

Search Overview

Search: search7
Date/Time done: Sun Nov 20 19:39:12 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

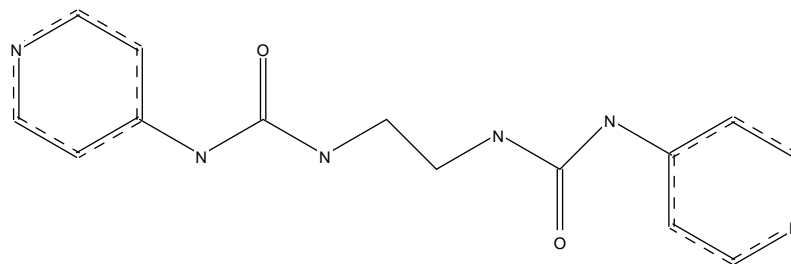
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

4M

Search: search7 (Sun Nov 20 19:39:12 2011): Hit 1

PUDROW

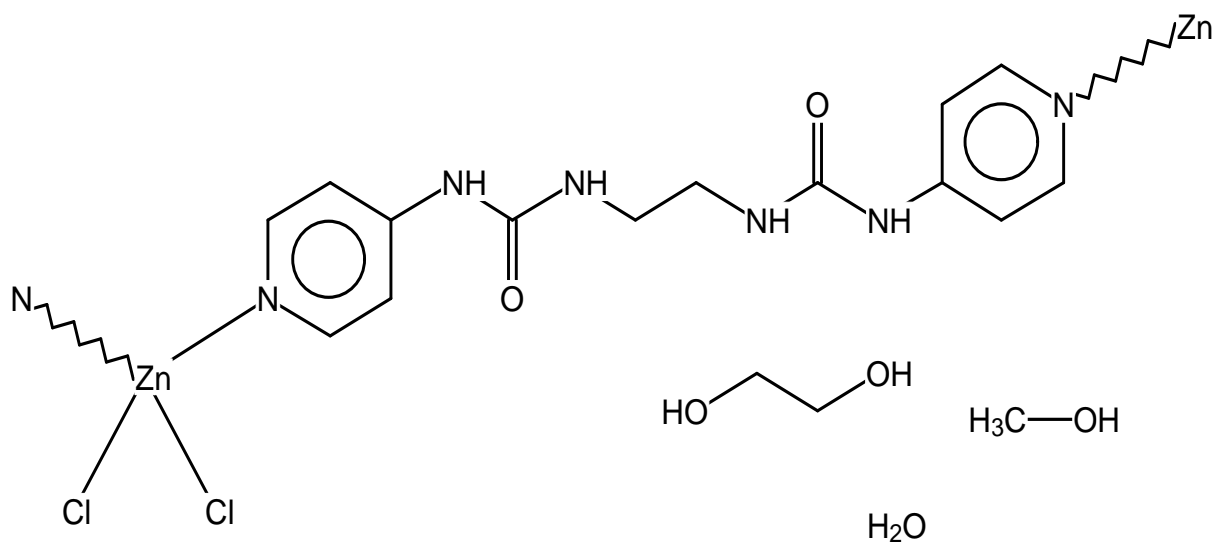
Reference: N.N.Adarsh, D.K.Kumar, P.Dastidar (2009)
Cryst.Growth Des. ,**9**,2979

Formula: $(C_{14} H_{16} Cl_2 N_6 O_2 Zn_1)_n, 0.5n(C_2 H_6 O_2), 0.5n(C_1 H_4 O_1), 2n(H_2 O_1)$

Compound Name: catena-((μ_2 -1,1'-(Ethane-1,2-diyl)-bis(3-(4-pyridinyl)urea)-N,N')-dichloro-zinc(ii) ethylene glycol methanol solvate dihydrate)

Space Group: P21/m **Cell:** **a** 7.702(1) **b** 15.578(3) **c** 10.475(2)
Space Group No.: 11 **(Å, °)** α 90.00 β 111.55(0) γ 90.00

R-Factor (%): 4.19 **Temperature(K):** 298 **Density(g/cm³):** 1.476



Search Overview

Search: search8
Date/Time done: Sun Nov 20 19:40:04 2011
Database(s): CSD version 5.32 (November 2010)
CSD version 5.32 updates (Nov 2010)
Restriction Info: No refcode restrictions applied
Filters: None
Percentage Completed: 100%
Number of Hits: 9

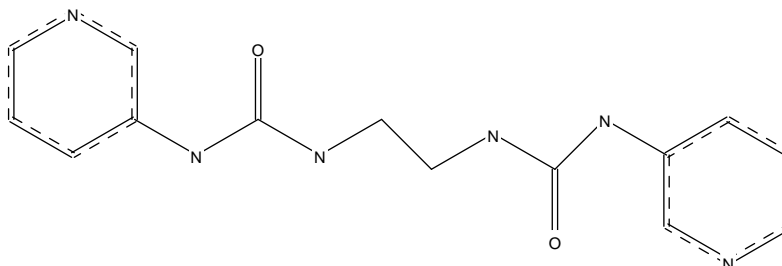
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

4M

Search: search8 (Sun Nov 20 19:40:04 2011): Hit 1

HEZLAA

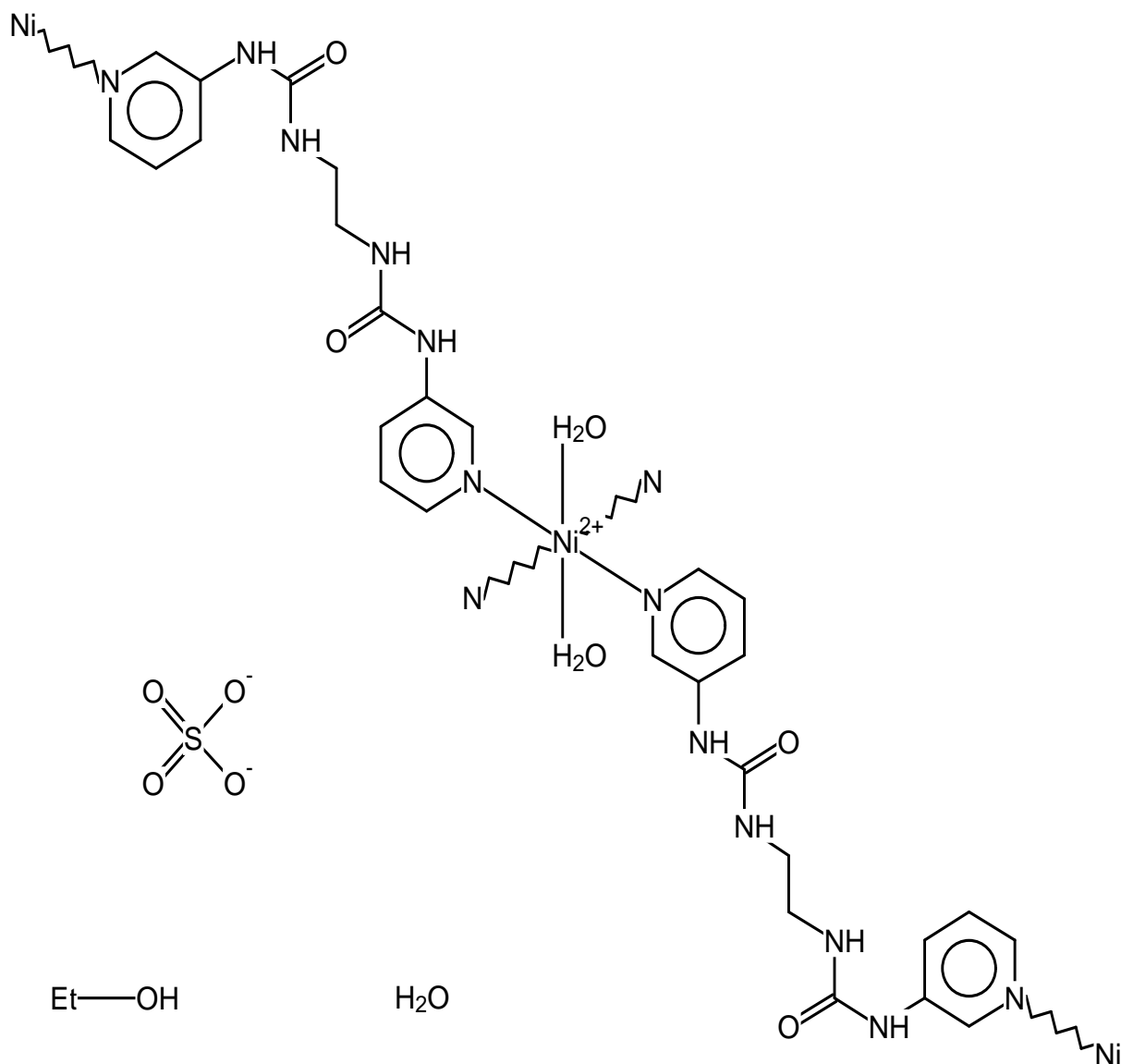
Reference: R.Custelcean, V.Sellin, B.A.Moyer (2007)
Chem.Commun. ,1541

Formula: $(C_{28} H_{36} N_{12} Ni_1 O_6^{2+})n, n(O_4 S_1^{2-}), 2.4n(C_2 H_6 O_1), 5.5n(H_2 O_1)$

Compound Name: catena-(bis(μ_2 -anti-Ethane-1,2-diylbis(N'-(3-pyridyl)urea))-diaqua-nickel(ii) sulfate ethanol solvate hydrate)

Space Group: P21/c **Cell:** **a** 13.237(3) **b** 13.908(3) **c** 23.358(5)
Space Group No.: 14 **(Å, °)** α 90.00 β 95.11(3) γ 90.00

