

Search Overview

Search: search1
Date/Time done: Wed Aug 10 21:04:46 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

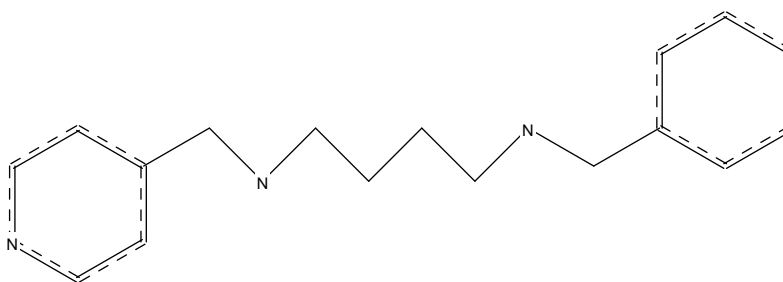
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

4M

Search: search1 (Wed Aug 10 21:04:46 2011): Hit 1

ADOFII

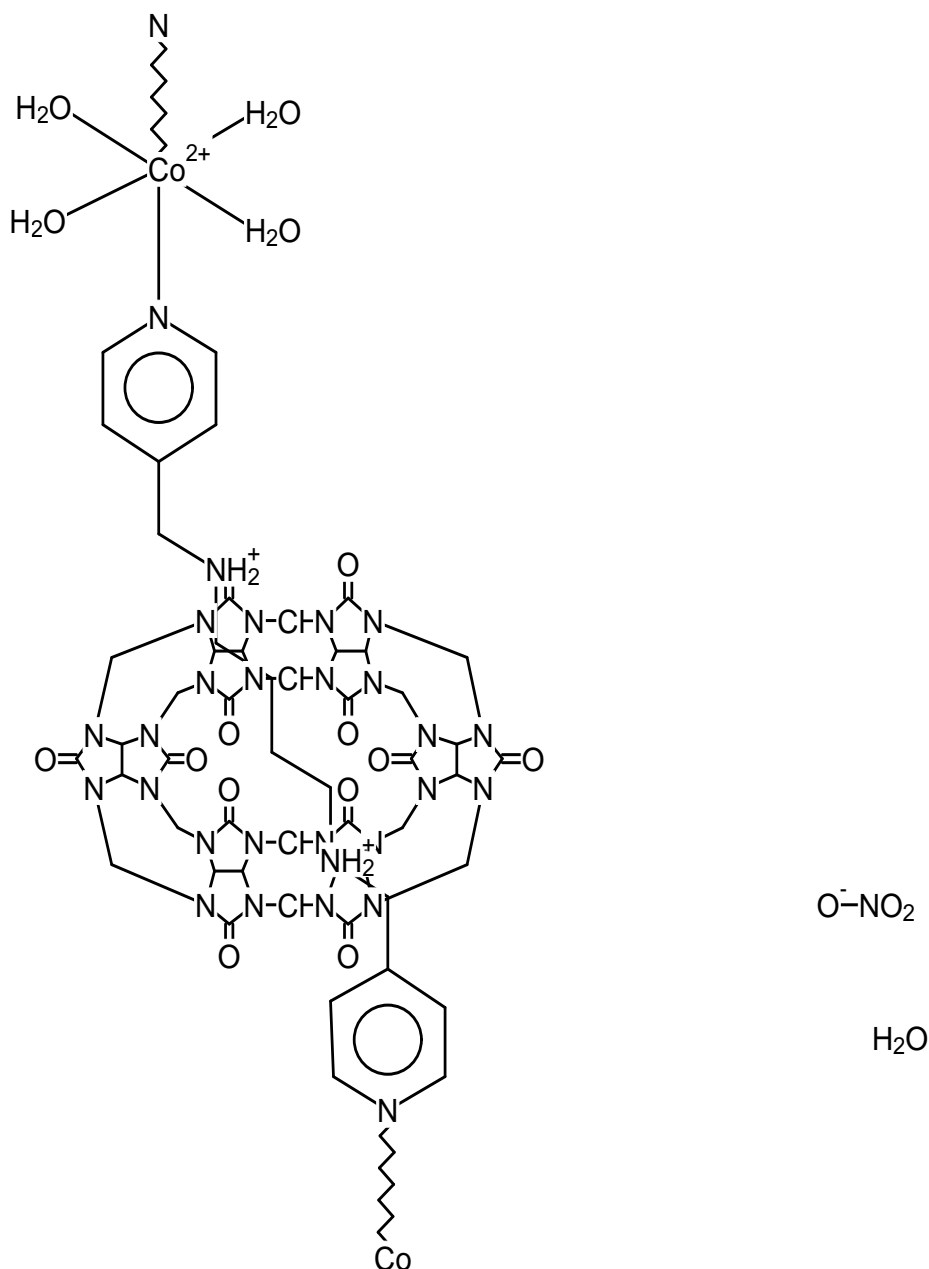
Reference: Ki-Min Park, Dongmok Whang, Eunsung Lee,
Jungseok Heo, Kimoon Kim (2002) *Chem.-Eur.J.* ,8,498

Formula: $(C_{36} H_{36} N_{24} O_{12})_n, n(C_{16} H_{32} Co_1 N_4 O_4^{4+}), 4n(N_1 O_3^{-1}), 13n(H_2 O_1)$

Compound Name: catena-(((μ_2 -N,N'-bis(4-Pyridylmethyl)butane-1,4-diammonium)-tetra-aqua-cobalt(ii))-(cucurbituril)-polyrotaxane tetranitrate tridecahydrate)

Space Group: P21/c **Cell:** **a** 12.446(0) **b** 21.324(0) **c** 29.040(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 91.42(0) γ 90.00

R-Factor (%): 7.98 **Temperature(K):** 293 **Density(g/cm³):** 1.623



Search: search1 (Wed Aug 10 21:04:46 2011): Hit 2

ADOFOO

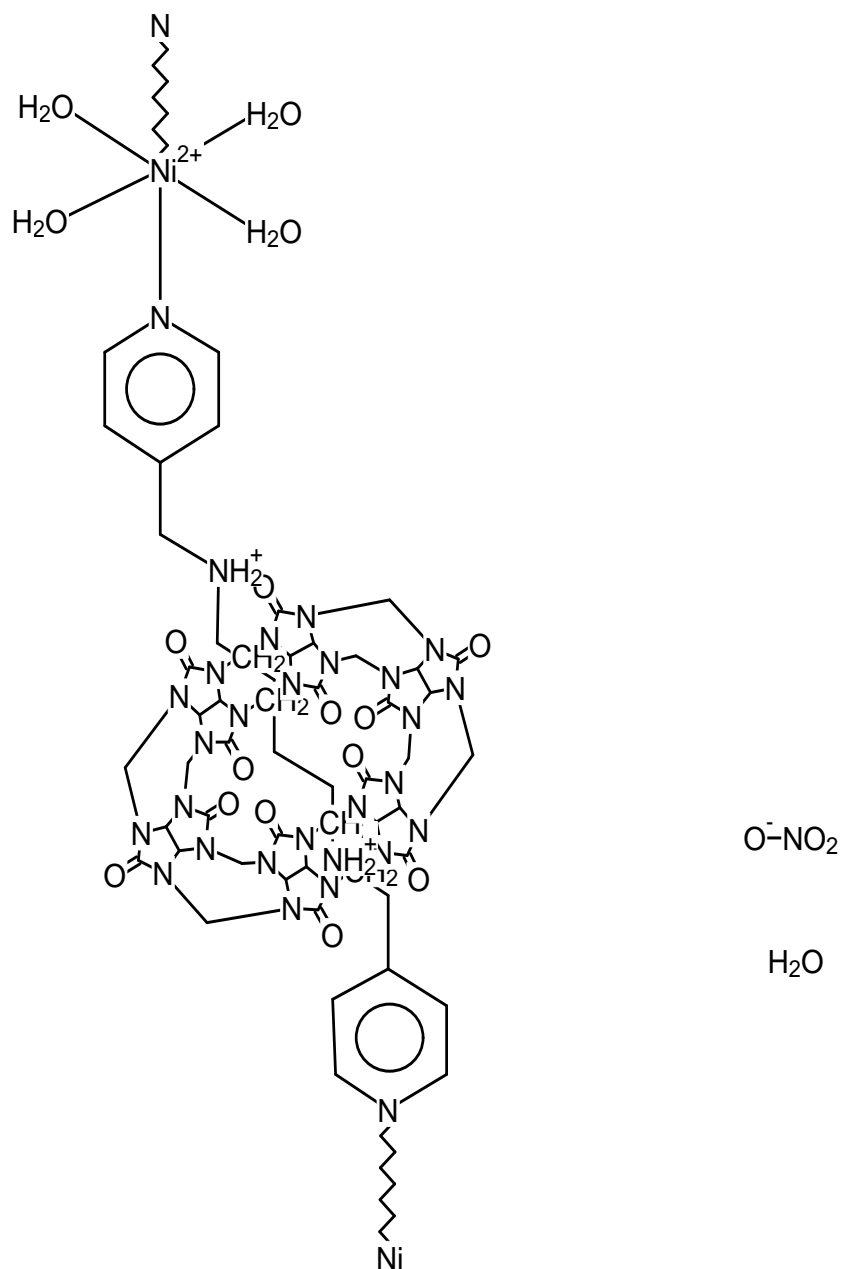
Reference: Ki-Min Park, Dongmok Whang, Eunsung Lee,
Jungseok Heo, Kimoon Kim (2002) *Chem.-Eur.J.* ,**8**,498

Formula: $(C_{36} H_{36} N_{24} O_{12})_n, n(C_{16} H_{32} N_4 Ni_1 O_4^{4+}), 4n(N_1 O_3^{1-}), 13n(H_2 O_1)$

Compound Name: catena-(((μ_2 -N,N'-bis(4-Pyridylmethyl)butane-1,4-diammonium)-tetra-aqua-nickel(ii))-(cucurbituril)-polyrotaxane tetranitrate tridecahydrate)

Space Group: P21/c **Cell:** **a** 12.430(3) **b** 21.318(4) **c** 29.012(6)
Space Group No.: 14 **(Å, °)** α 90.00 β 91.80(3) γ 90.00

R-Factor (%): 9.45 **Temperature(K):** 293 **Density(g/cm³):** 1.627



Search: search1 (Wed Aug 10 21:04:46 2011): Hit 3

REKHIY

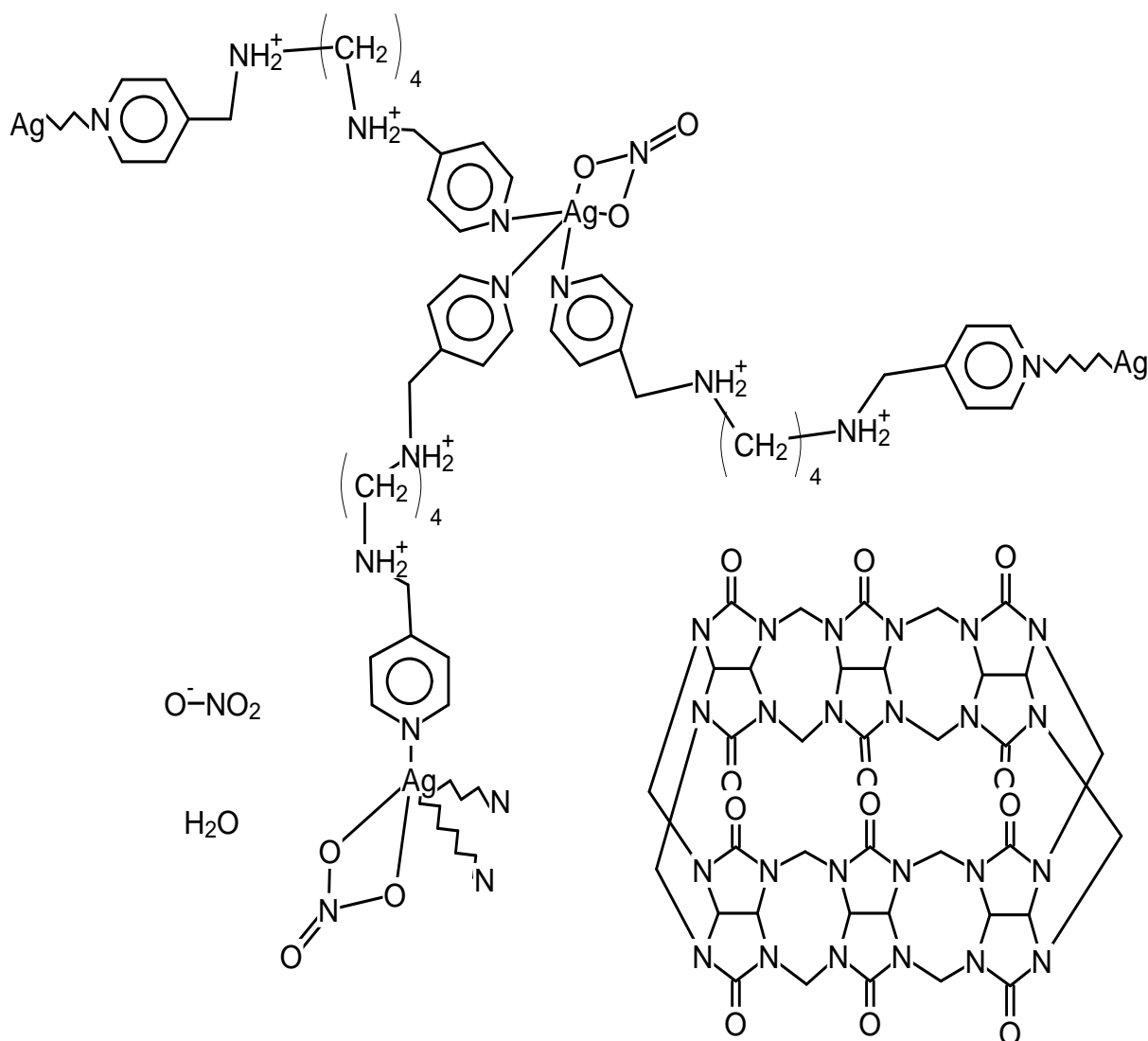
Reference: Dongmok Whang, Kimoon Kim (1997) *J.Am.Chem.Soc.* ,
119,451

