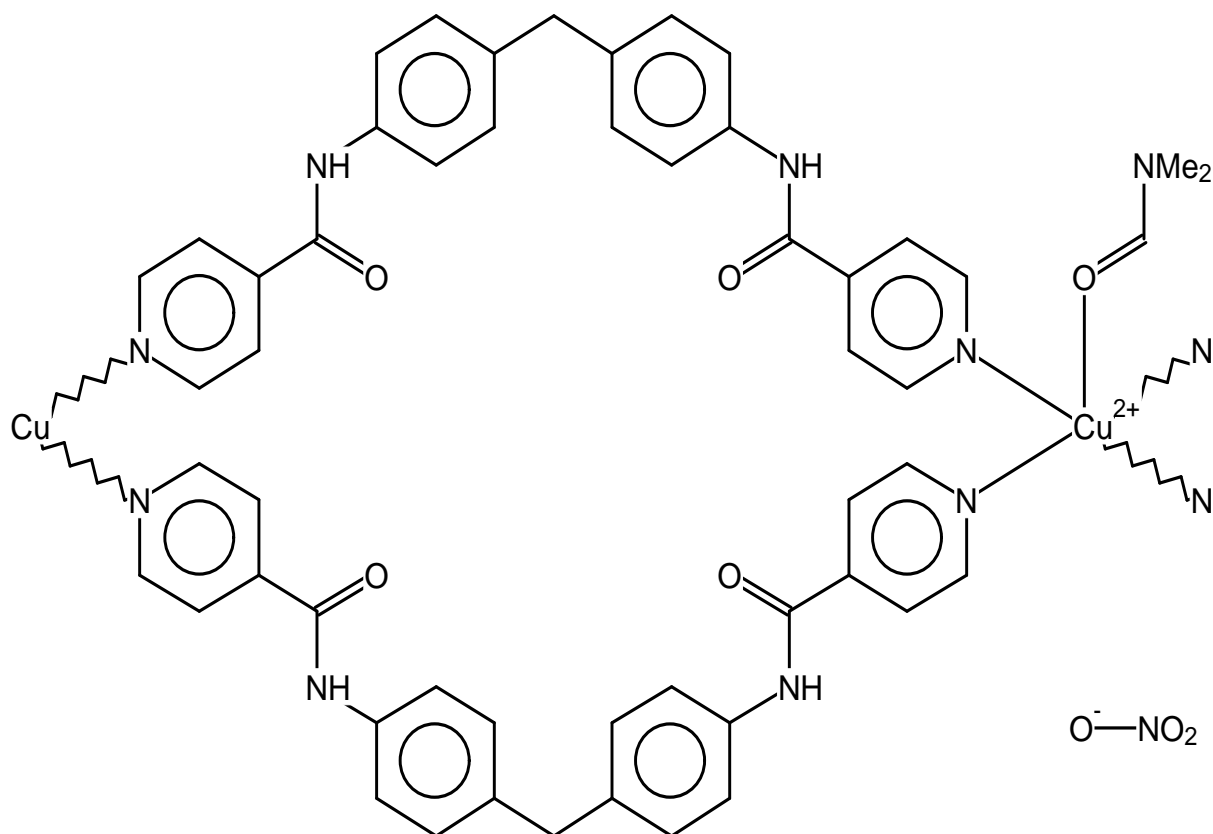
### LOKGOI

**Reference:** Chun-Wei Yeh, Jhy-Der Chen, Ju-Chun Wang (2008)  
*Polyhedron* ,27,3611

**Formula:**  $(C_{53} H_{47} Cu_1 N_9 O_5^{2+})_n, 2n(N_1 O_3^{1-})$

**Compound Name:** catena-[bis( $\mu_2$ -N,N'-(Methylenedi-p-phenylene)bis(pyridine-4-carboxamide))-(dimethylformamide)-copper(ii) dinitrate unknown solvate]

<b>Space Group:</b>	P-1	<b>Cell:</b>	<b>a</b> 13.079(1)	<b>b</b> 16.165(1)	<b>c</b> 16.828(1)
<b>Space Group No.:</b>	2	<b>(Å, °)</b>	$\alpha$ 105.66(0)	$\beta$ 94.35(0)	$\gamma$ 112.77(0)
<b>R-Factor (%):</b>	5.76	<b>Temperature(K):</b>	297	<b>Density(g/cm<sup>3</sup>):</b>	1.157