R-Factor (%): 8.25 **Temperature(K):** 173 **Density(g/cm³):** 1.552



Search: search8 (Sun Nov 20 19:40:04 2011): Hit 2

KOLNEF

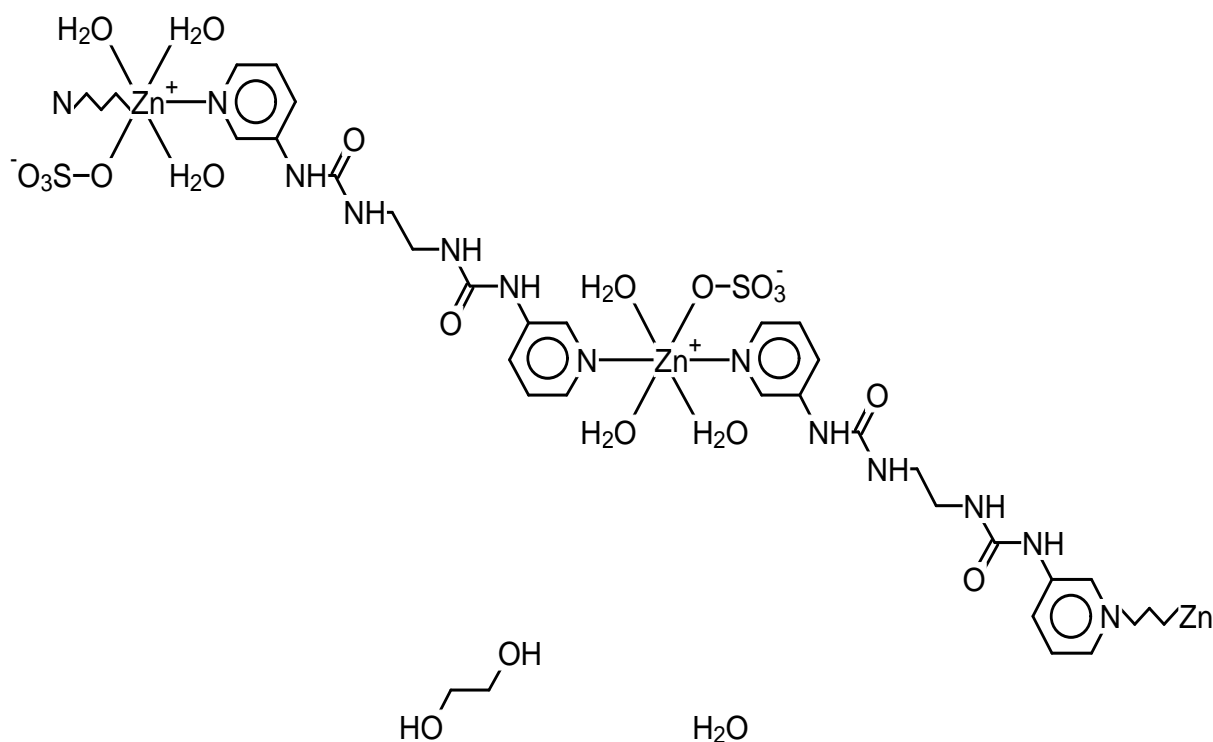
Reference: N.N.Adarsh, D.K.Kumar, P.Dastidar (2008)
CrystEngComm ,**10**,1565

Formula: (C₂₈ H₄₄ N₁₂ O₁₈ S₂ Zn₂)_n,2n(C₂ H₆ O₂),4n(H₂ O₁)

Compound Name: catena-(bis(μ₂-1,1'-(Ethane-1,2-diyl)bis(3-(3-pyridyl)urea-N,N'))-hexa-aqua-bis(sulfato-O)-di-zinc(ii) ethyleneglycol solvate tetrahydrate)

Space Group: P-1 **Cell:** **a** 7.693(0) **b** 9.756(0) **c** 17.286(1)
Space Group No.: 2 **(Å, °)** **α** 81.07(0) **β** 81.97(0) **γ** 86.10(0)

R-Factor (%): 4.09 **Temperature(K):** 100 **Density(g/cm³):** 1.608



Search: search8 (Sun Nov 20 19:40:04 2011): Hit 3

KOLNIJ

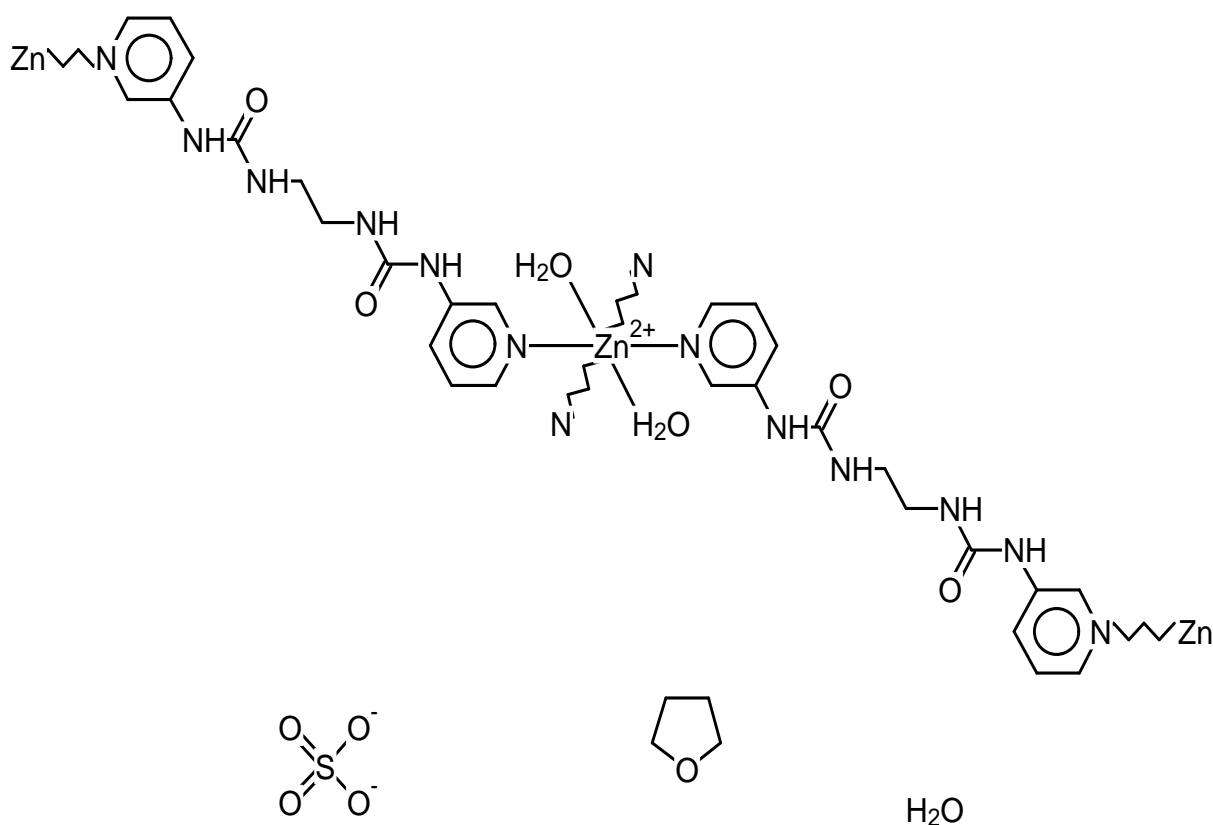
Reference: N.N.Adarsh, D.K.Kumar, P.Dastidar (2008)
CrystEngComm ,**10**,1565

Formula: (C₂₈ H₃₆ N₁₂ O₆ Zn₁²⁺)_n,n(O₄ S₁²⁻),2n(C₄ H₈ O₁),2n(H₂ O₁)

Compound Name: catena-(bis(μ₂-1,1'-(Ethane-1,2-diyl)bis(3-(3-pyridyl)urea-N,N'))-diaqua-zinc(ii) sulfate tetrahydrofuran solvate dihydrate)

Space Group: P21/n **Cell:** **a** 13.098(1) **b** 13.931(1) **c** 24.194(2)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 94.80(0) **γ** 90.00

R-Factor (%): 6.89 **Temperature(K):** 100 **Density(g/cm³):** 1.477



Search: search8 (Sun Nov 20 19:40:04 2011): Hit 4

KOLNOP

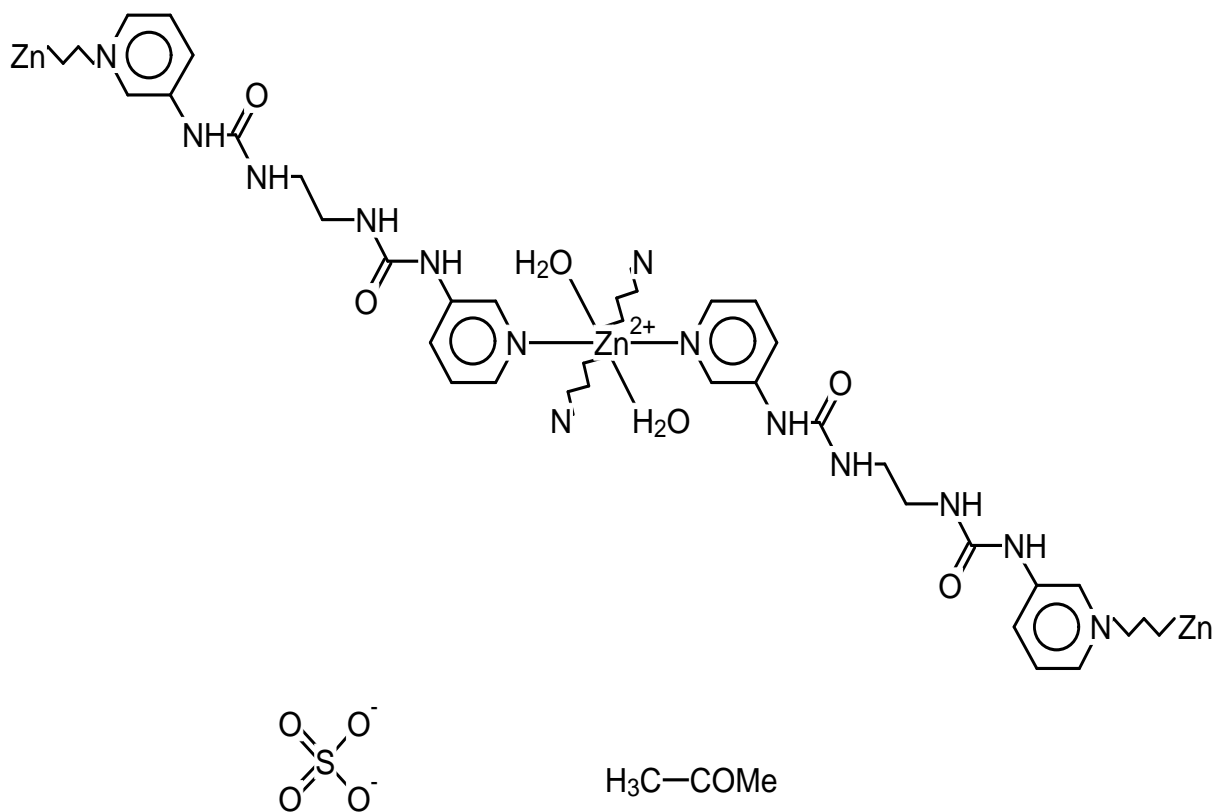
Reference: N.N.Adarsh, D.K.Kumar, P.Dastidar (2008)
CrystEngComm, **10**,1565