Formula: $(C_{48} H_{72} Ag_2 N_{14} O_6^{6+})_n, 3n(C_{36} H_{36} N_{24} O_{12}), 6n(N_1 O_3^{1-}), 40n(H_2 O_1)$

Compound Name: catena(μ_2 -tris(N,N'-bis(4-Pyridylmethyl)-1,4-diaminobutane)-di-nitrato-
di-silver tris(cucurbituril) hexanitrate hydrate)

Space Group: Cmca **Cell:** **a** 31.408(3) **b** 32.508(4) **c** 22.479(3)
Space Group No.: 64 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 11.81 **Temperature(K):** 295 **Density(g/cm³):** 1.516



Search: search1 (Wed Aug 10 21:04:46 2011): Hit 4

REKHOE

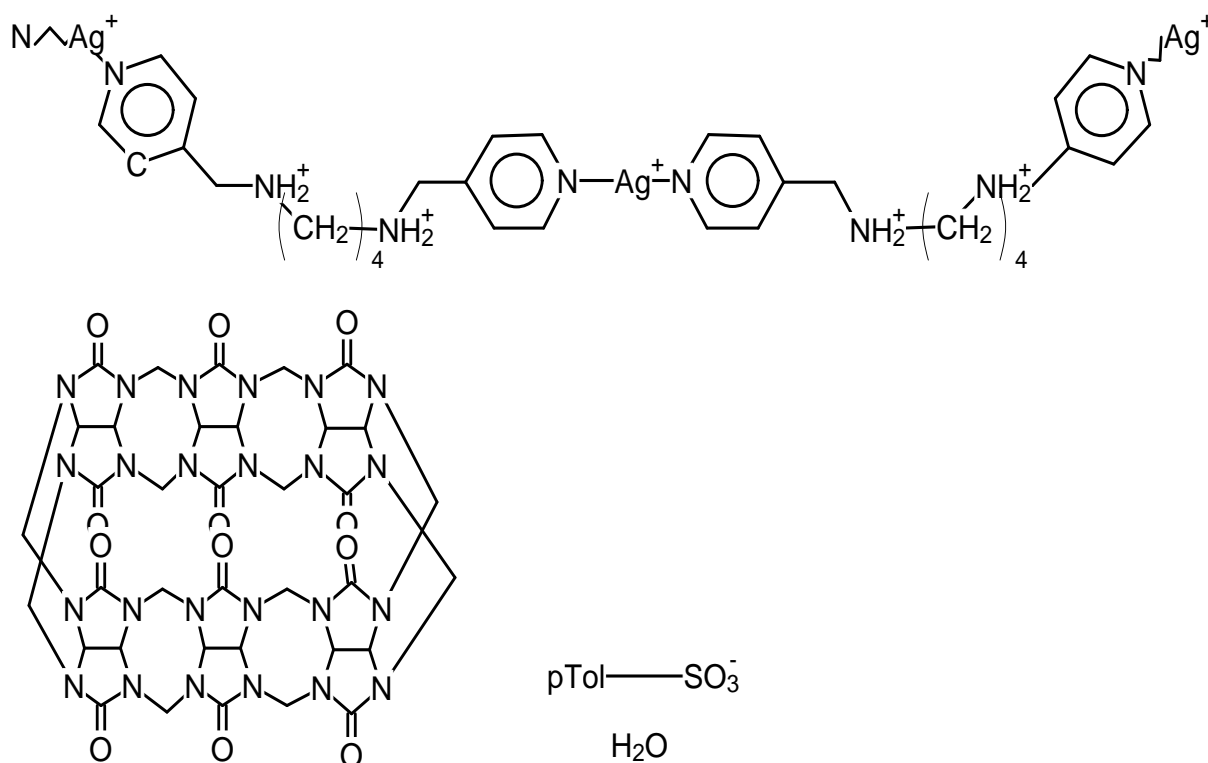
Reference: Dongmok Whang, Kimoon Kim (1997) *J.Am.Chem.Soc.* ,
119,451

Formula: $(C_{32} H_{48} Ag_2 N_8^{6+})_{0.5n}, n(C_{36} H_{36} N_{24} O_{12}), 3n(C_7 H_7 O_3 S_1^{1-}), 11n(H_2 O_1)$

Compound Name: catena(μ_2 -N,N'-bis(4-Pyridylmethyl-1,4-diaminobutane)-silver
cucurbituril tris(p-toluenesulfonate) undecahydrate)

Space Group: P-1 **Cell:** **a** 15.001(2) **b** 15.491(2) **c** 23.580(2)
Space Group No.: 2 **(Å, °)** α 91.90(1) β 105.54(0) γ 116.71(1)

R-Factor (%): 11.05 **Temperature(K):** 295 **Density(g/cm³):** 1.495



Search: search1 (Wed Aug 10 21:04:46 2011): Hit 5

SEWSES

Reference: Dongmok Whang, Ki-Min Park, Jungseok Heo, P.Ashton, K.Kim (1998) *J.Am.Chem.Soc.* ,**120**,4899

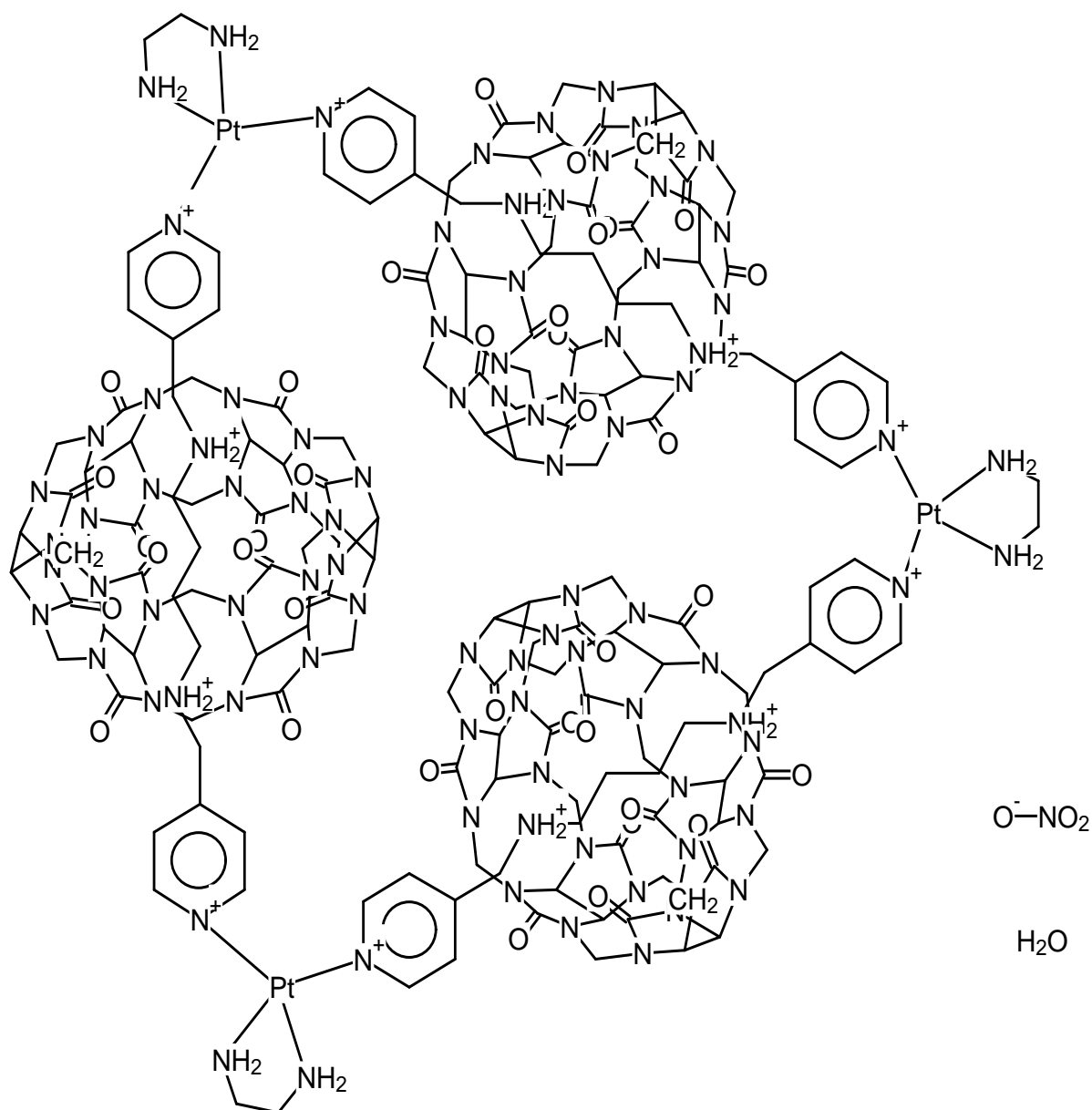
Formula: $C_{54} H_{96} N_{18} Pt_3^{12+}, C_{36} H_{36} N_{24} O_{12}, C_{36} H_{36} N_{24} O_{12}, C_{36} H_{36} N_{24} O_{12}, 12(N_1 O_3^{1-})$

Compound Name: (4)-tris((Cucurbituril)-(μ_2 -N,N'-bis(4-pyridylmethyl)-1,4-diaminobutane)-(ethylenediamine)-platinum)-cyclic-oligorotaxane dodecanitrate hydrate

Synonym: Cyclic oligorotaxane (4)MN molecular necklace dodecanitrate hydrate

Space Group: P63/m **Cell:** **a** 26.707(0) **b** 26.707(0) **c** 23.365(0)
Space Group No.: 176 **(Å, °)** α 90.00 β 90.00 γ 120.00

R-Factor (%): 9.57 **Temperature(K):** 188 **Density(g/cm³):** 1.584



Search: search1 (Wed Aug 10 21:04:46 2011): Hit 6

SEWSES01

Reference: Ki-Min Park, Soo-Young Kim, Jungseok Heo,
Dongmok Whang, S.Sakamoto, K.Yamaguchi, Kimoon Kim (2002)
J.Am.Chem.Soc. ,**124**,2140

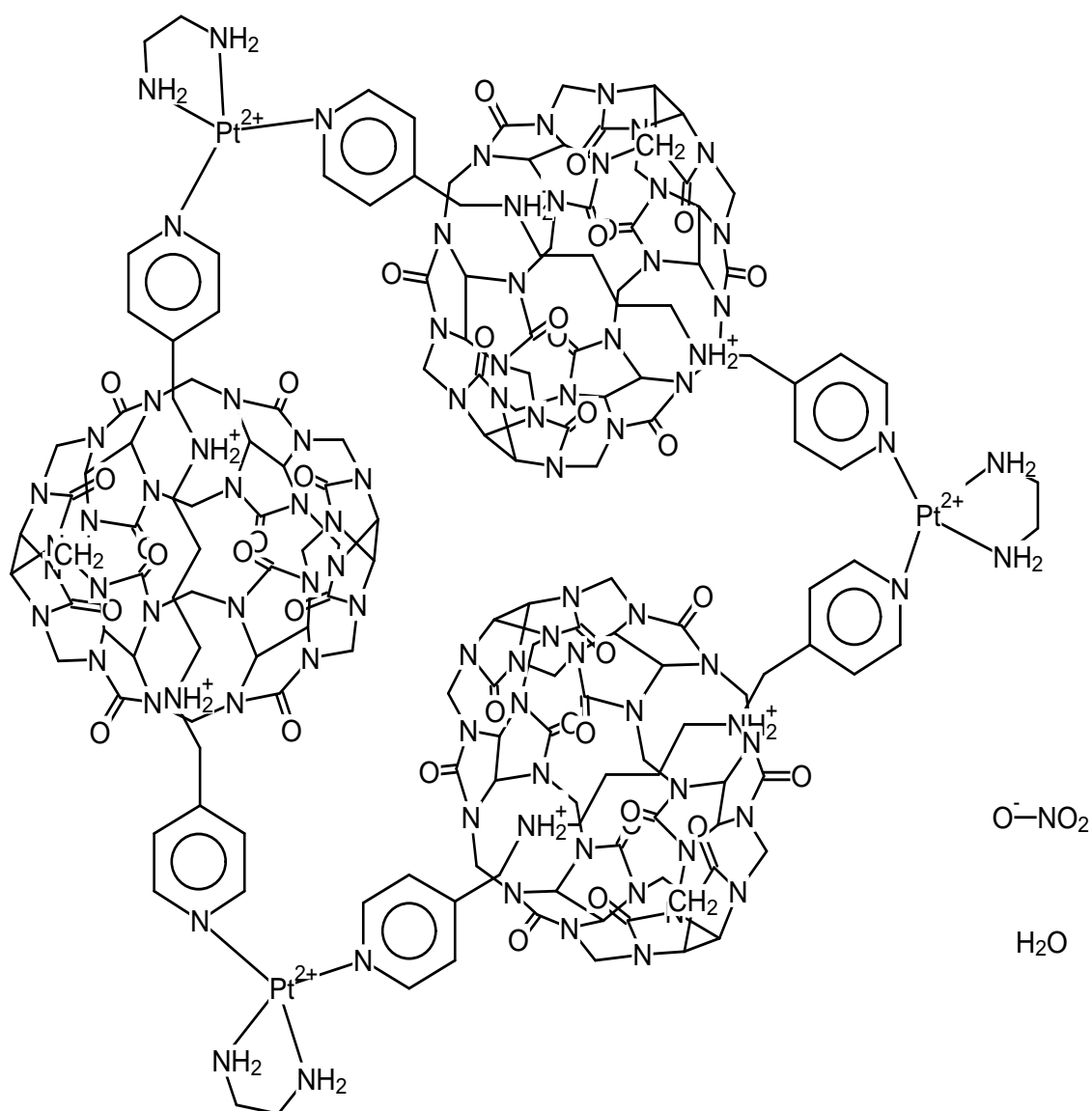
Formula: $C_{54}H_{96}N_{18}Pt_3^{12+}, C_{36}H_{36}N_{24}O_{12}, C_{36}H_{36}N_{24}O_{12}, C_{36}H_{36}N_{24}O_{12}, 12(N_1O_3^{1-})$