## Search: search24 (Thu May 26 18:36:16 2011): Hit 4

### LOKGUO

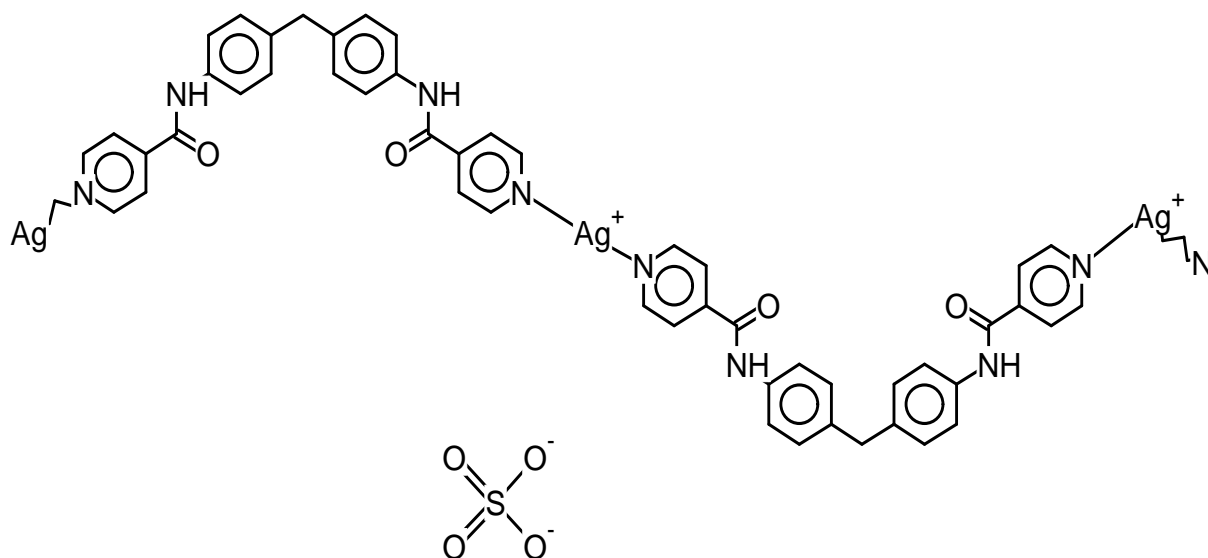
**Reference:** Chun-Wei Yeh, Jhy-Der Chen, Ju-Chun Wang (2008)  
*Polyhedron* ,27,3611

**Formula:** (C<sub>50</sub> H<sub>40</sub> Ag<sub>2</sub> N<sub>8</sub> O<sub>4</sub> 2<sup>+</sup>)<sub>n</sub>,n(O<sub>4</sub> S<sub>1</sub> 2<sup>-</sup>)

**Compound Name:** catena-[bis(μ<sub>2</sub>-N,N'-(Methylenedi-p-phenylene)bis(pyridine-4-carboxamide))-di-silver(i) sulfate unknown solvate]

**Space Group:** P-1      **Cell:**      **a** 8.986(1)      **b** 17.014(1)      **c** 20.087(3)  
**Space Group No.:** 2      (**Å, °**)      **α** 100.41(1)      **β** 101.13(1)      **γ** 90.54(1)