Formula: $(C_{28} H_{36} N_{12} O_6 Zn_1^{2+})n, n(O_4 S_1^{2-}), 2n(C_3 H_6 O_1), 2n(H_2 O_1)$

Compound Name: catena-(bis(μ_2 -1,1'-(Ethane-1,2-diyl)bis(3-(3-pyridyl)urea-N,N'))-diaqua-zinc(ii) sulfate acetone solvate dihydrate)

Space Group: P21/n **Cell:** **a** 13.196(1) **b** 13.998(1) **c** 23.607(3)
Space Group No.: 14 **(Å, °)** α 90.00 β 94.71(0) γ 90.00

R-Factor (%): 8.80 **Temperature(K):** 100 **Density(g/cm³):** 1.452



Search: search8 (Sun Nov 20 19:40:04 2011): Hit 5

KOLNUV

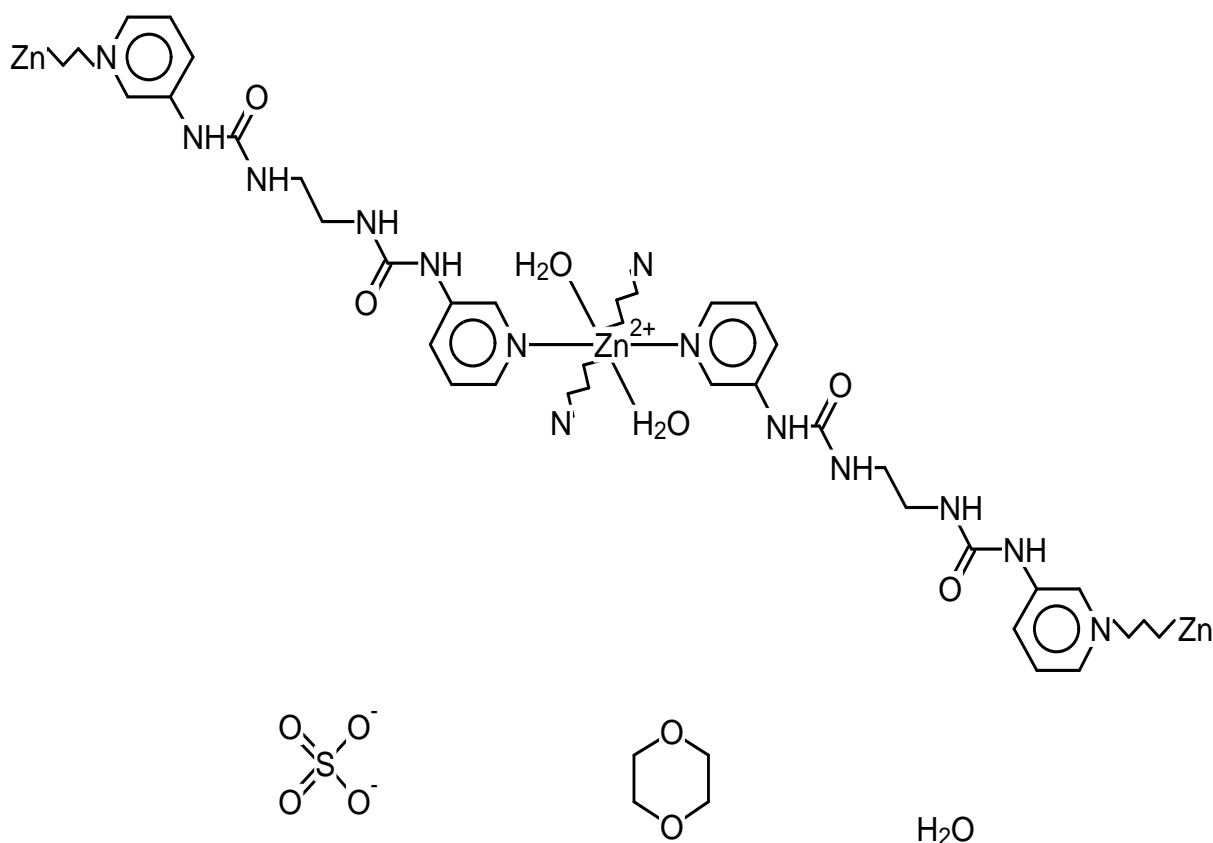
Reference: N.N.Adarsh, D.K.Kumar, P.Dastidar (2008)
CrystEngComm ,**10**,1565

Formula: (C₂₈ H₃₆ N₁₂ O₆ Zn₁²⁺)_n,n(O₄ S₁²⁻),2n(C₄ H₈ O₂),2n(H₂ O₁)

Compound Name: catena-(bis(μ₂-1,1'-(Ethane-1,2-diyl)bis(3-(3-pyridyl)urea-N,N'))-diaqua-zinc(ii) sulfate 1,4-dioxane solvate dihydrate)

Space Group: P21/n **Cell:** **a** 13.372(0) **b** 13.695(0) **c** 24.417(1)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 96.41(0) **γ** 90.00

R-Factor (%): 5.69 **Temperature(K):** 100 **Density(g/cm³):** 1.510



Search: search8 (Sun Nov 20 19:40:04 2011): Hit 6

PUDRIQ

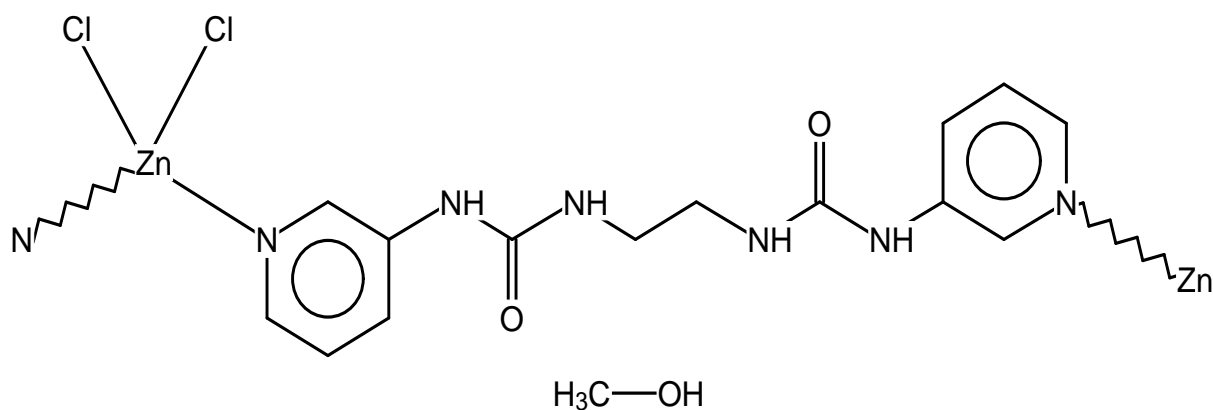
Reference: N.N.Adarsh, D.K.Kumar, P.Dastidar (2009)
Cryst.Growth Des. ,**9**,2979

Formula: (C₁₄ H₁₆ Cl₂ N₆ O₂ Zn₁)_n,2n(C₁ H₄ O₁)

Compound Name: catena-((μ₂-1,1'-(Ethane-1,2-diyl)-bis(3-(3-pyridinyl)urea)-N,N')-dichloro-zinc(ii) methanol solvate)

Space Group: C2/c **Cell:** **a** 17.904(3) **b** 6.532(1) **c** 19.129(4)
Space Group No.: 15 **(Å, °)** **α** 90.00 **β** 109.18(0) **γ** 90.00

R-Factor (%): 7.23 **Temperature(K):** 100 **Density(g/cm³):** 1.574



Search: search8 (Sun Nov 20 19:40:04 2011): Hit 7

RUSPAX

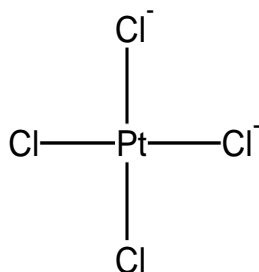
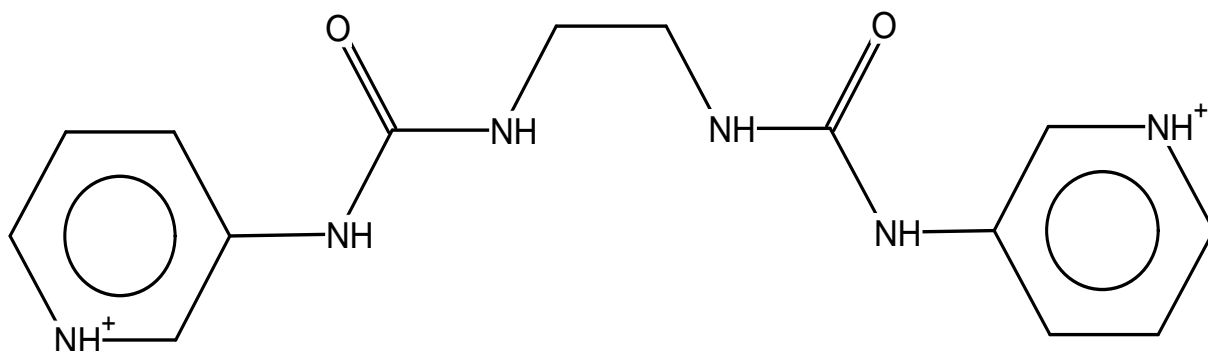
Reference: N.N.Adarsh, D.K.Kumar, P.Dastidar (2010)
Acta Crystallogr., Sect.E: Struct. Rep. Online ,**66**,m270