Compound Name: (4)-(tris((Cucurbituril)-(μ₂-N,N'-bis(4-pyridylmethyl)-1,4-diammonio-butane)-(ethylenediamine)-platinum))-cyclic-oligorotaxane dodecanitrate hydrate

Synonym: Cyclic oligorotaxane (4)MN molecular necklace dodecanitrate hydrate

Space Group: P63/m **Cell:** **a** 26.707(0) **b** 26.707(0) **c** 23.365(0)
Space Group No.: 176 **(Å, °)** **α** 90.00 **β** 90.00 **γ** 120.00

R-Factor (%): 9.57 **Temperature(K):** 188 **Density(g/cm³):** 1.584



Search: search1 (Wed Aug 10 21:04:46 2011): Hit 7

TUBVUH

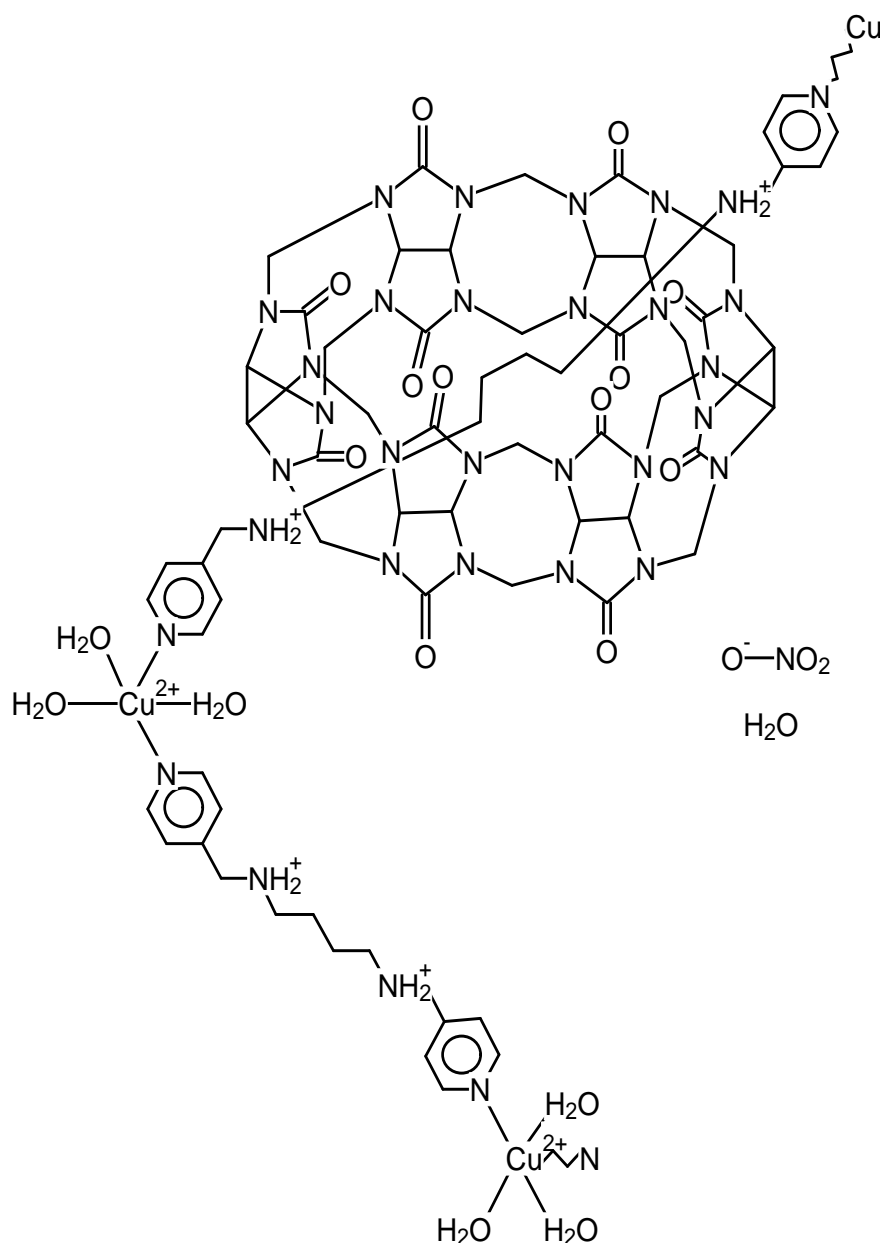
Reference: Dongmok Whang, You-Moon Jeon, Jungseok Heo, Kimoon Kim (1996) *J.Am.Chem.Soc.* ,**118**,11333

Formula: $(C_{36} H_{36} N_{24} O_{12})_2n, n(C_{32} H_{60} Cu_2 N_8 O_6^{8+}), 8n(N_1 O_3^{1-}), 28n(H_2 O_1)$

Compound Name: catena-((3)-bis(Cucurbituril)-(bis(μ_2 -N,N'-bis(4-pyridylmethyl)-1,4-diaminobutane)-hexa-aqua-di-copper))-polyrotaxane octanitrate hydrate

Space Group: P-1 **Cell:** **a** 14.690(2) **b** 14.923(2) **c** 19.665(3)
Space Group No.: 2 (**Å, °**) α 84.96(1) β 74.98(1) γ 68.90

R-Factor (%): 10.04 **Temperature(K):** 295 **Density(g/cm³):** 1.613



Search Overview

Search: search2
Date/Time done: Wed Aug 10 21:12:20 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

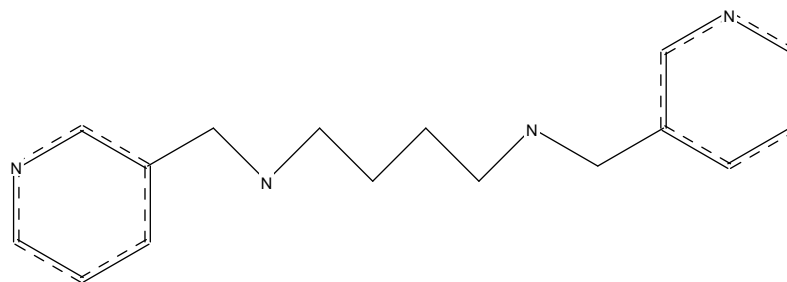
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

4M

Search: search2 (Wed Aug 10 21:12:20 2011): Hit 1

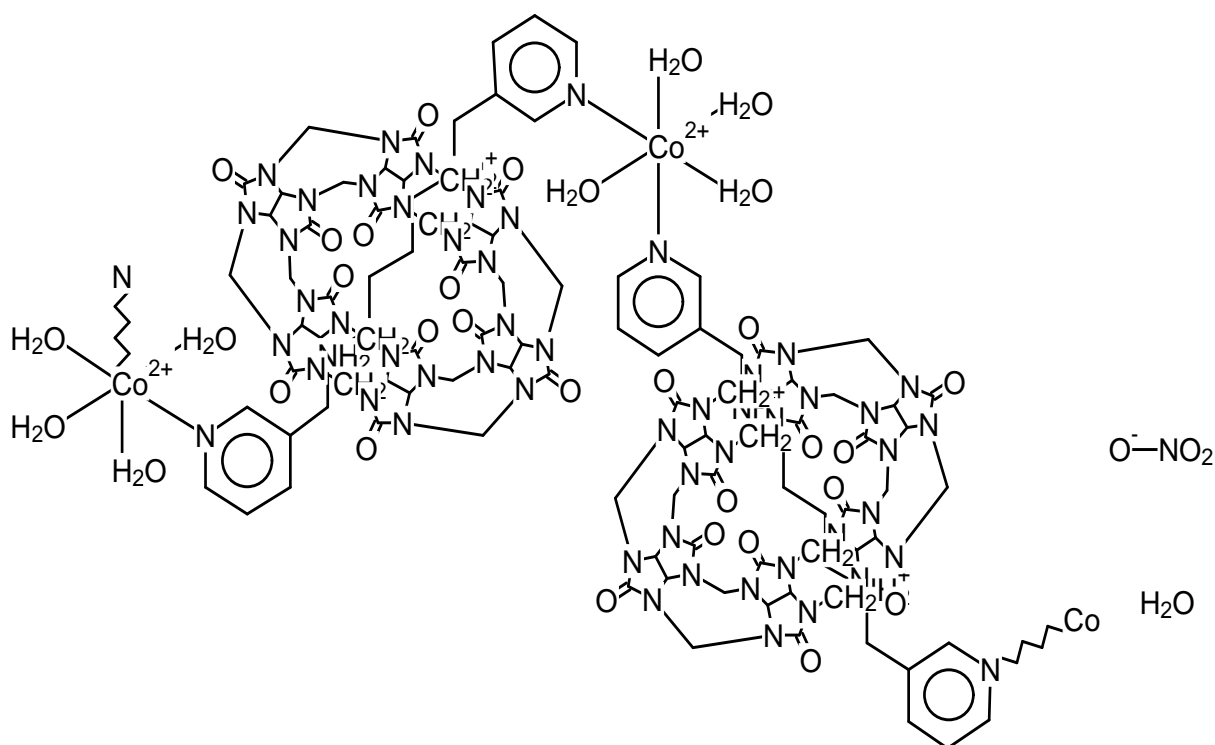
ADOFAA

Reference: Ki-Min Park, Dongmok Whang, Eunsung Lee,
Jungseok Heo, Kimoon Kim (2002) *Chem.-Eur.J.* ,**8**,498

Formula: $(C_{32} H_{64} Co_2 N_8 O_8^{8+})_n, n(C_{36} H_{36} N_{24} O_{12}), n(C_{36} H_{36} N_{24} O_{12}), 8n(N_1 O_3^{-1}), 30n(H_2O)$

Compound Name: catena-(cis-bis(μ_2 -N,N'-bis(3-Pyridylmethyl)butane-1,4-diammonium)-bis(tetra-aqua-cobalt(ii))-bis(cucurbituril)-polyrotaxane octanitrate hydrate)

Space Group:	P-1	Cell:	a 14.387(0)	b 14.709(0)	c 21.977(0)
Space Group No.:	2	(Å, °)	α 97.17(0)	β 97.34(0)	γ 115.94(0)
R-Factor (%):	7.42	Temperature(K):	293	Density(g/cm³):	1.569