**R-Factor (%):** 5.19      **Temperature(K):** 295      **Density(g/cm<sup>3</sup>):** 1.266





## Search: search24 (Thu May 26 18:36:16 2011): Hit 5

### LOKHAV

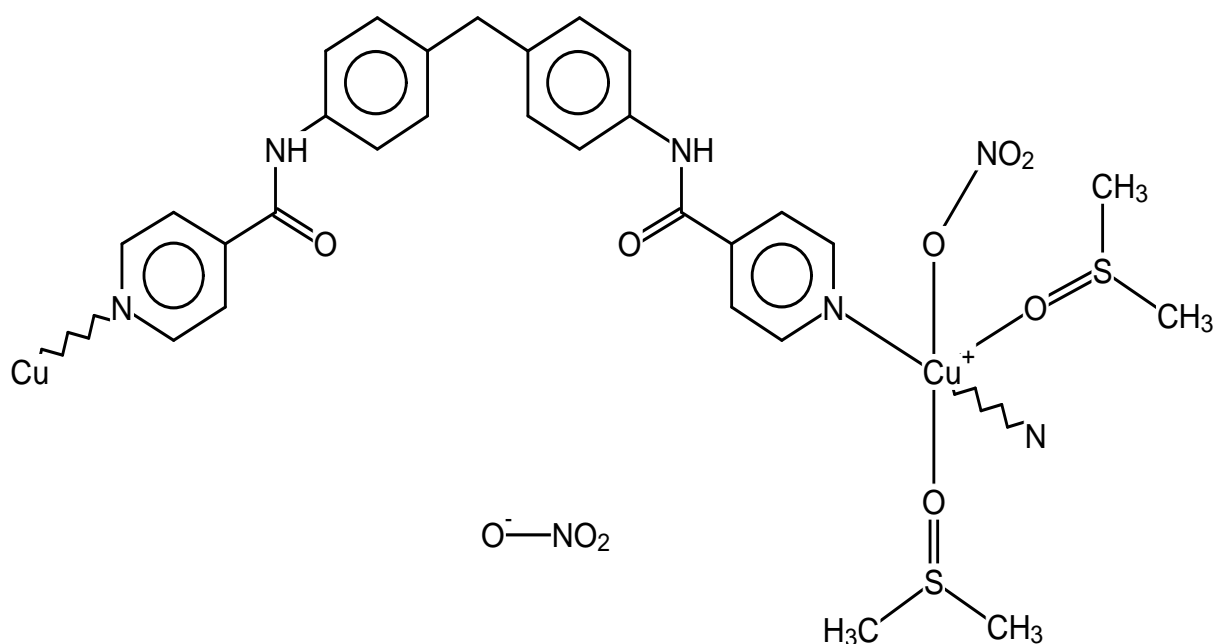
**Reference:** Chun-Wei Yeh, Jhy-Der Chen, Ju-Chun Wang (2008)  
*Polyhedron* ,27,3611

**Formula:** (C<sub>29</sub> H<sub>32</sub> Cu<sub>1</sub> N<sub>5</sub> O<sub>7</sub> S<sub>2</sub><sup>1+</sup>)<sub>n</sub>,n(N<sub>1</sub> O<sub>3</sub><sup>1-</sup>)

**Compound Name:** catena-[(μ<sub>2</sub>-N,N'-(Methylenedi-p-phenylene)bis(pyridine-4-carboxamide)  
)-bis(dimethylsulfoxide)-nitrate-copper(ii) nitrate unknown solvate]

**Space Group:** Pbcm      **Cell:**      **a** 8.802(0)      **b** 22.706(0)      **c** 17.165(0)  
**Space Group No.:** 57      **(Å, °)**      **α** 90.00      **β** 90.00      **γ** 90.00

**R-Factor (%):** 7.61      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.457



## Search Overview

**Search:** search2  
**Date/Time done:** Fri May 27 14:15:58 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:** 3

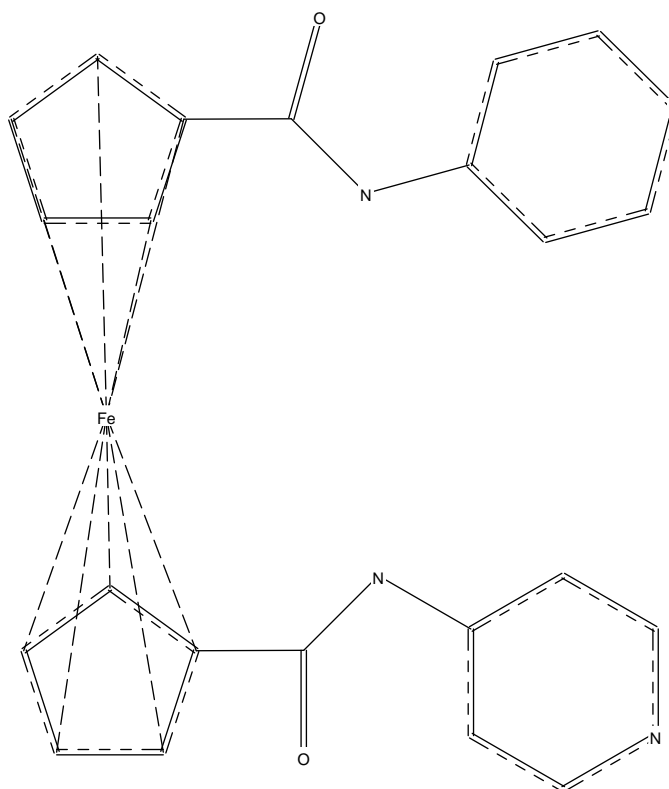
*Summary of queries used. Search found structures that:*