Formula: C₁₄ H₁₈ N₆ O₂ 2⁺, Cl₄ Pt₁ 2⁻

Compound Name: 3,3'-(Ethane-1,2-diylbis[carbonylbis(azanediyl)])dipyridinium tetrachlorido-platinum(ii)

Space Group: C2/c **Cell:** **a** 17.813(1) **b** 7.080(0) **c** 15.577(1)
Space Group No.: 15 **(Å, °)** **α** 90.00 **β** 103.33(0) **γ** 90.00

R-Factor (%): 2.52 **Temperature(K):** 100 **Density(g/cm³):** 2.221



Search: search8 (Sun Nov 20 19:40:04 2011): Hit 8

WOCXIW

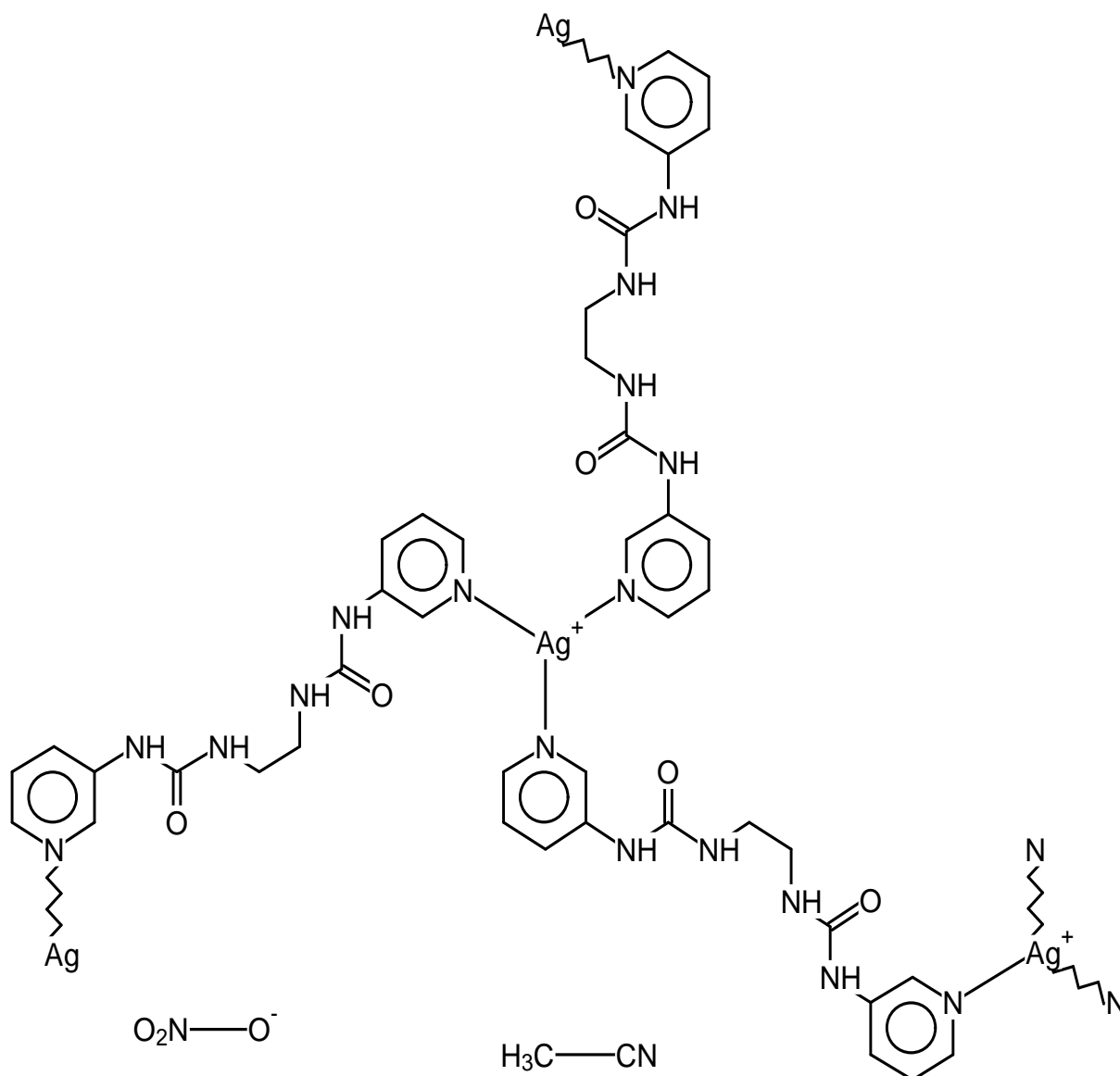
Reference: P.Byrne, G.O.Lloyd, N.Clarke, J.W.Steed (2008)
Angew.Chem.,Int.Ed. ,**47**,5761

Formula: (C₄₂ H₄₈ Ag₂ N₁₈ O₆²⁺)_n,2n(N₁ O₃¹⁻),2n(C₂ H₃ N₁)

Compound Name: catena-(tris(μ₂-N,N''-ethane-1,2-diylbis(3-pyridin-3-ylurea))-di-silver(i) dinitrate acetonitrile solvate)

Synonym: borromean weave 2

Space Group:	C2/c	Cell:	a 15.727(2)	b 27.878(4)	c 12.963(1)
Space Group No.:	15	(Å, °)	α 90.00	β 103.92(0)	γ 90.00
R-Factor (%):	6.39	Temperature(K):	120	Density(g/cm³):	1.593



Search: search8 (Sun Nov 20 19:40:04 2011): Hit 9

WOCXOC

Reference: P.Byrne, G.O.Lloyd, N.Clarke, J.W.Steed (2008)
Angew.Chem.,Int.Ed. ,**47**,5761

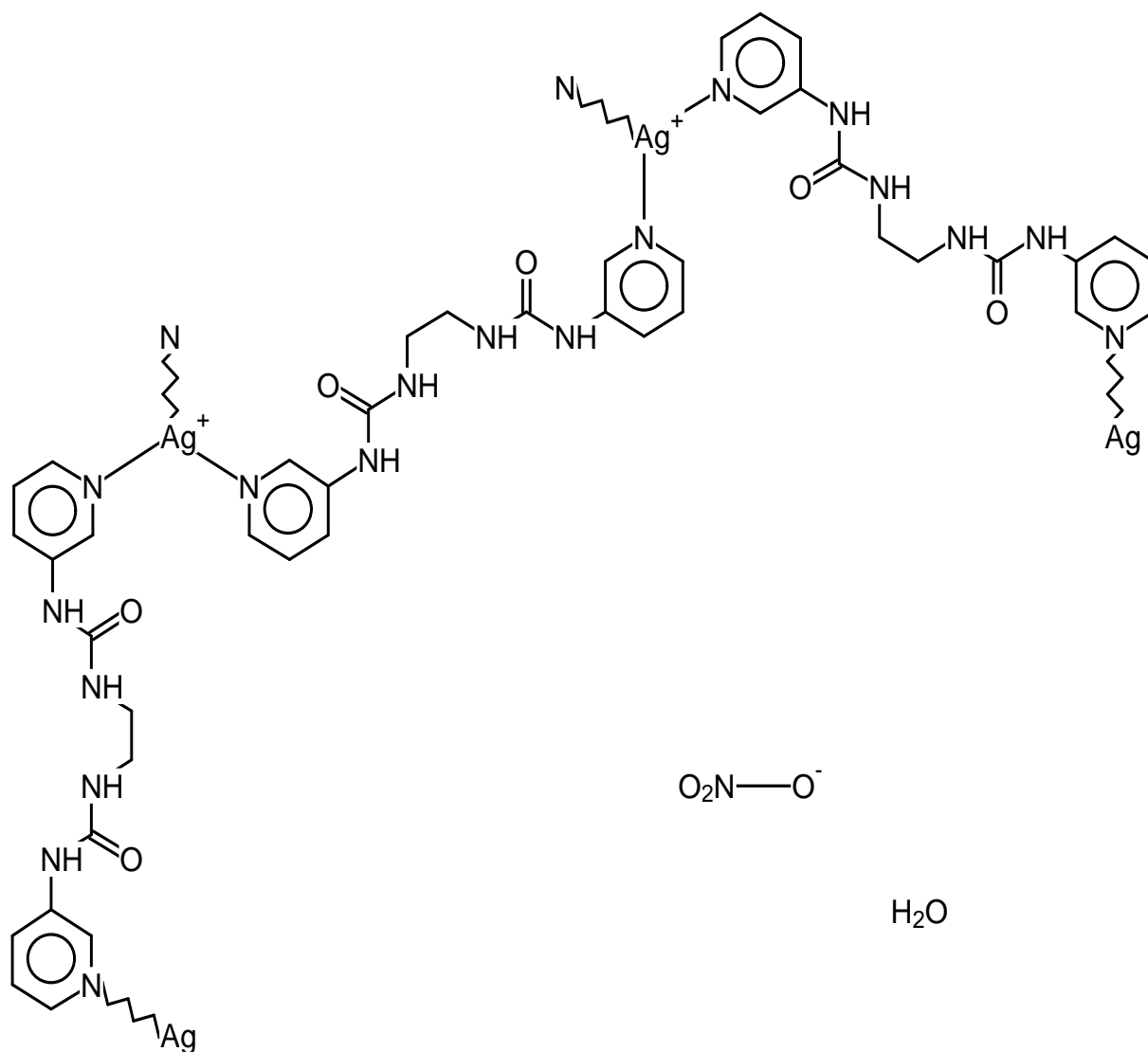
Formula: (C₄₂ H₄₈ Ag₂ N₁₈ O₆²⁺)_n,2n(N₁ O₃¹⁻),7n(H₂ O₁)

Compound Name: catena-(tris(μ₂-N,N''-ethane-1,2-diylbis(3-pyridin-3-ylurea))-di-silver(i) dinitrate heptahydrate)

Synonym: borromean weave 1

Space Group: P21/c **Cell:** **a** 15.683(4) **b** 27.326(6) **c** 12.807(3)
Space Group No.: 14 **(Å, °)** α 90.00 β 96.98(0) γ 90.00

R-Factor (%): 6.98 **Temperature(K):** 120 **Density(g/cm³):** 1.666



Search Overview

Search: search10
Date/Time done: Sun Nov 20 19:42:06 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