Search: search2 (Wed Aug 10 21:12:20 2011): Hit 2

ADOFEE

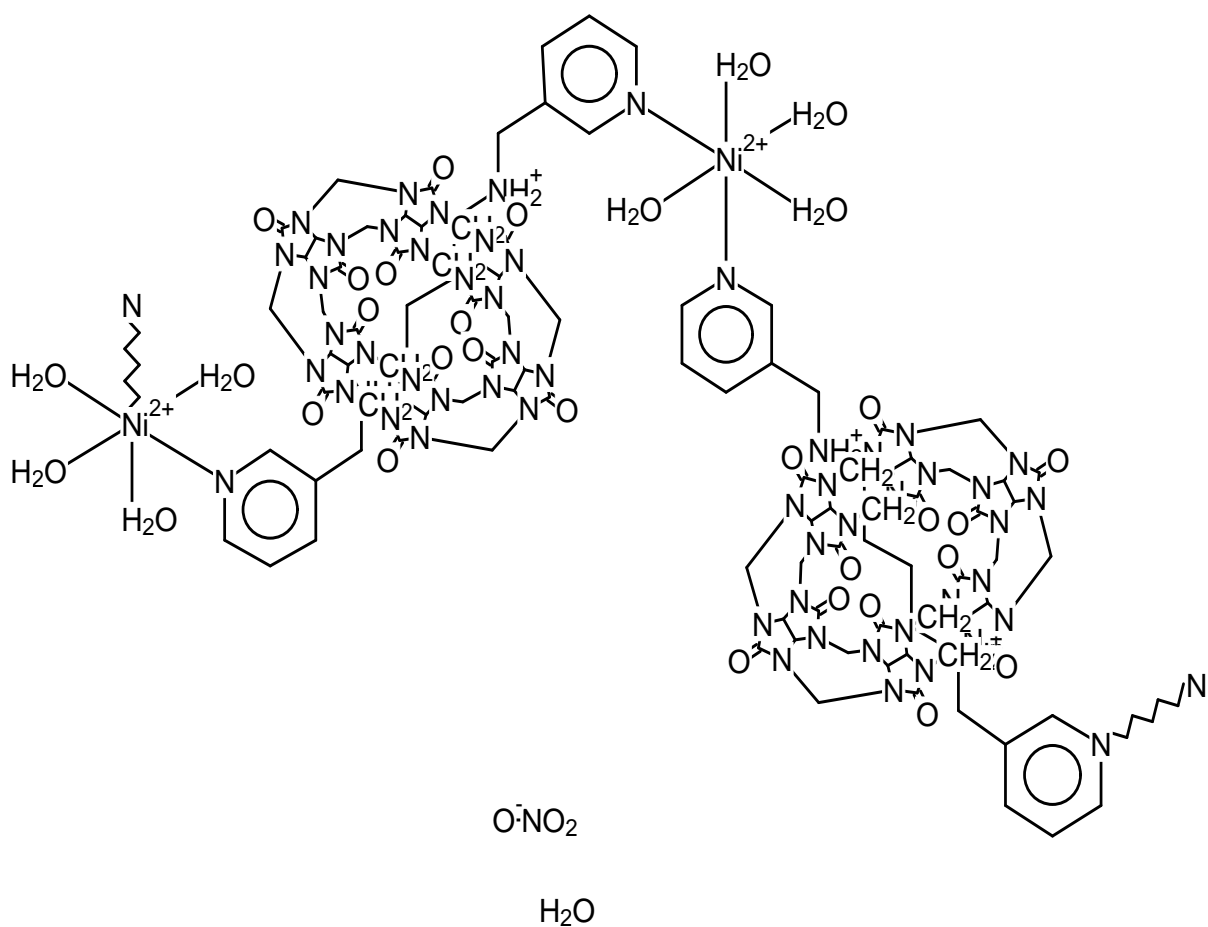
Reference: Ki-Min Park, Dongmok Whang, Eunsung Lee,
Jungseok Heo, Kimoon Kim (2002) *Chem.-Eur.J.* ,8,498

Formula: $(C_{32}H_{64}N_8Ni_2O_8^{8+})_n, n(C_{36}H_{36}N_{24}O_{12}), n(C_{36}H_{36}N_{24}O_{12}), 8n(N_1O_3^{1-}), 30n(H_2O)$

Compound Name: catena-(cis-bis(μ_2 -N,N'-bis(3-Pyridylmethyl)butane-1,4-diammonium)-bis(tetra-aqua-nickel(ii))-bis(cucurbituril)-polyrotaxane octanitrate hydrate)

Space Group: P-1 **Cell:** **a** 14.168(0) **b** 14.551(0) **c** 21.545(0)
Space Group No.: 2 (**Å, °**) α 99.05(0) β 94.68(0) γ 114.82

R-Factor (%): 13.22 **Temperature(K):** 188 **Density(g/cm³):** 1.622



Search: search2 (Wed Aug 10 21:12:20 2011): Hit 3

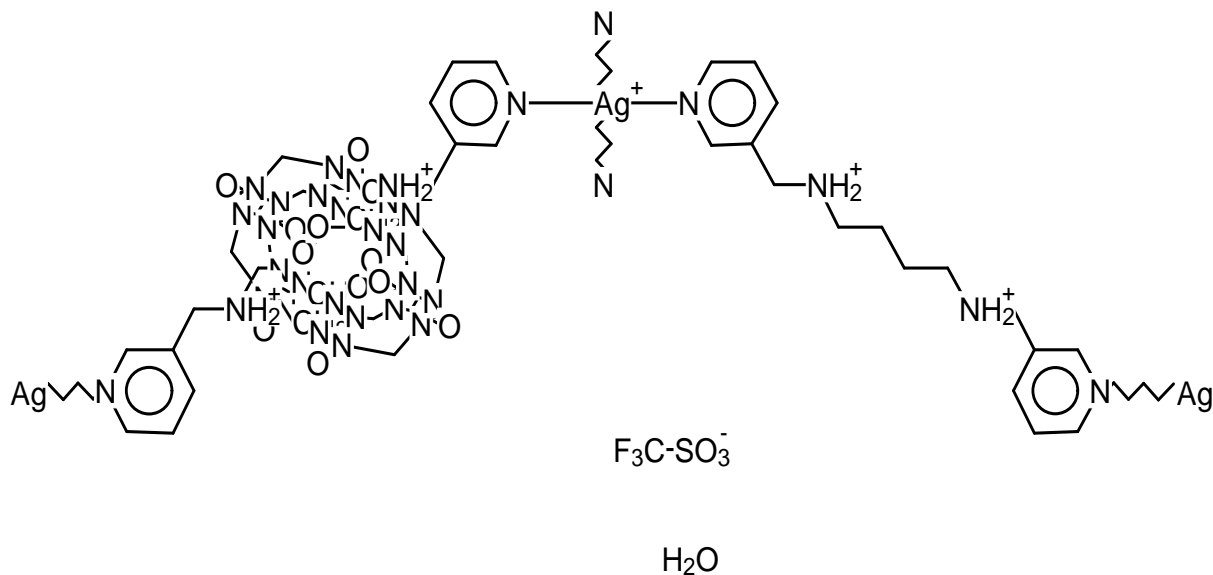
ADOGAB

Reference: Ki-Min Park, Dongmok Whang, Eunsung Lee,
Jungseok Heo, Kimoon Kim (2002) *Chem.-Eur.J.* ,**8**,498

Formula: $(C_{36} H_{36} N_{24} O_{12})_{2n,n}(C_{32} H_{48} Ag_1 N_8^{5+}),5n(C_1 F_3 O_3 S_1^{1-}),20n(H_2 O_1)$

Compound Name: catena-((bis(μ_2 -N,N'-bis(3-Pyridylmethyl)butane-1,4-diammonium)-
silver(i))-bis(cucurbituril)-polyrotaxane
pentakis(trifluoromethanesulfonate) icosahydrate)

Space Group:	P4/n	Cell:	a 24.453(0)	b 24.453(0)	c 12.691(0)
Space Group No.:	85	(Å, °)	α 90.00	β 90.00	γ 90.00
R-Factor (%):	5.63	Temperature(K):	293	Density(g/cm³):	1.642



Search: search2 (Wed Aug 10 21:12:20 2011): Hit 4

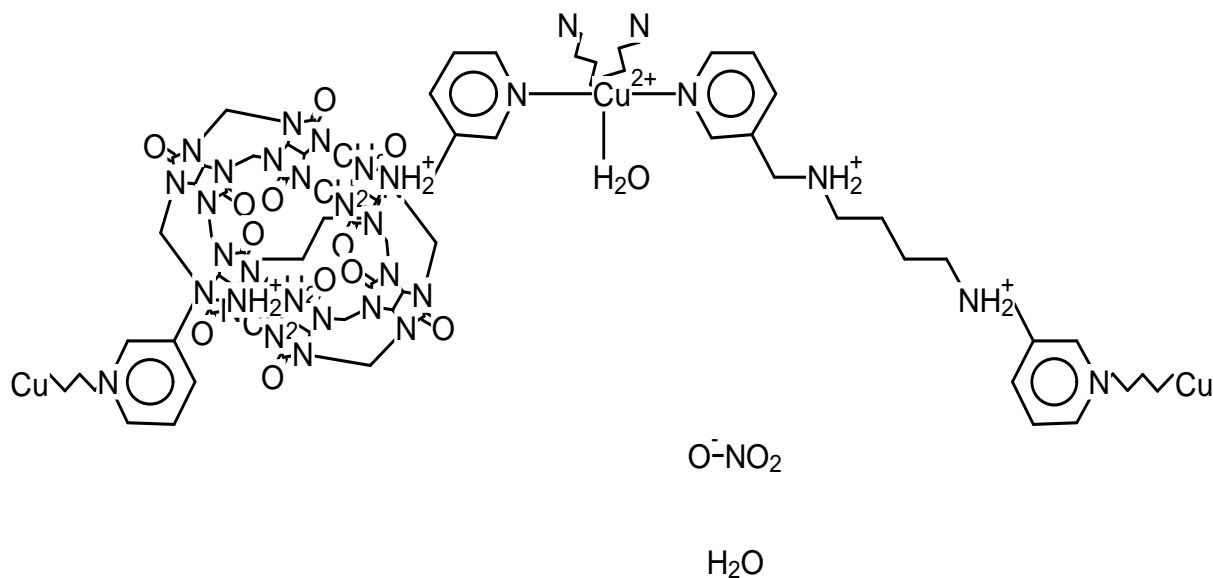
ADOGEF

Reference: Ki-Min Park, Dongmok Whang, Eunsung Lee,
Jungseok Heo, Kimoon Kim (2002) *Chem.-Eur.J.*, **8**,498

Formula: $(C_{36} H_{36} N_{24} O_{12})_2 n, n(C_{32} H_{50} Cu_1 N_8 O_1^{6+}), 6n(N_1 O_3^{1-}), 2 \cdot 3.5n(H_2 O_1)$

Compound Name: catena-(bis(μ_2 -N,N'-bis(3-Pyridylmethyl)butane-1,4-diammonium)-aqua-copper(ii) bis(cucurbituril) polyrotaxane hexanitrate hydrate)

Space Group:	P4/n	Cell:	a 23.751(0)	b 23.751(0)	c 14.116(0)
Space Group No.:	85	(Å, °)	α 90.00	β 90.00	γ 90.00
R-Factor (%):	10.89	Temperature(K):	170	Density(g/cm³):	1.425



Search: search2 (Wed Aug 10 21:12:20 2011): Hit 5

XIGXIU

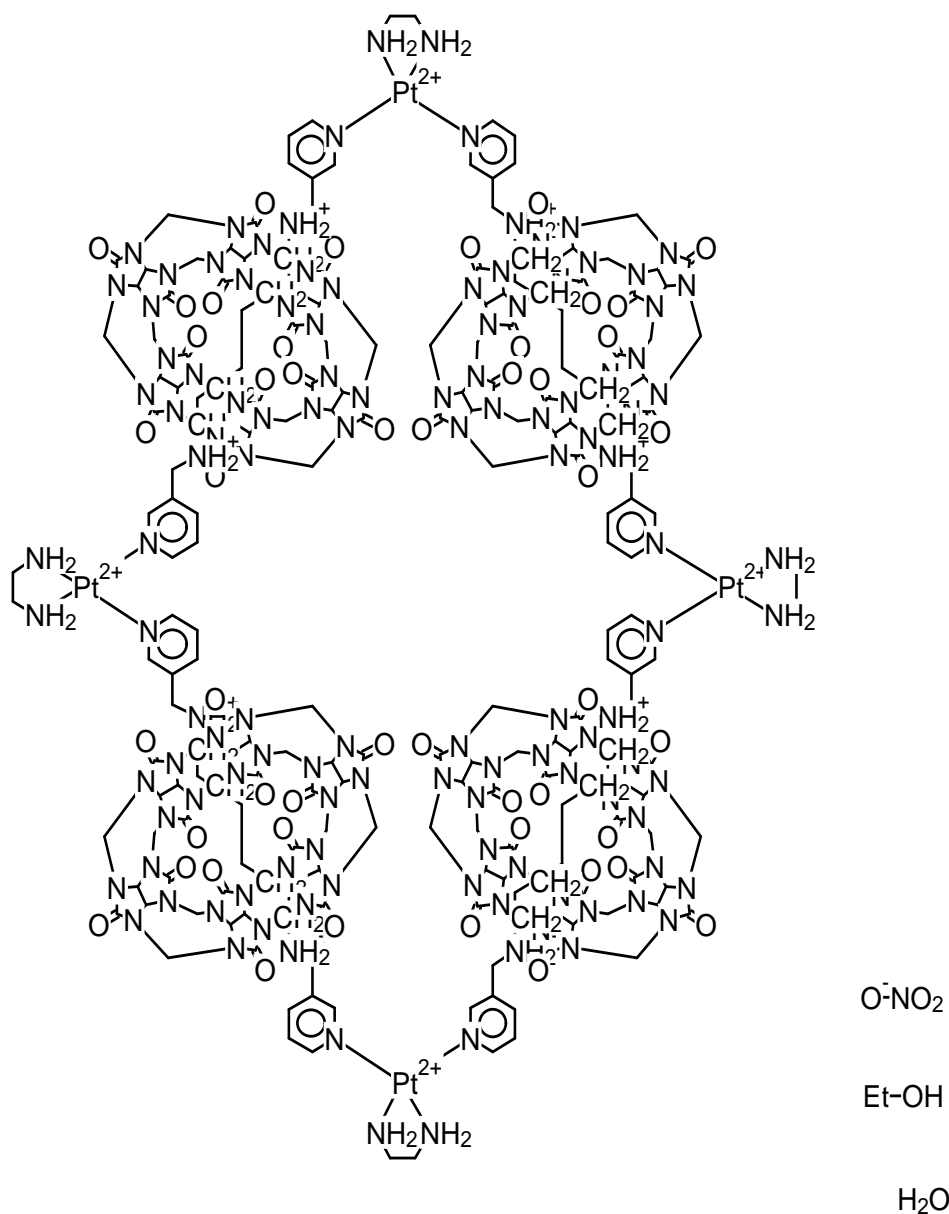
Reference: Ki-Min Park, Soo-Young Kim, Jungseok Heo,
Dongmok Whang, S.Sakamoto, K.Yamaguchi, Kimoon Kim (2002)
J.Am.Chem.Soc. ,**124**,2140