match

**Query 1**

**Query 2**

**Query 1**



**Query 2**

4M

## Search: search2 (Fri May 27 14:15:58 2011): Hit 1

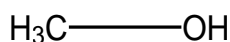
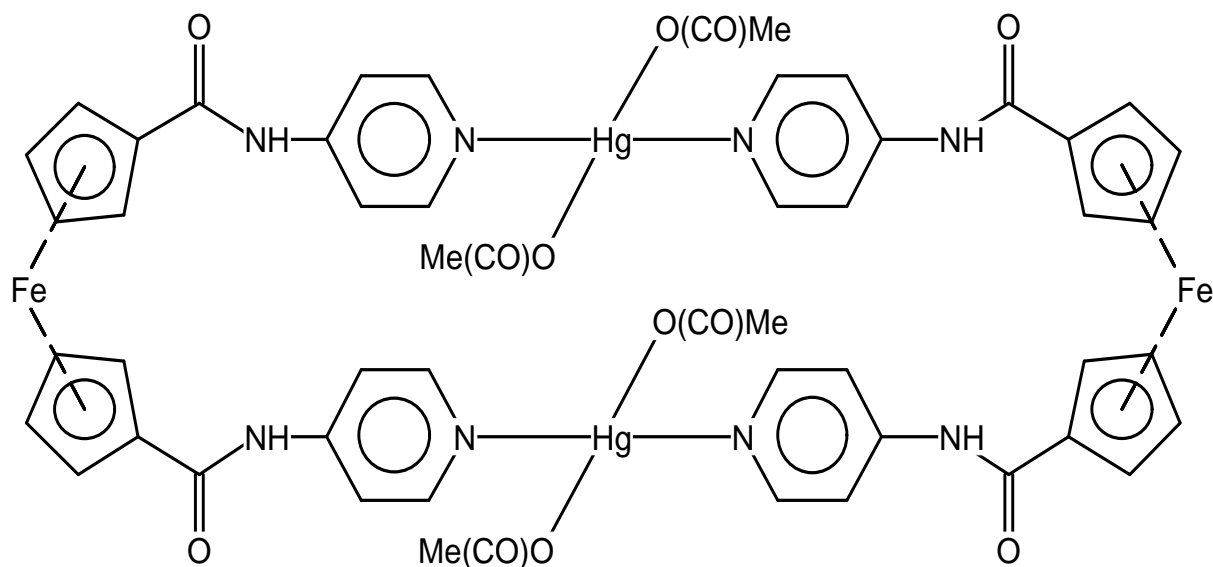
### TABBOO

**Reference:** Gang Li, Yinglin Song, Hongwei Hou, Linke Li, Yaoting Fan, Yu Zhu, Xiangru Meng, Liwei Mi (2003) *Inorg.Chem.* ,**42**, 913

**Formula:** C<sub>52</sub> H<sub>48</sub> Fe<sub>2</sub> Hg<sub>2</sub> N<sub>8</sub> O<sub>12</sub>, 2(C<sub>1</sub> H<sub>4</sub> O<sub>1</sub>)

**Compound Name:** bis( $\mu_2$ -1,1'-bis((4-pyridylamino)carbonyl)ferrocenyl)-tetrakis(methoxycarbonyl)-di-mercury methanol solvate

<b>Space Group:</b>	P-1	<b>Cell:</b>	<b>a</b> 10.067(2)	<b>b</b> 10.344(2)	<b>c</b> 13.959(3)
<b>Space Group No.:</b>	2	<b>(Å, °)</b>	$\alpha$ 108.52(3)	$\beta$ 99.03(3)	$\gamma$ 94.28(3)
<b>R-Factor (%):</b>	6.87	<b>Temperature(K):</b>	291	<b>Density(g/cm<sup>3</sup>):</b>	1.913