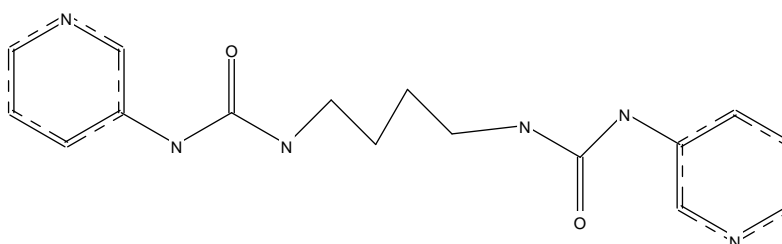
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

4M

Search: search10 (Sun Nov 20 19:42:06 2011): Hit 1

NUCFAT

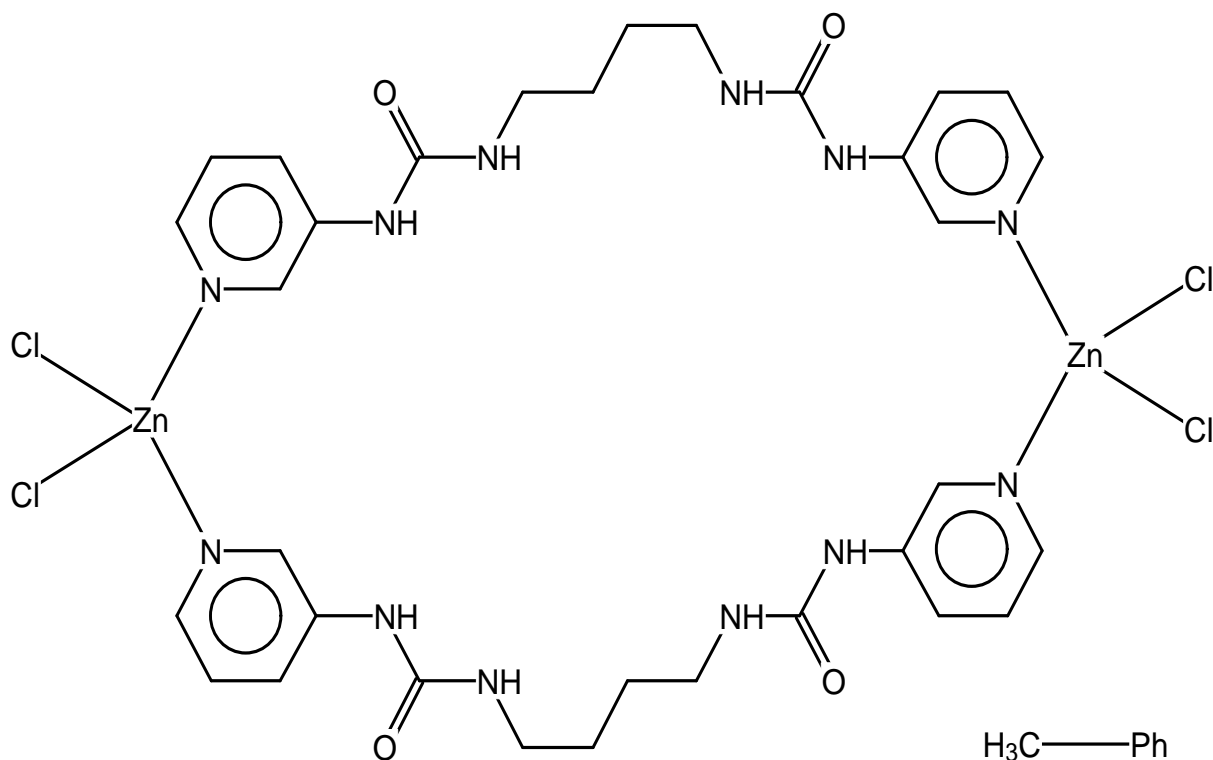
Reference: Jianjun Liang, Biao Wu, Chuandong Jia, Xiao-Juan Yang
(2009) *CrystEngComm*, **11**,975

Formula: C₃₂ H₄₀ Cl₄ N₁₂ O₄ Zn₂·C₇ H₈

Compound Name: bis(μ₂-1,4-bis(3-(3-Pyridyl)urea-1-yl)butane-N,N')-tetrachloro-di-zinc(ii)
toluene clathrate

Space Group: Aba2 **Cell:** **a** 12.950(0) **b** 41.020(3) **c** 8.887(0)
Space Group No.: 41 **(Å, °)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 4.75 **Temperature(K):** 293 **Density(g/cm³):** 1.437



Search: search10 (Sun Nov 20 19:42:06 2011): Hit 2

NUCFEX

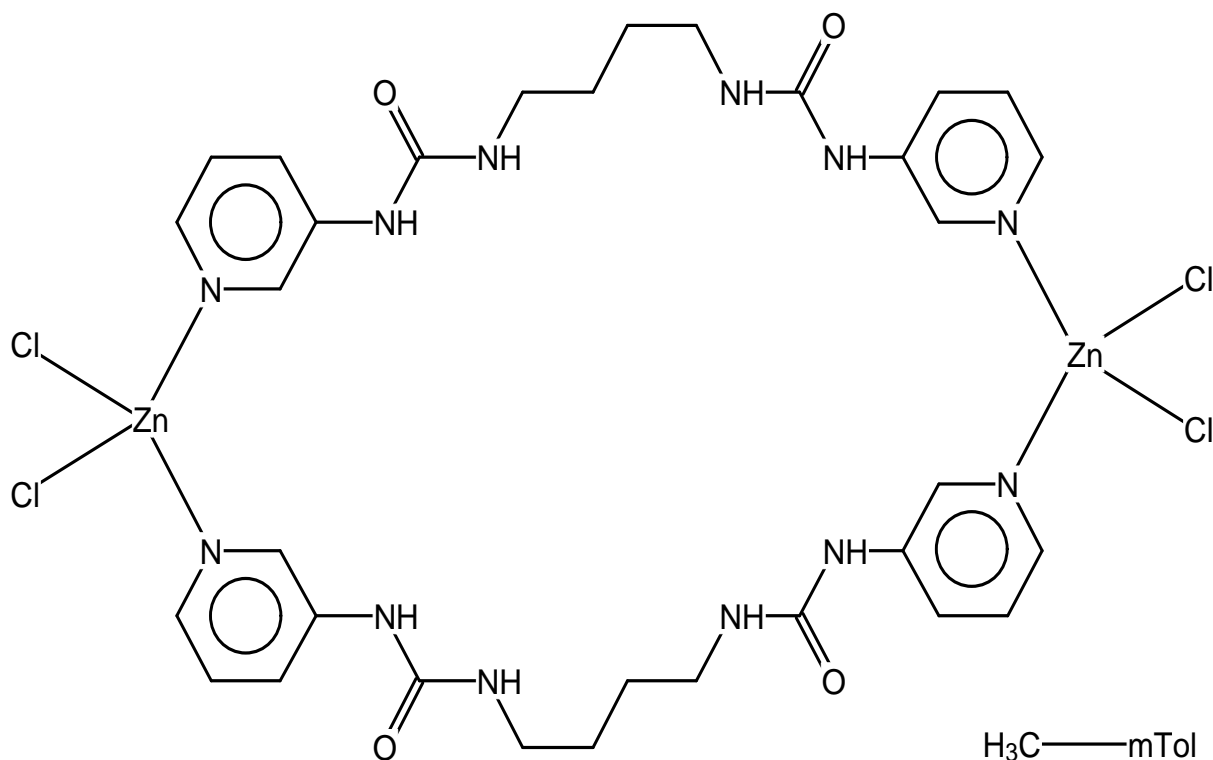
Reference: Jianjun Liang, Biao Wu, Chuandong Jia, Xiao-Juan Yang
(2009) *CrystEngComm*, **11**,975

Formula: C₃₂ H₄₀ Cl₄ N₁₂ O₄ Zn₂, C₈ H₁₀

Compound Name: bis(μ_2 -1,4-bis(3-(3-Pyridyl)urea-1-yl)butane-N,N')-tetrachloro-di-zinc(ii) m-xylene clathrate

Space Group: Aba2 **Cell:** **a** 12.965(3) **b** 40.535(8) **c** 8.805(1)
Space Group No.: 41 (**Å, °**) α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.25 **Temperature(K):** 293 **Density(g/cm³):** 1.486