Formula: $C_{36} H_{36} N_{24} O_{12}$, $C_{72} H_{128} N_{24} Pt_4^{16+}$, $C_{36} H_{36} N_{24} O_{12}$, $C_{36} H_{36} N_{24} O_{12}$, $C_{36} H_{36} N_{24} O_{12}$

Compound Name: (5)-(tetrakis((Cucurbituril)-(μ_2 -N,N'-bis(3-pyridylmethyl)-1,4-diammoniumbutane)-(ethylenediamine)-platinum))-cyclic-oligorotaxane hexadecanitate ethanol solvate hydrate

Space Group: P21 **Cell:** **a** 15.756(0) **b** 26.462(0) **c** 43.249(0)
Space Group No.: 4 (**Å, °**) α 90.00 β 94.43(0) γ 90.00

R-Factor (%): 8.01 **Temperature(K):** 188 **Density(g/cm³):** 1.574



Search Overview

Search: search3
Date/Time done: Wed Aug 10 21:17:39 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

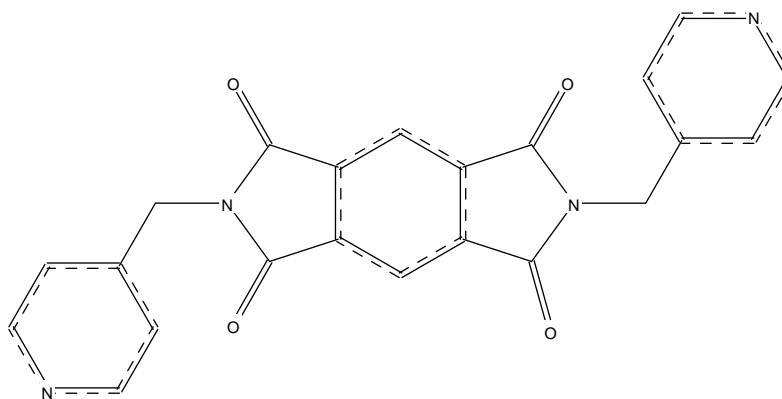
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

4M

Search: search3 (Wed Aug 10 21:17:39 2011): Hit 1

JIQXUD

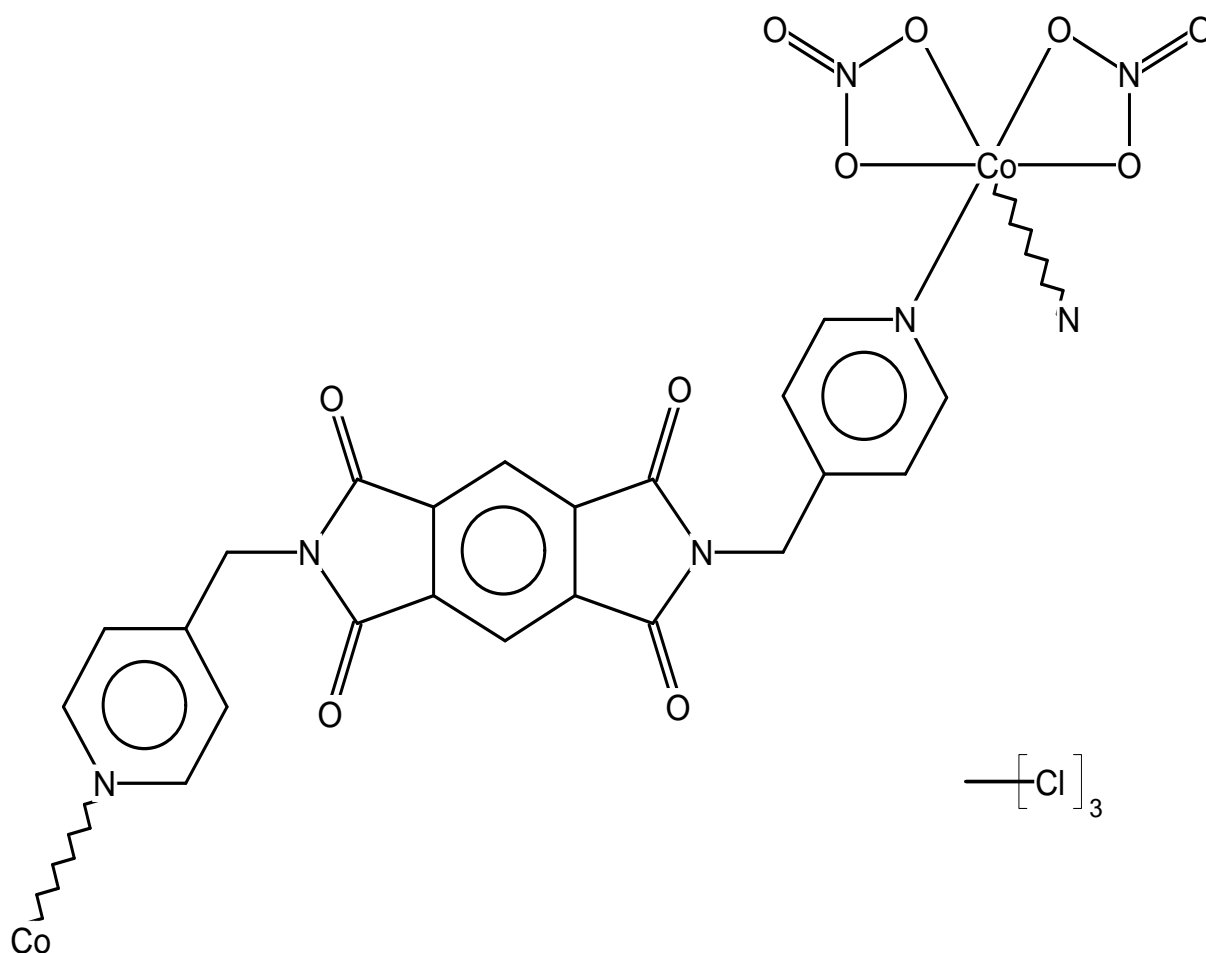
Reference: Yu-Qin Qiao, Xing-Qiang Lu, Cheng-Yong Su,
Bei-Sheng Kang (2007) *Z.Anorg.Allg.Chem.* ,**633**,2453

Formula: (C₂₂ H₁₄ Co₁ N₆ O₁₀)_n,n(C₁ H₁ Cl₃)

Compound Name: catena-[(μ₂-N,N'-bis(4-Pyridylmethyl) pyromellitic diimide-N,N')-
bis(nitrato-O,O')-cobalt(ii) chloroform solvate]

Space Group: C2/c **Cell:** **a** 16.720(3) **b** 17.232(3) **c** 12.175(2)
Space Group No.: 15 **(Å, °)** **α** 90.00 **β** 128.90(0) **γ** 90.00

R-Factor (%): 6.93 **Temperature(K):** 293 **Density(g/cm³):** 1.705



Search: search3 (Wed Aug 10 21:17:39 2011): Hit 2

PALYOR

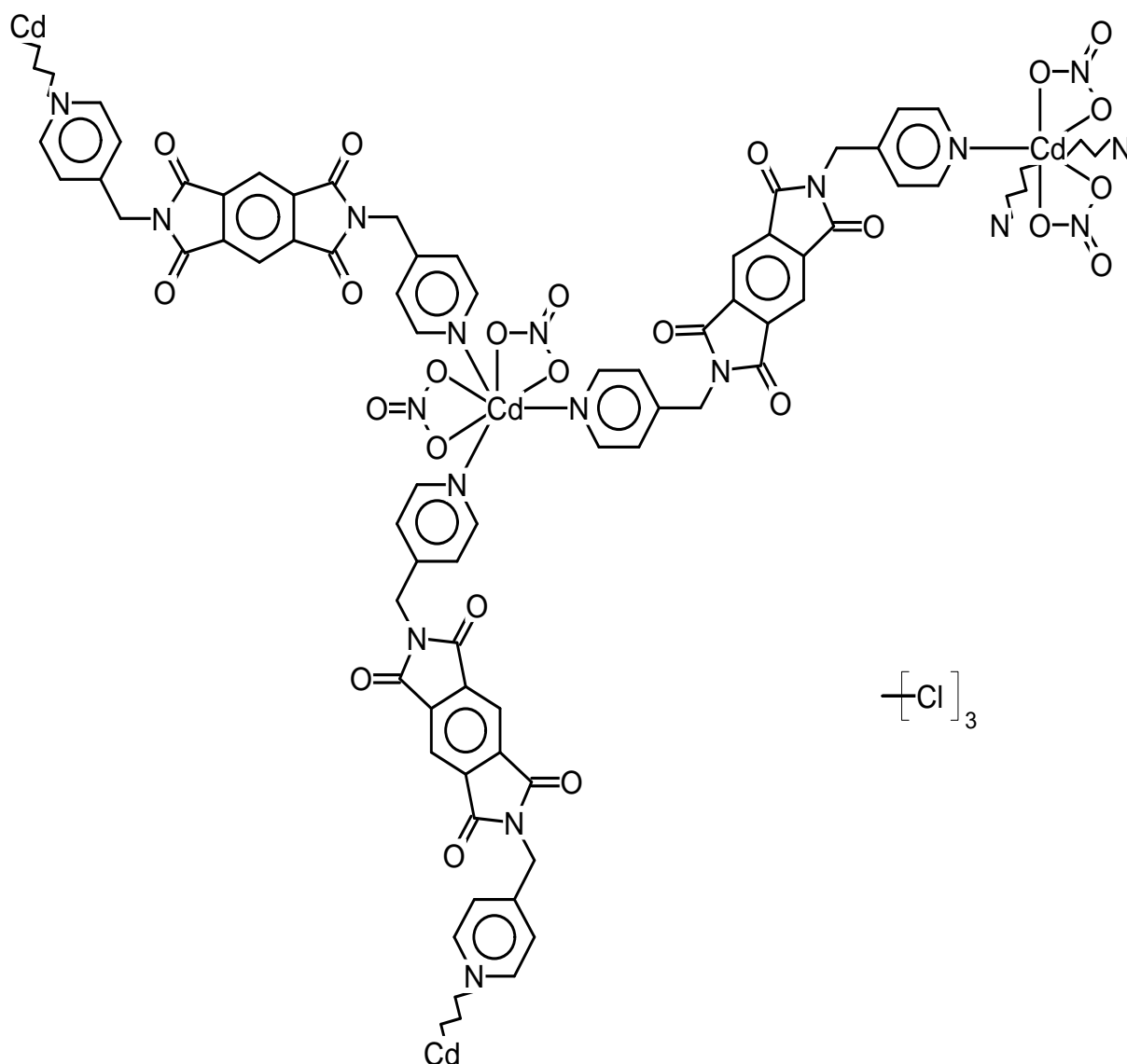
Reference: Xing-Qiang Lu, Ji-Jun Jiang, H.-C.zur Loye,
Bei-Sheng Kang, Cheng-Yong Su (2005) *Inorg.Chem.* ,**44**,1810

Formula: $(C_{66} H_{42} Cd_2 N_{16} O_{24})_n, 2n(C_1 H_1 Cl_3)$

Compound Name: catena-(tris(μ_2 -N,N'-bis(4-Pyridylmethyl)pyromellitic diimide)-
tetrakis(nitrato-O,O')-di-cadmium(ii) chloroform solvate)

Space Group: P-1 **Cell:** **a** 11.012(1) **b** 13.190(2) **c** 13.934(2)
Space Group No.: 2 **(Å, °)** α 95.10(0) β 106.14(0) γ 99.00(0)