## Search Overview

**Search:** search3  
**Date/Time done:** Fri May 27 14:17:54 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:** 4

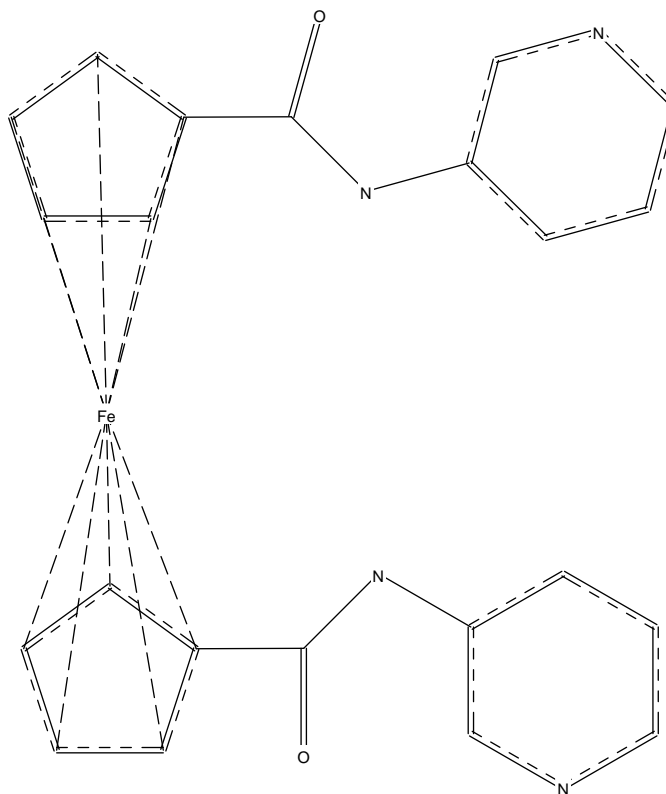
*Summary of queries used. Search found structures that:*