Search: search10 (Sun Nov 20 19:42:06 2011): Hit 3

NUCFIB

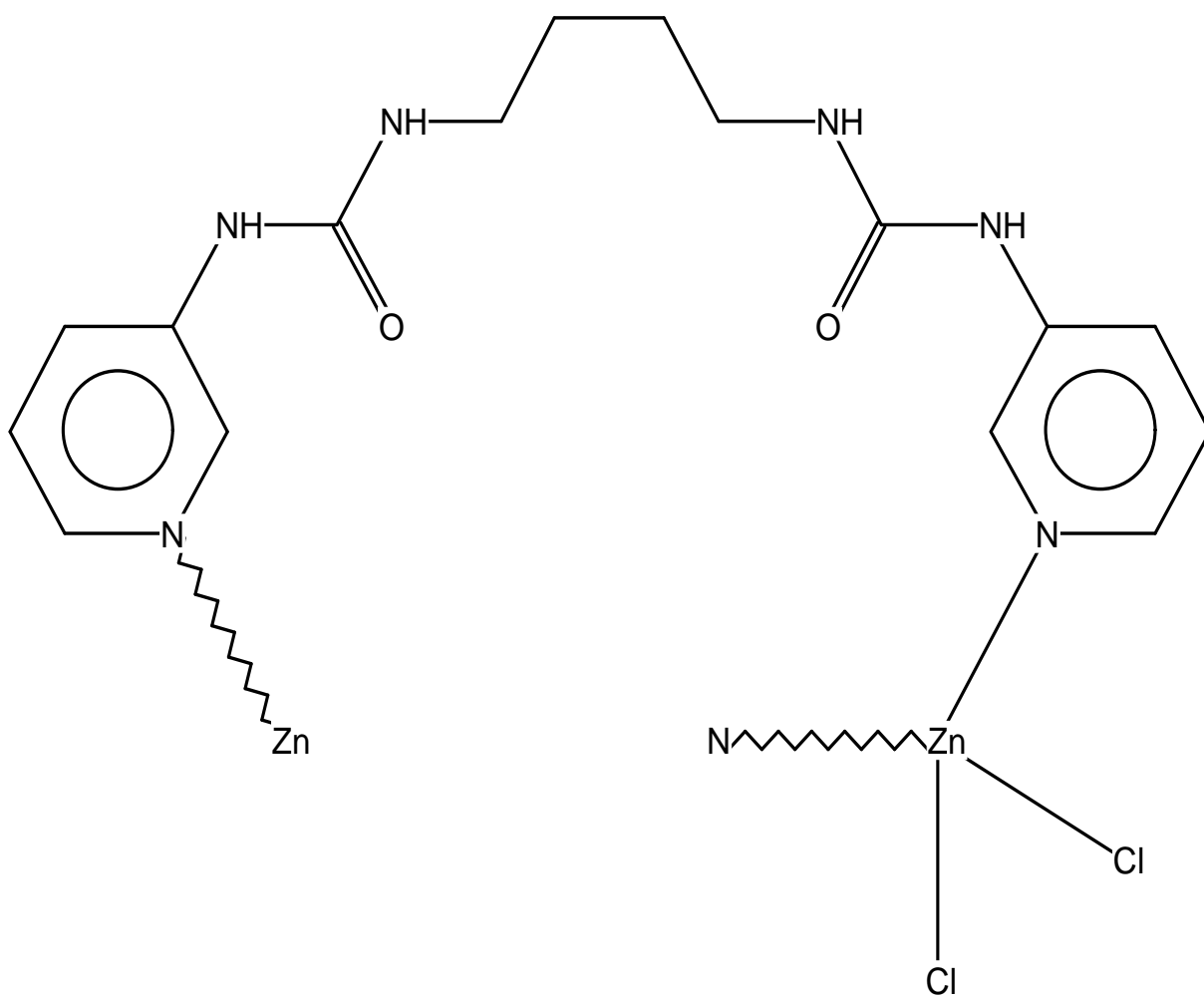
Reference: Jianjun Liang, Biao Wu, Chuandong Jia, Xiao-Juan Yang
(2009) *CrystEngComm*, **11**,975

Formula: (C₁₆ H₂₀ Cl₂ N₆ O₂ Zn₁)_n

Compound Name: catena-[(μ₂-1,4-bis(3-(3-Pyridyl)urea-1-yl)butane-N,N')-dichloro-zinc(ii)]

Space Group:	C2/c	Cell:	a 10.734(1)	b 14.345(1)	c 13.728(1)
Space Group No.:	15	(Å, °)	α 90.00	β 104.84(0)	γ 90.00

R-Factor (%):	3.01	Temperature(K):	293	Density(g/cm³):	1.510
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Search Overview

Search: search11
Date/Time done: Sun Nov 20 19:43:27 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: 2

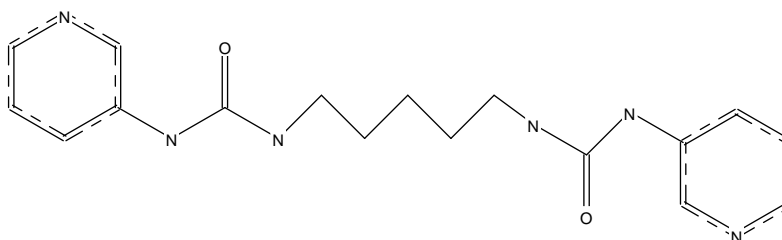
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

4M

Search: search11 (Sun Nov 20 19:43:27 2011): Hit 1

JOHYIP

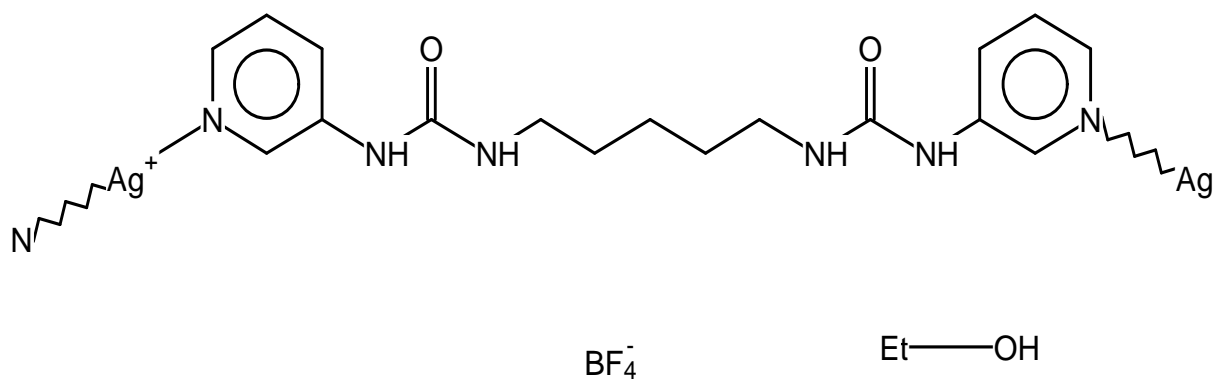
Reference: P.Byrne, G.O.Lloyd, K.M.Anderson, N.Clarke, J.W.Steed
(2008) *Chem.Commun.* ,3720

Formula: (C₁₇ H₂₂ Ag₁ N₆ O₂¹⁺)_n,n(B₁ F₄¹⁻),n(C₂ H₆ O₁)

Compound Name: catena-[(μ₂-N,N'-Pentanediylbis(N-(3-pyridin-3-yl)urea))-silver(i)
tetrafluoroborate ethanol solvate]

Space Group: P21/n **Cell:** **a** 15.479(1) **b** 7.394(0) **c** 21.154(2)
Space Group No.: 14 **(Å, °)** α 90.00 β 96.13(0) γ 90.00

R-Factor (%): 12.64 **Temperature(K):** 100 **Density(g/cm³):** 1.609



Search: search11 (Sun Nov 20 19:43:27 2011): Hit 2

JOHYOV

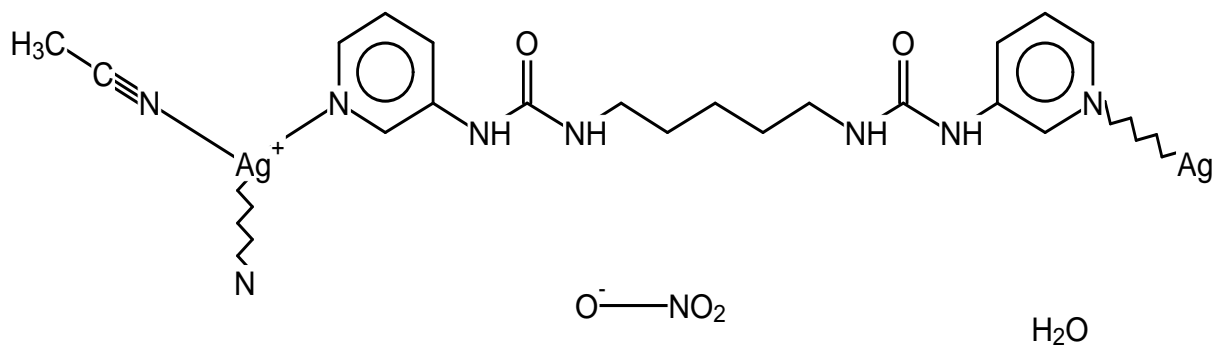
Reference: P.Byrne, G.O.Lloyd, K.M.Anderson, N.Clarke, J.W.Steed
(2008) *Chem.Commun.* ,3720

Formula: (C₁₉ H₂₅ Ag₁ N₇ O₂¹⁺)_n,n(N₁ O₃¹⁻),1.75n(H₂ O₁)

Compound Name: catena-[(μ₂-N,N'-Pentanediylbis(N-(3-pyridin-3-yl)urea))-acetonitrile-silver(i) nitrate hydrate]

Space Group: Pna21 **Cell:** **a** 34.975(3) **b** 12.561(1) **c** 5.754(0)
Space Group No.: 33 **(Å, °)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 3.78 **Temperature(K):** 120 **Density(g/cm³):** 1.537



Search Overview

Search: search13
Date/Time done: Sun Nov 20 19:45:52 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

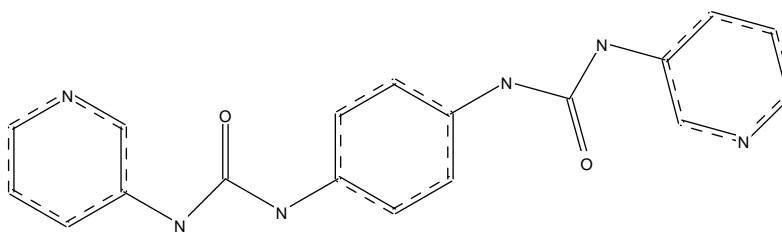
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