R-Factor (%): 4.00 **Temperature(K):** 298 **Density(g/cm³):** 1.665



Search: search3 (Wed Aug 10 21:17:39 2011): Hit 3

RESHUT

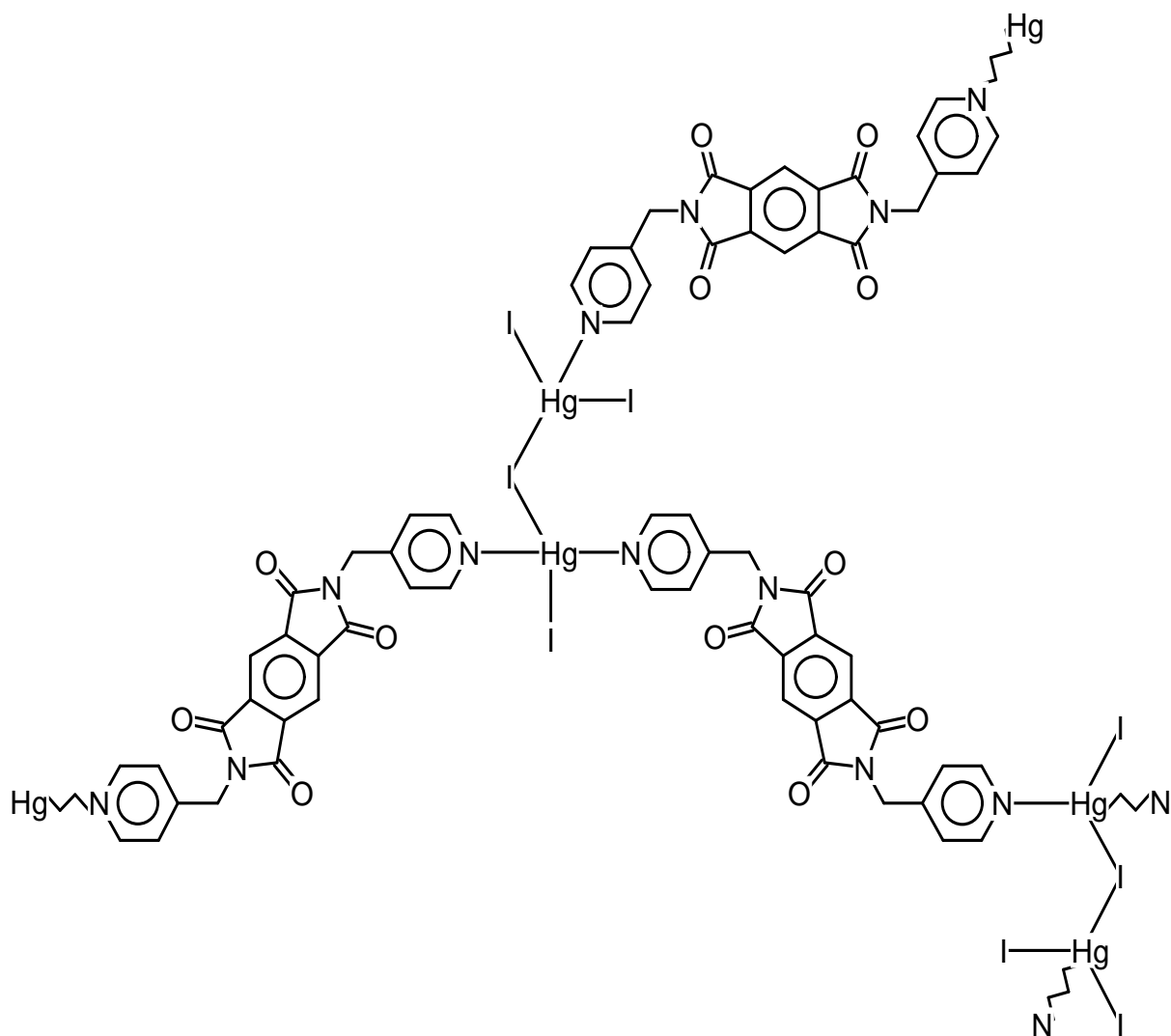
Reference: Xing-Qiang Lu, Mei Pan, Jian-Rong He, Yue-Peng Cai,
Bei-Sheng Kang, Cheng-Yong Su (2006) *CrystEngComm* ,8,827

Formula: (C₆₆ H₄₂ Hg₄ I₈ N₁₂ O₁₂)_n

Compound Name: catena-(bis(μ₂-Iodo)-tris(μ₂-N,N'-bis(4-pyridylmethyl)pyromellitic diimide-N,N')-octakis(iodo)-tetra-mercury)

Space Group: P-1 **Cell:** **a** 10.882(4) **b** 14.319(5) **c** 14.827(5)
Space Group No.: 2 **(Å, °)** **α** 62.90(0) **β** 89.98(0) **γ** 69.69(0)

R-Factor (%): 4.23 **Temperature(K):** 293 **Density(g/cm³):** 2.642



Search: search3 (Wed Aug 10 21:17:39 2011): Hit 4

TAJCEN

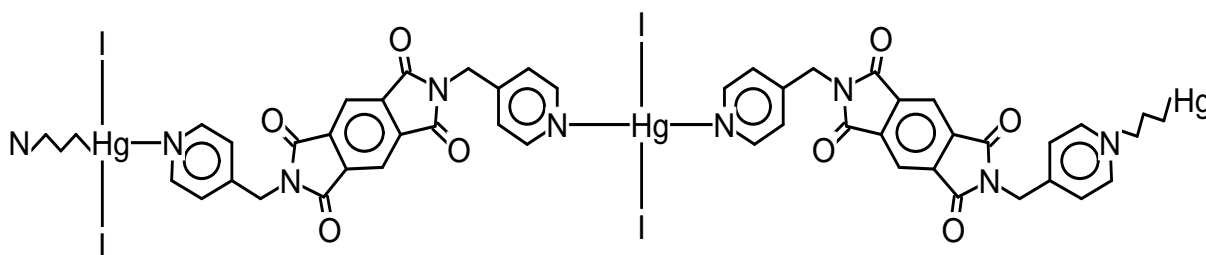
Reference: Yun-Hui Li, Cheng-Yong Su, A.M.Goforth, K.D.Shimizu, K.D.Gray, M.D.Smith, H.-C.zur Loye (2003) *Chem.Commun.* ,1630

Formula: (C₄₄ H₂₈ Hg₂ I₄ N₈ O₈)_n

Compound Name: catena-(bis(μ₂-2,6-bis(4-Pyridylmethyl)benzo(1,2-c:4,5-c')dipyrrole-1,3,5,7(2H,6H)-tetrone)-bis(di-iodo-mercury(ii)))

Space Group: P21/n **Cell:** **a** 11.668(0) **b** 12.226(0) **c** 17.444(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 103.51(0) γ 90.00

R-Factor (%): 2.96 **Temperature(K):** 150 **Density(g/cm³):** 2.341



Search Overview

Search: search4
Date/Time done: Wed Aug 10 21:26:39 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

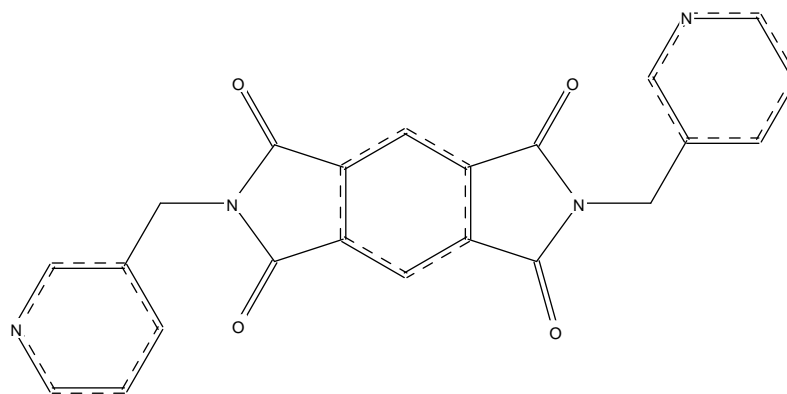
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

4M

Search: search4 (Wed Aug 10 21:26:39 2011): Hit 1

FISCAM

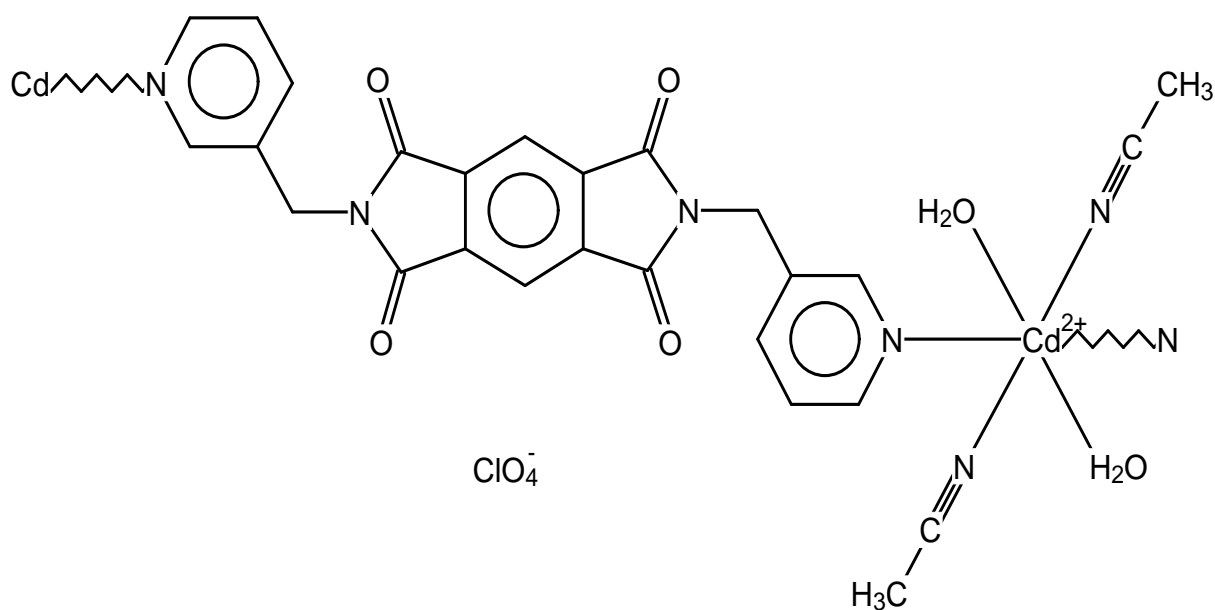
Reference: Xing-Qiang Lu, Li Zhang, Chun-Long Chen,
Cheng-Yong Su, Bei-Sheng Kang (2005) *Inorg.Chim.Acta* ,**358**,1771

Formula: $(C_{26} H_{24} Cd_1 N_6 O_6^{2+})_n, 2n(Cl_1 O_4^{1-})$

Compound Name: catena-((μ_2 -N,N'-bis(3-Pyridylmethyl)pyromellitic di-imide-N,N')-bis(acetonitrile)-diaqua-cadmium diperchlorate)

Space Group: P21/c **Cell:** **a** 13.545(1) **b** 8.135(1) **c** 14.882(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 95.57(0) γ 90.00

R-Factor (%): 3.70 **Temperature(K):** 298 **Density(g/cm³):** 1.685



Search: search4 (Wed Aug 10 21:26:39 2011): Hit 2

FISCEQ

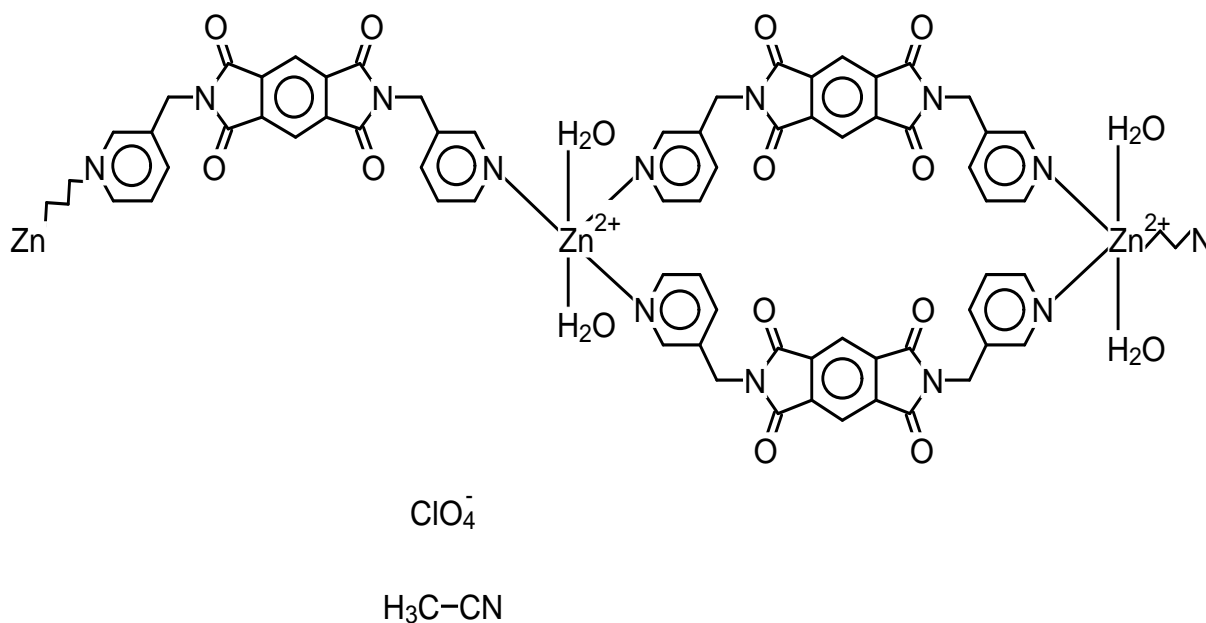
Reference: Xing-Qiang Lu, Li Zhang, Chun-Long Chen,
Cheng-Yong Su, Bei-Sheng Kang (2005) *Inorg.Chim.Acta* ,**358**,1771

Formula: $(C_{66} H_{50} N_{12} O_{16} Zn_2^{4+})n, 4n(Cl_1 O_4^{1-}), 2n(C_2 H_3 N_1)$

Compound Name: catena-(tris(μ_2 -N,N'-bis(3-Pyridylmethyl)pyromellitic di-imide-N,N')-tetra-aqua-di-zinc tetraperchlorate acetonitrile solvate)

Space Group: P-1 **Cell:** **a** 7.797(1) **b** 8.706(1) **c** 28.893(4)
Space Group No.: 2 (**Å, °**) α 81.94(0) β 89.38(0) γ 86.81(0)