match

**Query 1**

**Query 2**

**Query 1**



**Query 2**

4M

## Search: search3 (Fri May 27 14:17:54 2011): Hit 1

GIJKIU

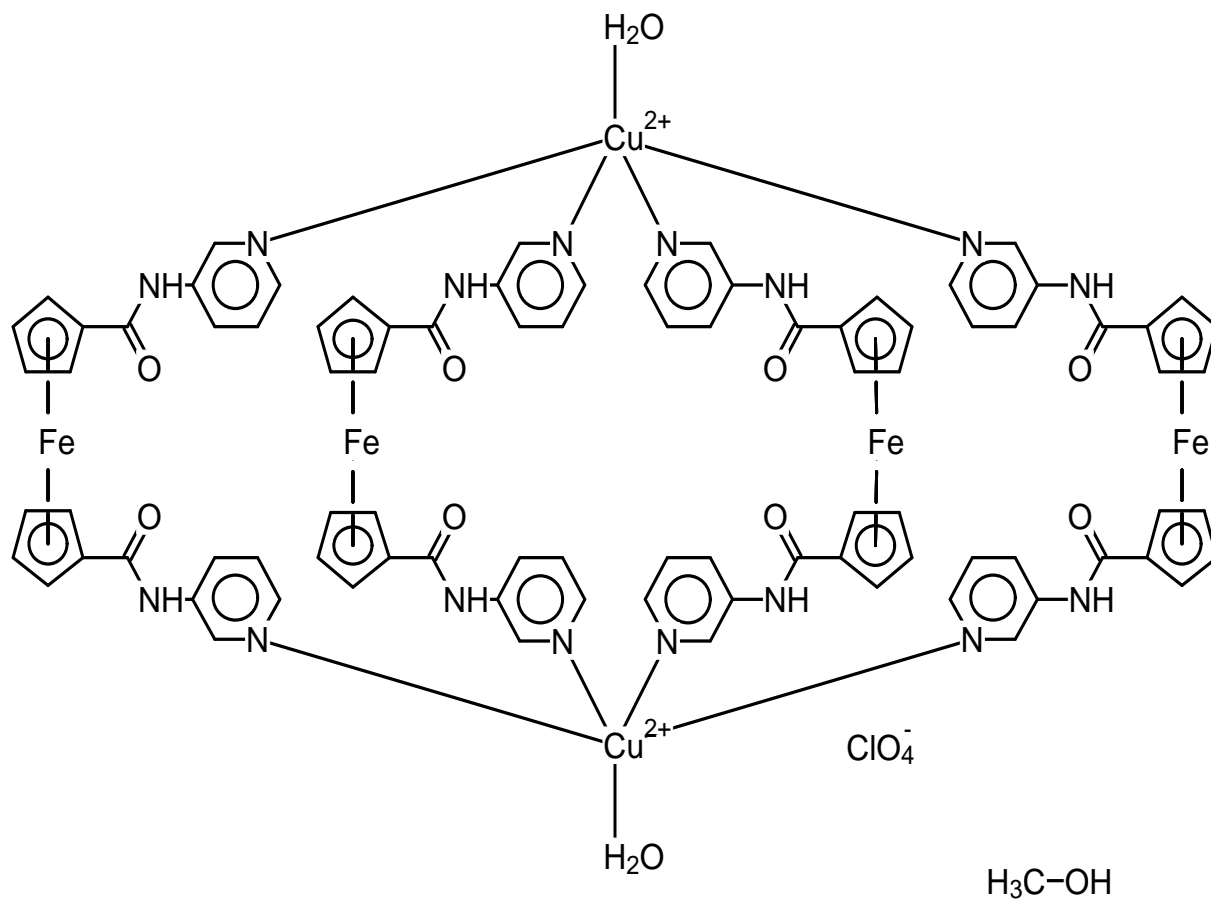
**Reference:** Kai-Ju Wei, Jia Ni, Yong-Shu Xie, Yangzhong Liu, Qing-Liang Liu (2007) *Dalton Trans.* ,3390

**Formula:**  $C_{88} H_{76} Cu_2 Fe_4 N_{16} O_{10}^{4+}, 4(Cl_1 O_4^{1-}), 4(C_1 H_4 O_1)$

**Compound Name:** tetrakis( $\mu_2$ -1,1'-bis((3-Pyridylamino)carbonyl)ferrocene-N,N')-diaqua-dicopper(ii) tetraeperchlorate methanol solvate

**Space Group:** Fddd      **Cell:**      **a** 17.472(1)      **b** 22.079(1)      **c** 51.605(4)  
**Space Group No.:** 70      **(Å, °)**       $\alpha$  90.00       $\beta$  90.00       $\gamma$  90.00