4M

Search: search13 (Sun Nov 20 19:45:52 2011): Hit 1

PUNRUM

Reference: N.N.Adarsh, P.Dastidar (2010) *Cryst.Growth Des.* ,**10**,483

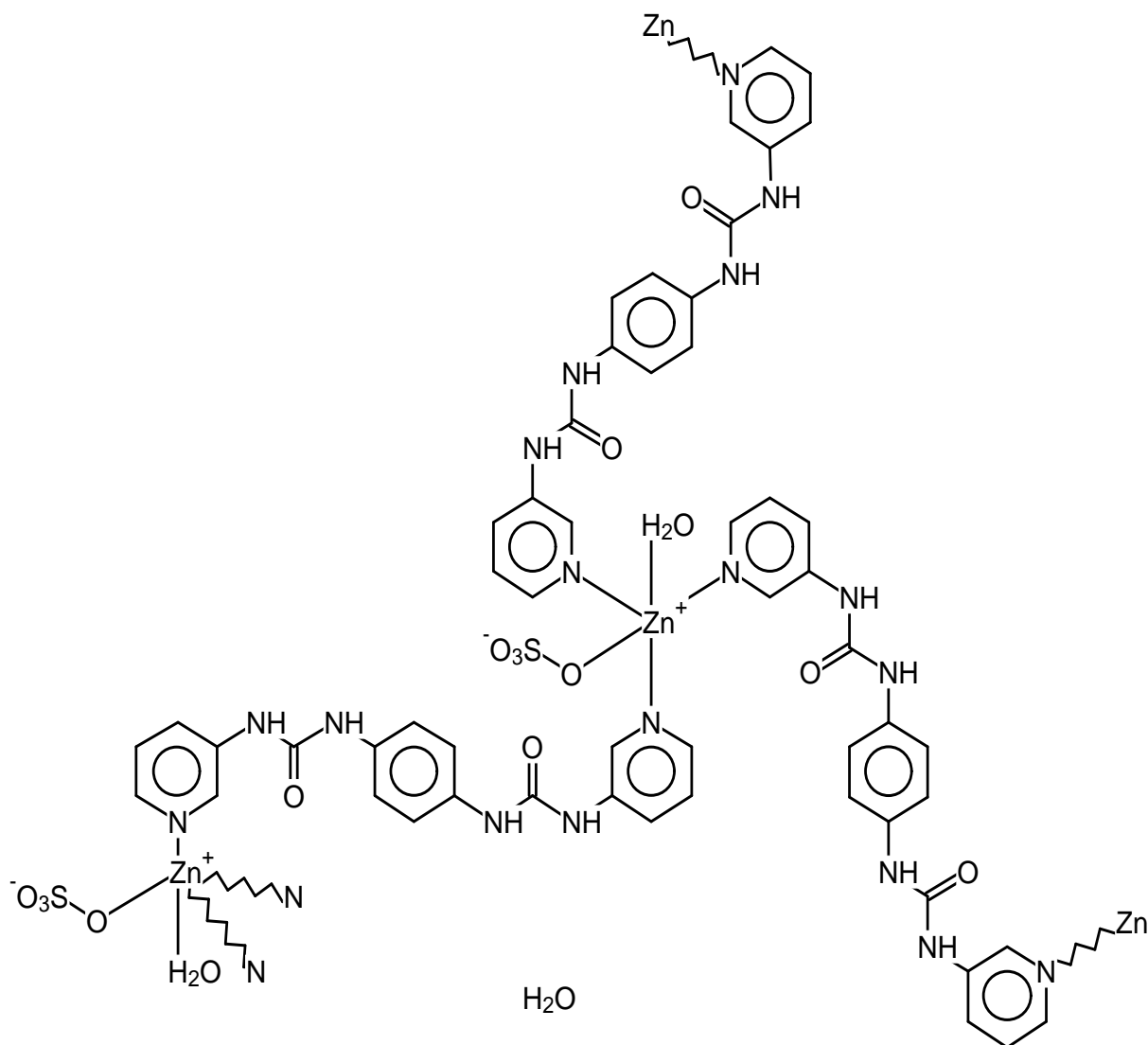
Formula: $(C_{54} H_{52} N_{18} O_{16} S_2 Zn_2)_n, 10n(H_2 O_1)$

Compound Name: catena-(tris(μ_2 -N,N'-bis(3-Pyridyl)-p-phenylene-bis(urea))-diaqua-bis(sulfato-O)-di-zinc decahydrate)

Space Group: R-3 **Cell:** **a** 15.080(1) **b** 15.080(1) **c** 35.075(9)

Space Group No.: 148 **(Å, °)** α 90.00 β 90.00 γ 120.00

R-Factor (%): 10.20 **Temperature(K):** 100 **Density(g/cm³):** 1.142



Search Overview

Search: search14
Date/Time done: Sun Nov 20 19:47:09 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

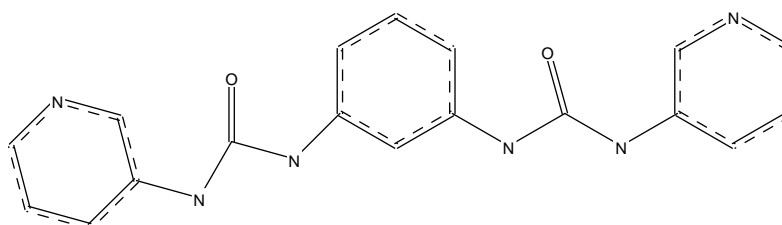
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

4M

Search: search14 (Sun Nov 20 19:47:09 2011): Hit 1

KURTUN

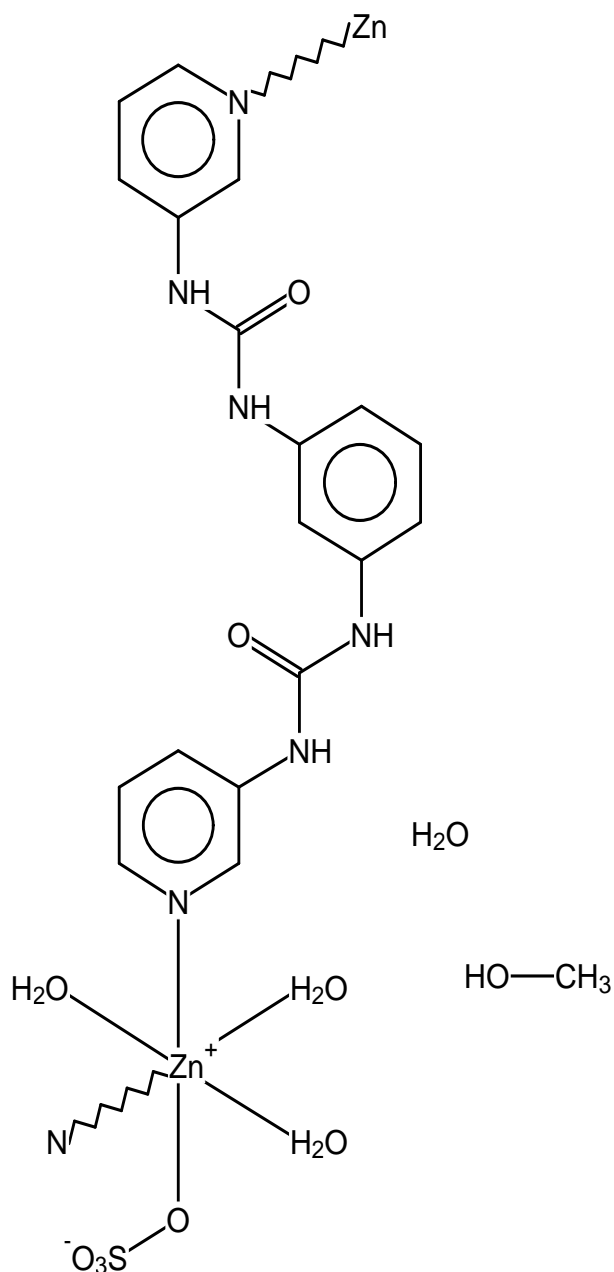
Reference: N.N.Adarsh, P.Dastidar (2010)
Acta Crystallogr., Sect.E:Struct.Rep.Online ,**66**,m413

Formula: (C₁₈ H₂₂ N₆ O₉ S₁ Zn₁)_n,n(C₁ H₄ O₁),n(H₂ O₁)

Compound Name: catena-((μ₂-3,3'-bis(3-pyridyl)-1,1'-(m-phenylene)diurea)-triqua-(sulfato)-zinc(ii) methanol solvate monohydrate)

Space Group: P21 **Cell:** **a** 6.483(0) **b** 19.265(2) **c** 9.706(1)
Space Group No.: 4 **(Å, °)** **α** 90.00 **β** 98.85(0) **γ** 90.00

R-Factor (%): 3.14 **Temperature(K):** 100 **Density(g/cm³):** 1.702



Search Overview

Search: search1
Date/Time done: Sun Nov 20 21:10:56 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: 3

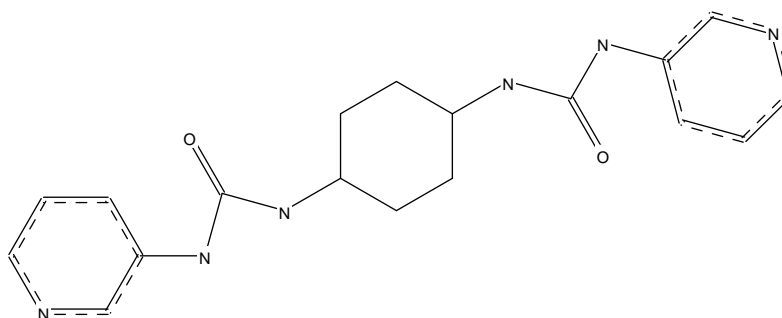
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

4M

Search: search1 (Sun Nov 20 21:10:56 2011): Hit 1

NANZAE

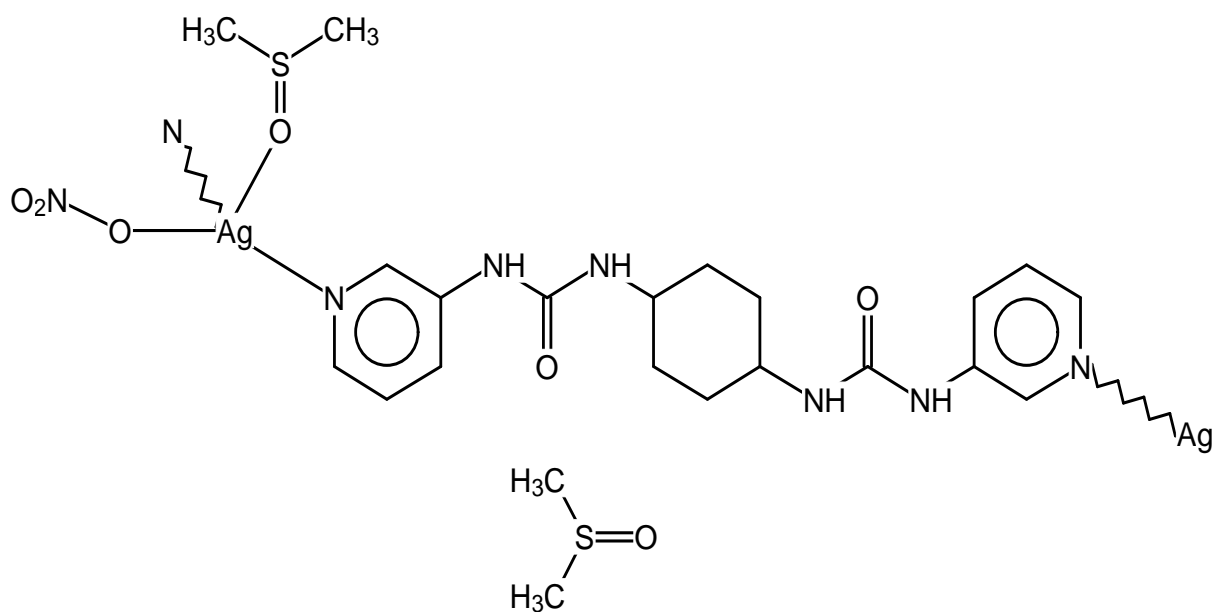
Reference: L.Applegarth, A.E.Goeta, J.W.Steed (2005)
Chem.Commun. ,2405