R-Factor (%): 5.25 **Temperature(K):** 298 **Density(g/cm³):** 1.608



Search: search4 (Wed Aug 10 21:26:39 2011): Hit 3

PALYIL

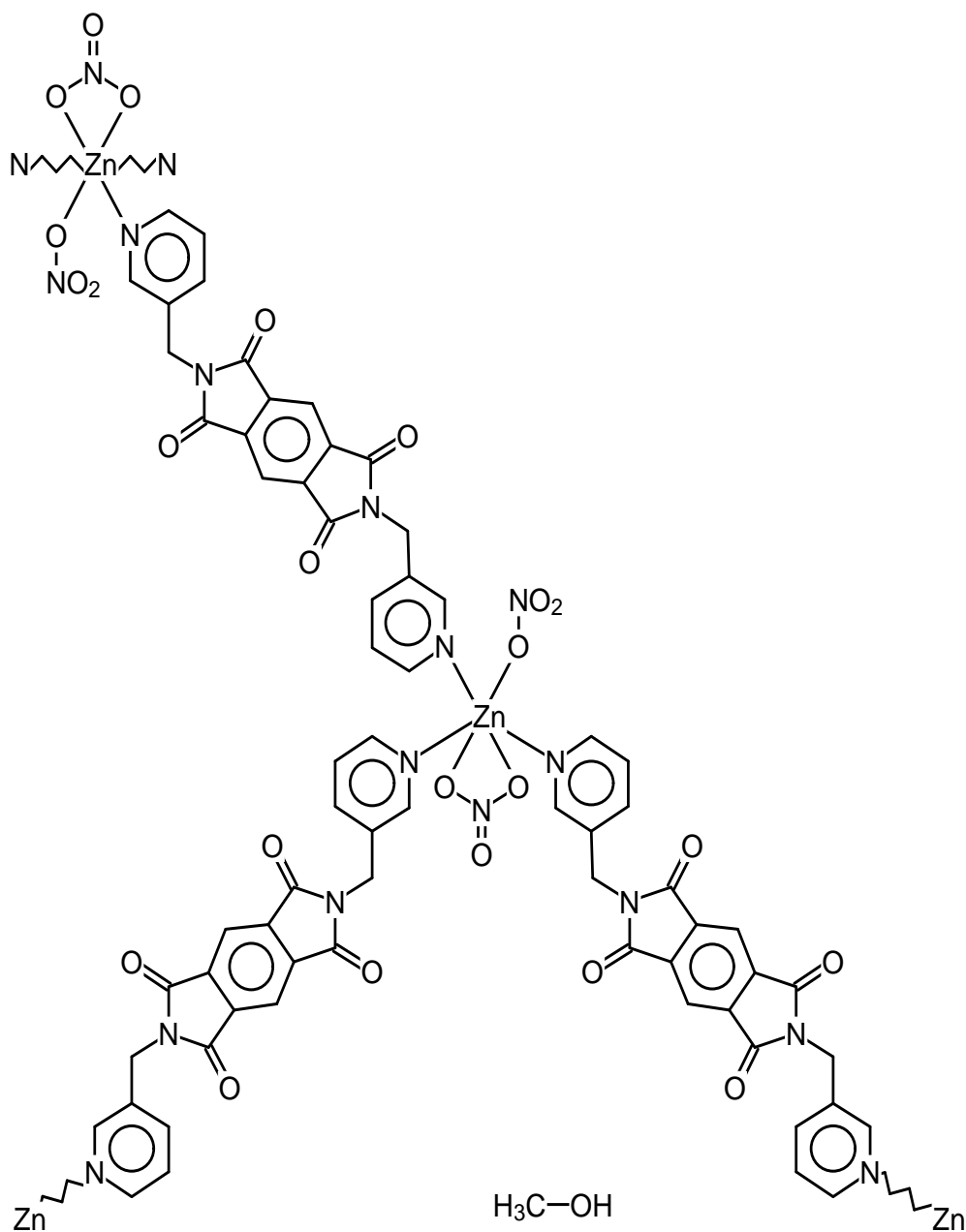
Reference: Xing-Qiang Lu, Ji-Jun Jiang, H.-C.zur Loye,
Bei-Sheng Kang, Cheng-Yong Su (2005) *Inorg.Chem.* ,**44**,1810

Formula: (C₆₆ H₄₂ N₁₆ O₂₄ Zn₂)_n,2n(C₁ H₄ O₁)

Compound Name: catena-(tris(μ₂-N,N'-bis(3-Pyridylmethyl)pyromellitic diimide)-bis(nitrato-O)-bis(nitrato-O,O')-di-zinc(ii) methanol solvate)

Space Group: P21/a **Cell:** **a** 15.361(4) **b** 13.388(4) **c** 17.105(5)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 103.43(0) **γ** 90.00

R-Factor (%): 4.09 **Temperature(K):** 293 **Density(g/cm³):** 1.590



Search: search4 (Wed Aug 10 21:26:39 2011): Hit 4

PALYUX

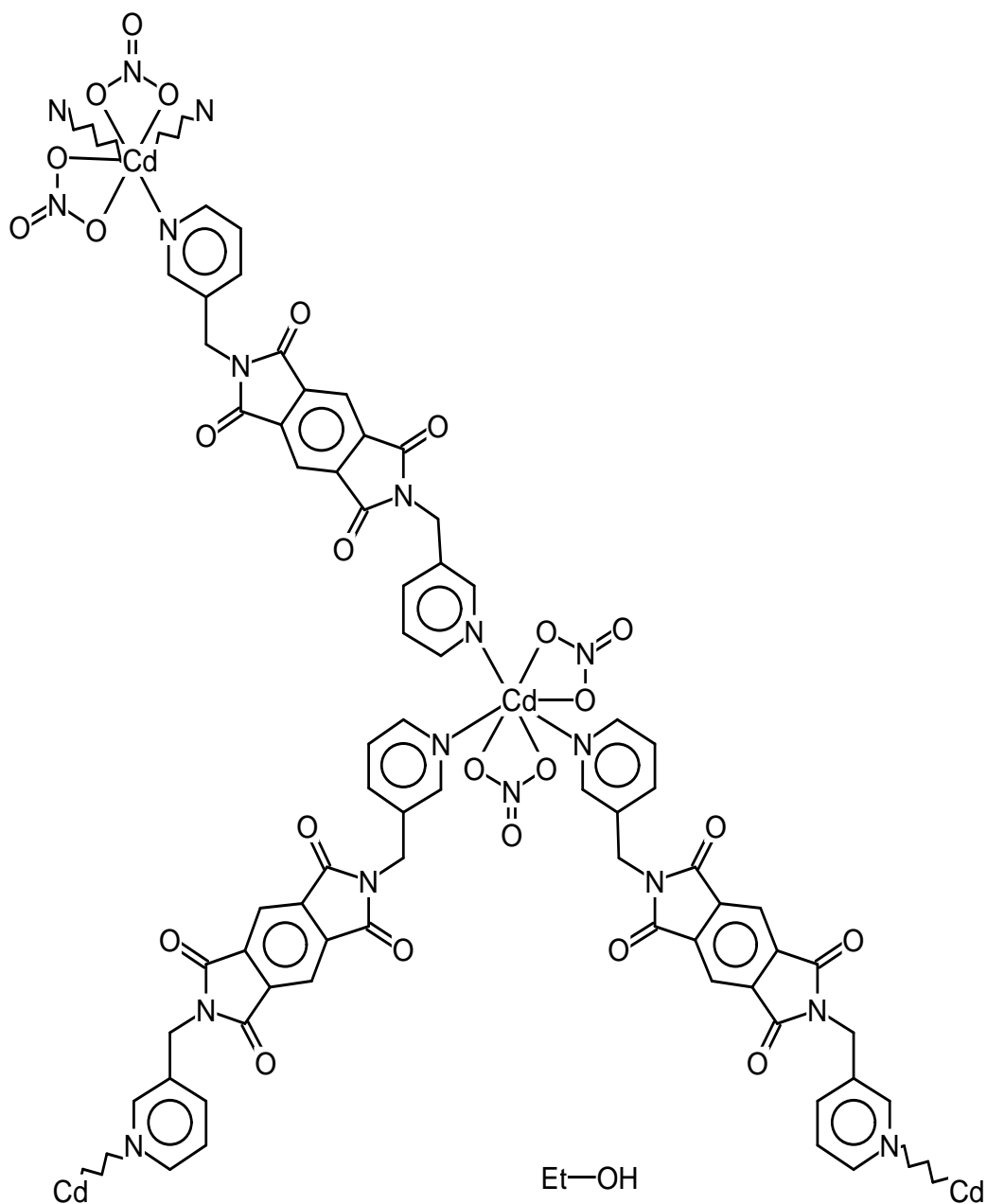
Reference: Xing-Qiang Lu, Ji-Jun Jiang, H.-C.zur Loye,
Bei-Sheng Kang, Cheng-Yong Su (2005) *Inorg.Chem.* ,**44**,1810

Formula: $(C_{66} H_{42} Cd_2 N_{16} O_{24})_n, 2n(C_2 H_6 O_1)$

Compound Name: catena-(tris(μ_2 -N,N'-bis(3-Pyridylmethyl)pyromellitic diimide)-bis(nitrato-O)-bis(nitrato-O,O')-di-cadmium(ii) ethanol solvate)

Space Group: P21/a **Cell:** **a** 15.403(1) **b** 13.614(1) **c** 17.400(2)
Space Group No.: 14 **(Å, °)** α 90.00 β 103.25(0) γ 90.00

R-Factor (%): 3.93 **Temperature(K):** 293 **Density(g/cm³):** 1.646



Search: search4 (Wed Aug 10 21:26:39 2011): Hit 5

PEVYUL

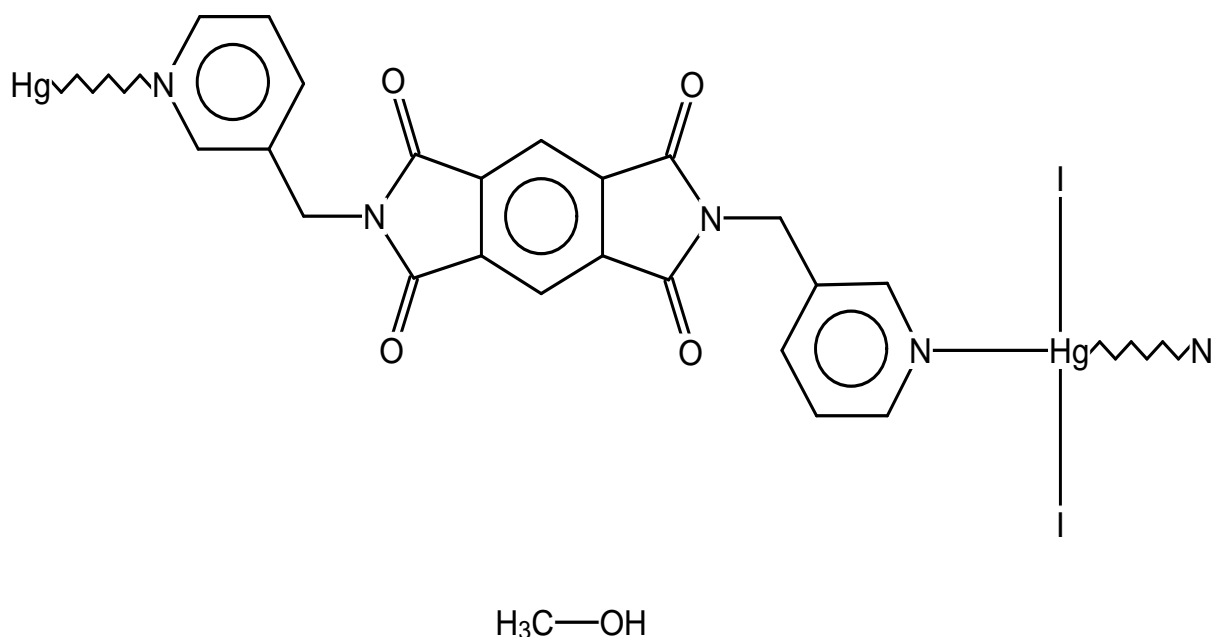
Reference: Xiaokang Li, Xialin Fan, Qingdao Zeng (2007)
Int.J.Mol.Sci. ,**8**,29

Formula: (C₂₂ H₁₄ Hg₁ I₂ N₄ O₄)_n,0.4n(C₁ H₄ O₁)

Compound Name: catena-((μ₂-N,N'-bis(3-Pyridylmethyl)diphthalic di-imide))-di-iodo-mercury(ii) methanol solvate

Space Group: P2/n **Cell:** **a** 10.812(2) **b** 6.226(1) **c** 19.627(4)
Space Group No.: 13 **(Å, °)** **α** 90.00 **β** 98.11(3) **γ** 90.00

R-Factor (%): 4.28 **Temperature(K):** 293 **Density(g/cm³):** 2.198



Search Overview

Search: search5
Date/Time done: Wed Aug 10 21:31:08 2011
Database(s): CSD version 5.32 (November 2010)
CSD version 5.32 updates (Nov 2010)
Restriction Info: No refcode restrictions applied
Filters: None
Percentage Completed: 100%
Number of Hits: 13

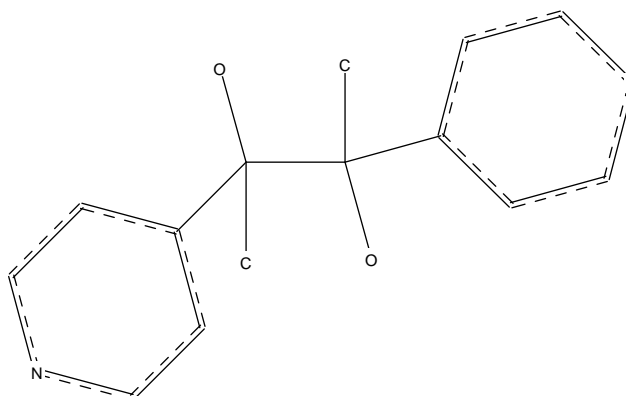
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