**R-Factor (%):** 5.78      **Temperature(K):** 123      **Density(g/cm<sup>3</sup>):** 1.598



## Search: search3 (Fri May 27 14:17:54 2011): Hit 2

GIJKOA

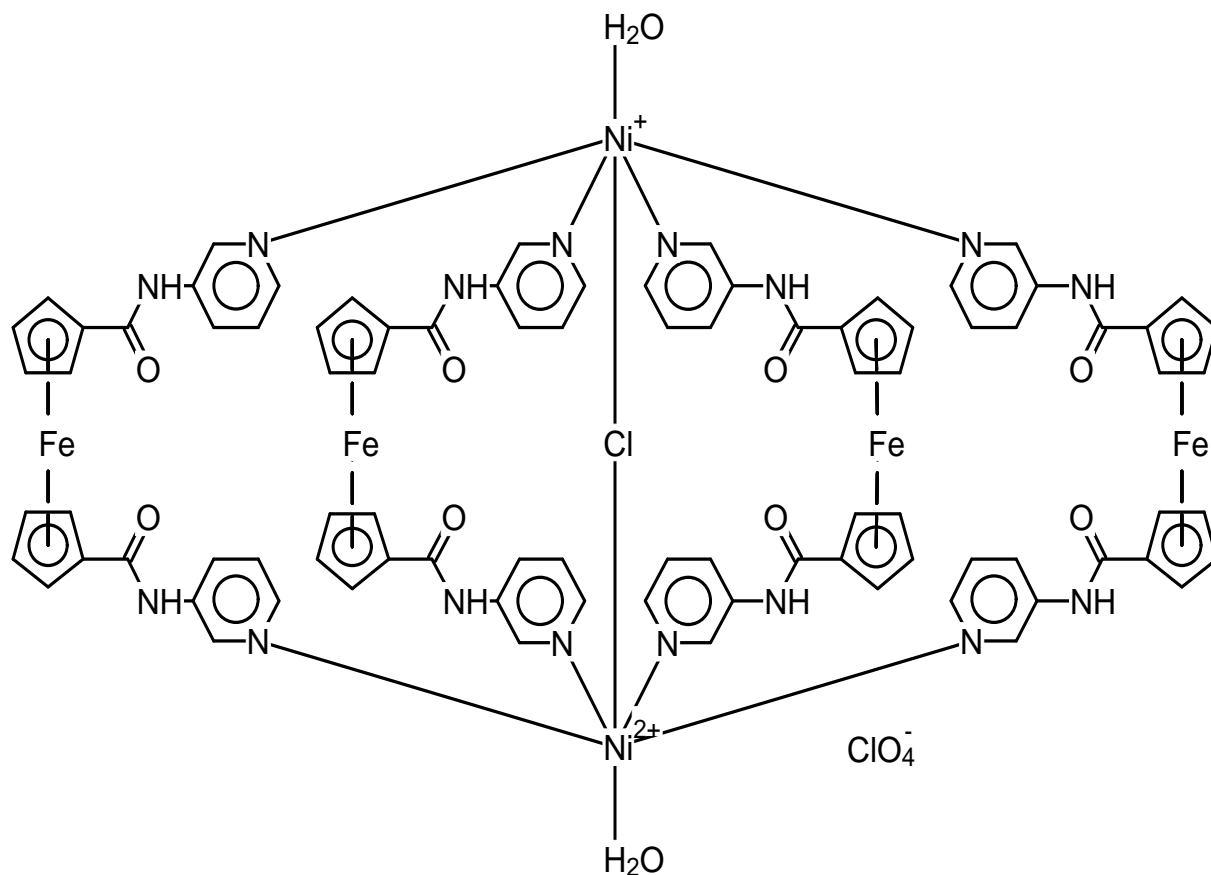
**Reference:** Kai-Ju Wei, Jia Ni, Yong-Shu Xie, Yangzhong Liu, Qing-Liang Liu (2007) *Dalton Trans.* ,3390

**Formula:**  $C_{88} H_{76} Cl_1 Fe_4 N_{16} Ni_2 O_{10}^{3+}, 3(Cl_1 O_4^{1-})$

**Compound Name:** tetrakis( $\mu_2$ -1,1'-bis((3-Pyridylamino)carbonyl)ferrocene-N,N')-( $\mu_2$ -chloro)-diaqua-di-nickel(ii) triperchlorate

**Space Group:** Fddd      **Cell:**    **a** 18.450(20)    **b** 22.310(20)    **c** 54.770(70)  
**Space Group No.:** 70      **(Å, °)**     $\alpha$  90.00       $\beta$  90.00       $\gamma$  90.00

**R-Factor (%):** 10.12      **Temperature(K):** 298      **Density(g/cm<sup>3</sup>):** 1.292



## Search: search3 (Fri May 27 14:17:54 2011): Hit 3

GIJKUG

**Reference:** Kai-Ju Wei, Jia Ni, Yong-Shu Xie, Yangzhong Liu, Qing-Liang Liu (2007) *Dalton Trans.* ,3390

**Formula:**  $C_{88} H_{76} Cl_1 Co_2 Fe_4 N_{16} O_{10}^{3+}, 3(Cl_1 O_4^{1-}), 4(C_1 H_4 O_1)$

**Compound Name:** tetrakis( $\mu_2$ -1,1'-bis((3-Pyridylamino)carbonyl)ferrocene-N,N')-( $\mu_2$ -chloro)-diaqua-di-cobalt(ii) triperchlorate methanol solvate

**Space Group:** Fddd      **Cell:**    **a** 17.906(0)    **b** 21.430(0)    **c** 53.006(2)  
**Space Group No.:** 70      **(Å, °)**     $\alpha$  90.00       $\beta$  90.00       $\gamma$  90.00

**R-Factor (%):** 8.69      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.516