Formula: (C₂₀ H₂₈ Ag₁ N₇ O₆ S₁)_n,n(C₂ H₆ O₁ S₁)

Compound Name: catena-((μ₂-1,4-bis(N'-(3-Pyridyl)-N-ureayl)cyclohexane)-
(dimethylsulfoxide)-(nitrate)-silver(i) dimethylsulfoxide solvate)

Space Group: P21/c **Cell:** **a** 12.927(0) **b** 13.329(0) **c** 16.547(0)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 105.36(0) **γ** 90.00

R-Factor (%): 2.54 **Temperature(K):** 120 **Density(g/cm³):** 1.644



Search: search1 (Sun Nov 20 21:10:56 2011): Hit 2

NANZEI

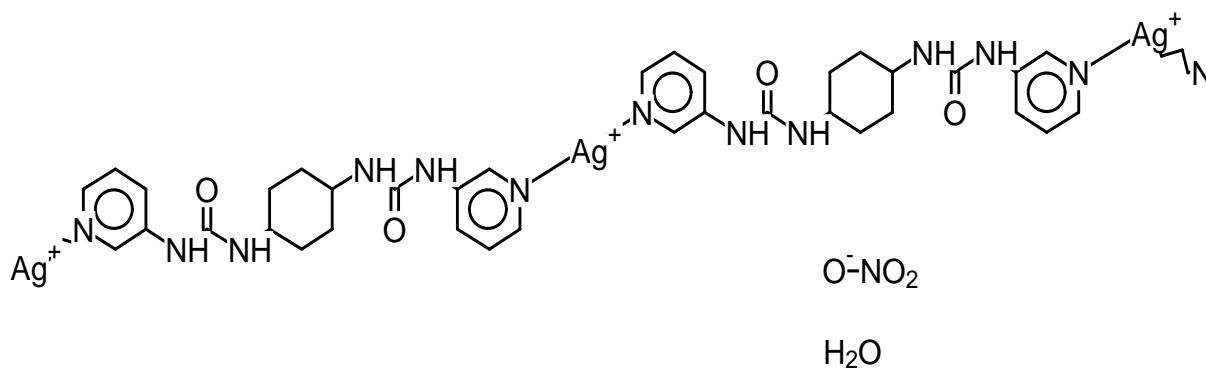
Reference: L.Applegarth, A.E.Goeta, J.W.Steed (2005)
Chem.Commun. ,2405

Formula: $(C_{36} H_{44} Ag_2 N_{12} O_4^{2+})_n, 2n(N_1 O_3^{1-}), 6n(H_2 O_1)$

Compound Name: catena-(bis(μ_2 -1,4-bis(N'-(3-Pyridyl)-N-ureayl)cyclohexane)-di-silver(i) dinitrate hexahydrate)

Space Group: P-1 **Cell:** **a** 9.414(0) **b** 10.913(0) **c** 12.381(1)
Space Group No.: 2 (**Å, °**) α 110.43(0) β 95.57(0) γ 102.52(0)

R-Factor (%): 5.75 **Temperature(K):** 120 **Density(g/cm³):** 1.681



Search: search1 (Sun Nov 20 21:10:56 2011): Hit 3

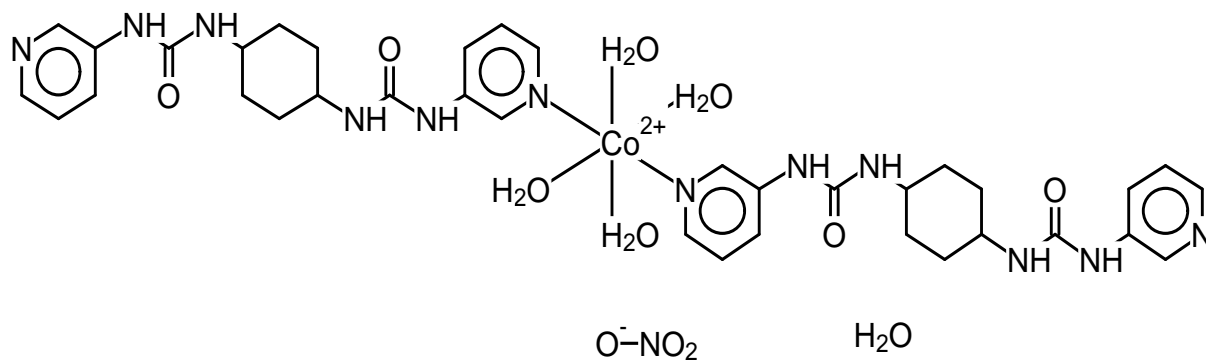
XAXFU Y

Reference: L.Applegarth, N.Clark, A.C.Richardson, A.D.M.Parker,
I.Radosavljevic-Evans, A.E.Goeta, J.A.K.Howard, J.W.Steed (2005)
Chem.Commun. ,5423

Formula: C₃₆ H₅₂ Co₁ N₁₂ O₈ ²⁺,2(N₁ O₃ ¹⁻),2(H₂ O₁)

Compound Name: trans-Tetra-aqua-bis(1,4-bis(3-(3-pyridyl)ureido)cyclohexane-N)-cobalt(ii)
dinitrate dihydrate

Space Group:	P-1	Cell:	a 9.338(0)	b 11.332(0)	c 11.410(0)
Space Group No.:	2	(Å, °)	α 74.17(0)	β 71.29(0)	γ 80.36(0)
R-Factor (%):	4.36	Temperature(K):	120	Density(g/cm³):	1.515



Search Overview

Search: search16
Date/Time done: Sun Nov 20 19:52:15 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

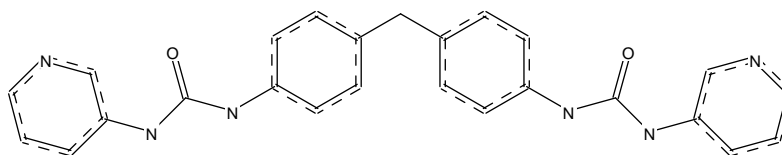
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

4M

Search: search16 (Sun Nov 20 19:52:15 2011): Hit 1

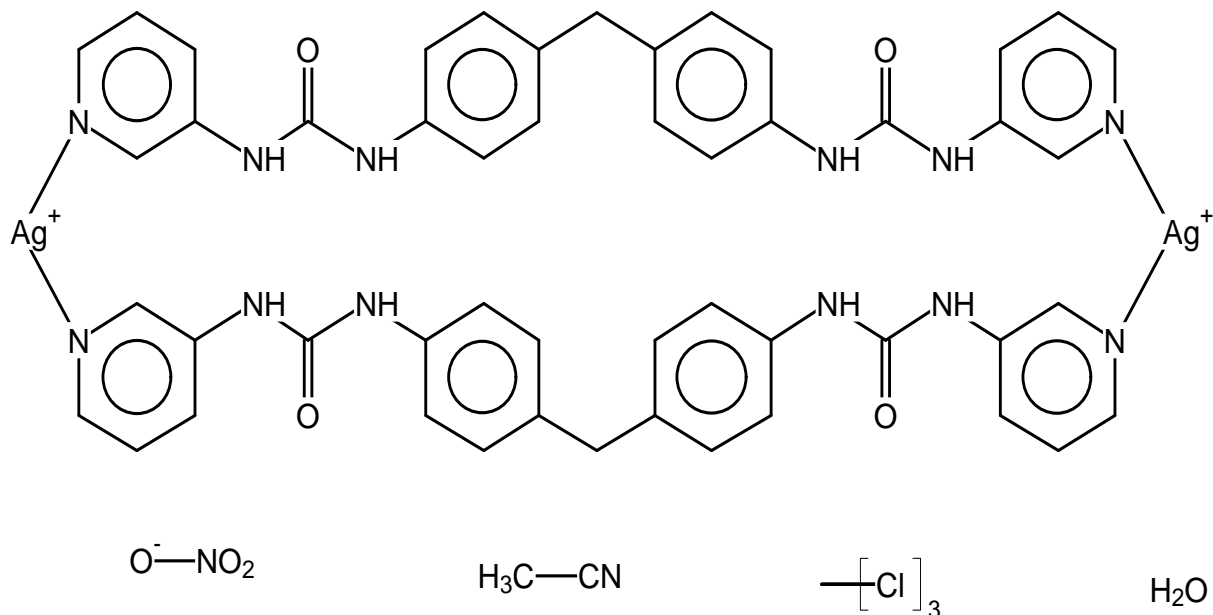
XAXFOS

Reference: L.Applegarth, N.Clark, A.C.Richardson, A.D.M.Parker,
I.Radosavljevic-Evans, A.E.Goeta, J.A.K.Howard, J.W.Steed (2005)
Chem.Commun. ,5423

Formula: $C_{50}H_{44}Ag_2N_{12}O_4^{2+}, 2(N_1O_3^{1-}), 2(C_2H_3N_1), 2(C_1H_1Cl_3), 1.5(H_2O_1)$

Compound Name: bis(μ_2 -bis(4-(3-(3-Pyridyl)ureido)phenyl)methane-N,N')-di-silver(i)
dinitrate acetonitrile chloroform solvate sesquihydrate

Space Group: Pmn21 **Cell:** **a** 43.826(4) **b** 5.261(0) **c** 14.096(1)
Space Group No.: 31 **(Å, °)** α 90.00 β 90.00 γ 90.00
R-Factor (%): 4.73 **Temperature(K):** 120 **Density(g/cm³):** 1.599



For **L50**, please refer M-O. M. Piepenbrock, N. Clarke and J. W. Steed, *Soft Matter*, 2010, **6**, 3541–3547