4M

Search: search5 (Wed Aug 10 21:31:08 2011): Hit 1

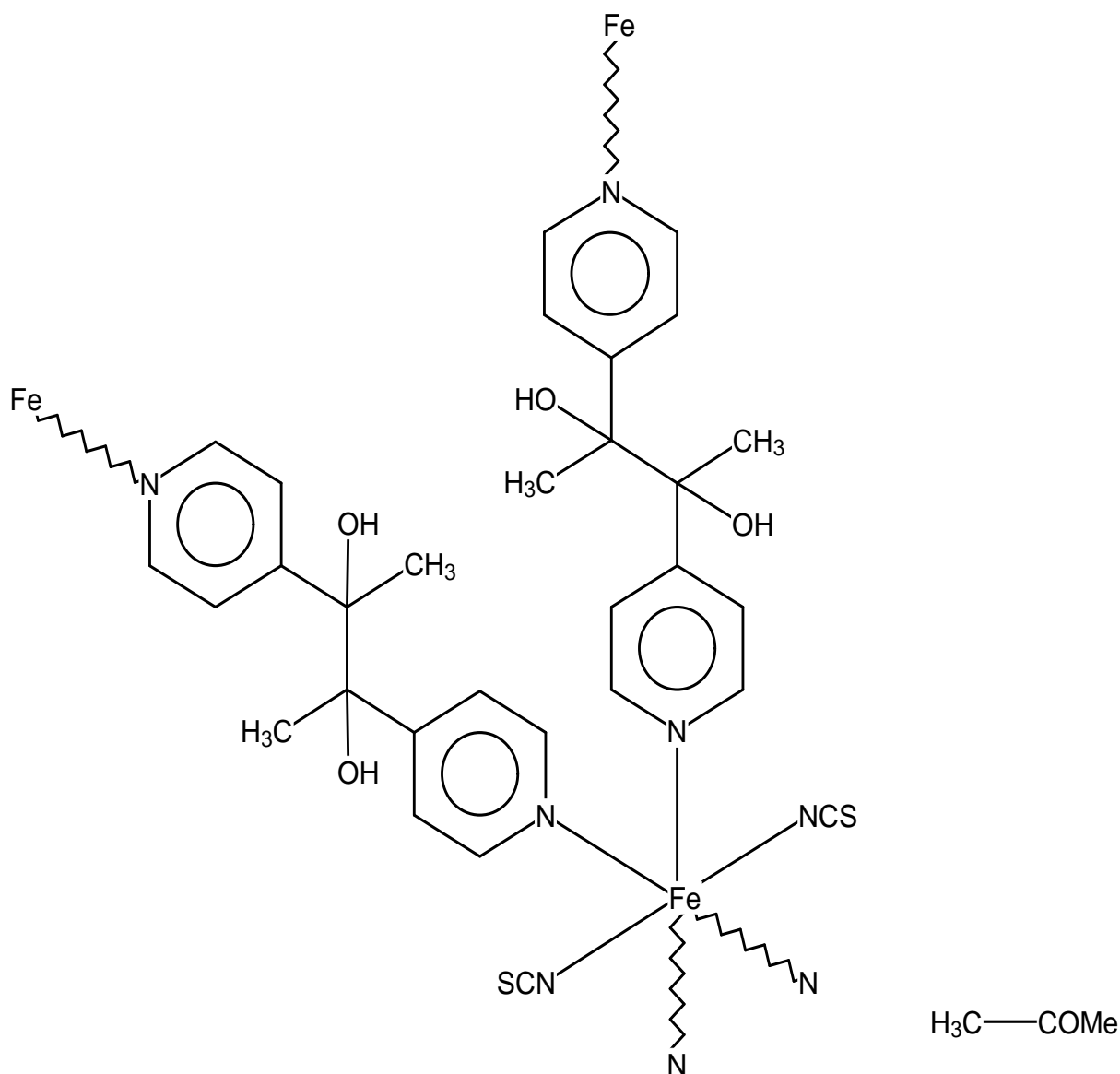
CEZDAN

Reference: S.M.Neville, B.Moubaraki, K.S.Murray, C.J.Keper (2007)
Angew.Chem.,Int.Ed. ,**46**,2059

Formula: $(C_{30} H_{32} Fe_1 N_6 O_4 S_2)_n, 0.5n(C_3 H_6 O_1)$

Compound Name: catena-(bis(μ_2 -meso-2,3-bis(4-Pyridyl)butane-2,3-diol)-dithiocyanato-iron(ii) hemikis(acetone) clathrate)

Space Group:	P4/ncc	Cell:	a 14.574(3)	b 14.574(3)	c 17.964(4)
Space Group No.:	130	(Å, °)	α 90.00	β 90.00	γ 90.00
R-Factor (%):	7.11	Temperature(K):	220	Density(g/cm³):	1.201



Search: search5 (Wed Aug 10 21:31:08 2011): Hit 2

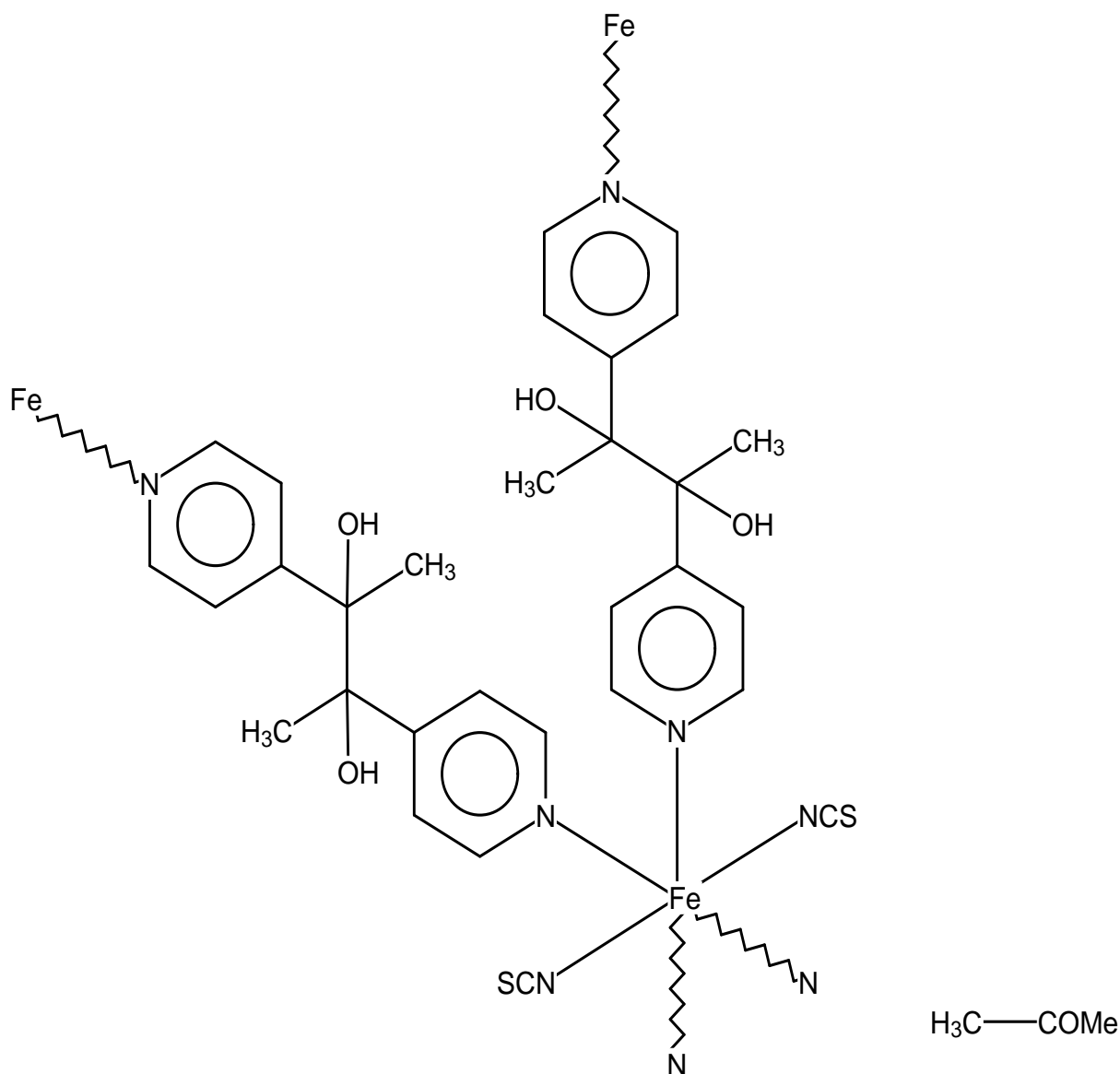
CEZDAN01

Reference: S.M.Neville, B.Moubaraki, K.S.Murray, C.J.Keper (2007)
Angew.Chem.,Int.Ed. ,**46**,2059

Formula: (C₃₀ H₃₂ Fe₁ N₆ O₄ S₂)_n,0.5n(C₃ H₆ O₁)

Compound Name: catena-(bis(μ₂-meso-2,3-bis(4-Pyridyl)butane-2,3-diol)-dithiocyanato-iron(ii) hemikis(acetone) clathrate)

Space Group:	P4/ncc	Cell:	a 14.224(1)	b 14.224(1)	c 17.580(4)
Space Group No.:	130	(Å, °)	α 90.00	β 90.00	γ 90.00
R-Factor (%):	8.31	Temperature(K):	173	Density(g/cm³):	1.288



Search: search5 (Wed Aug 10 21:31:08 2011): Hit 3

CIDGEC

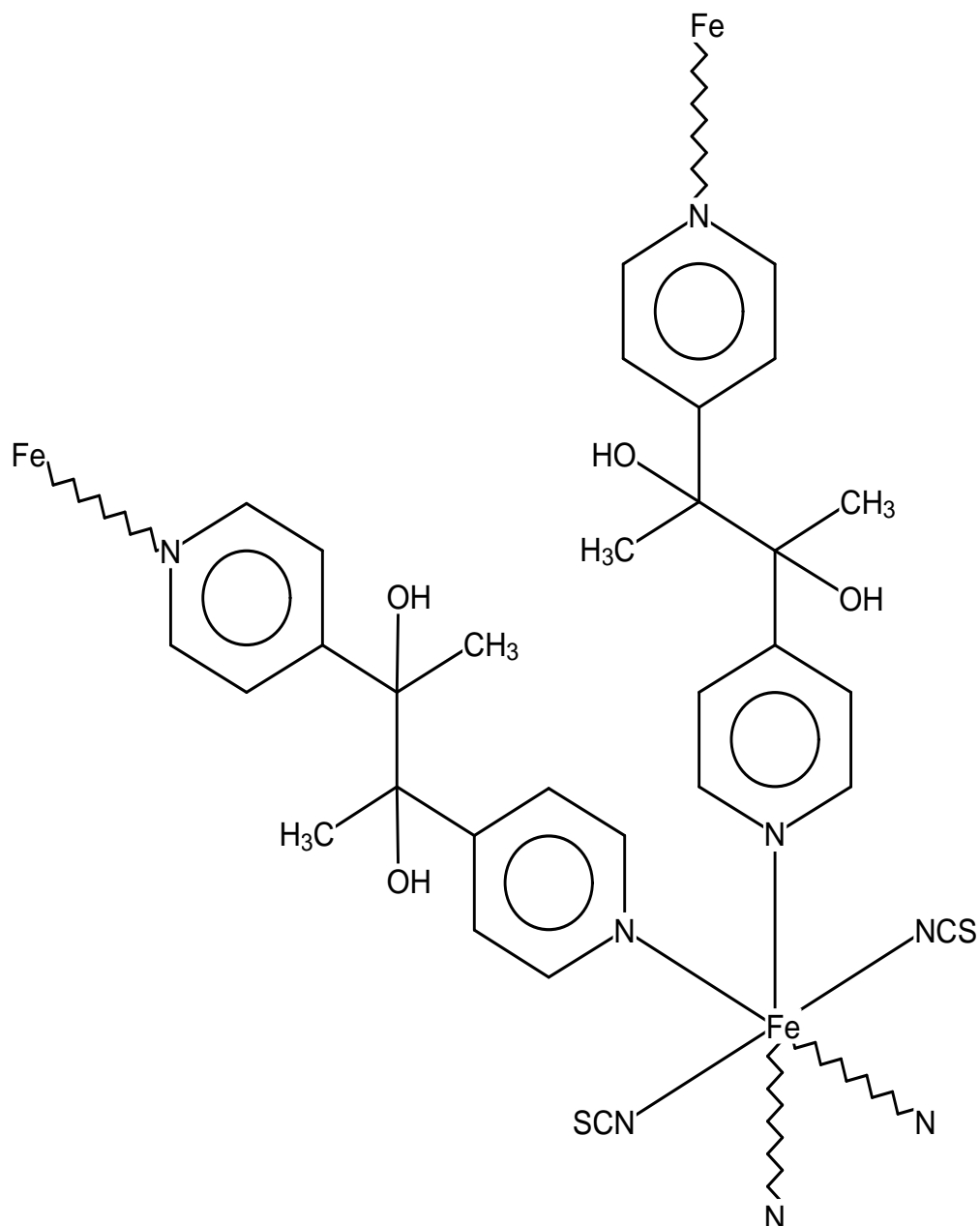
Reference: S.M.Neville, B.Moubaraki, K.S.Murray, C.J.Kepert (2007)
Angew.Chem.,Int.Ed. ,**46**,2059

Formula: (C₃₀ H₃₂ Fe₁ N₆ O₄ S₂)_n

Compound Name: catena-(bis(μ₂-meso-2,3-bis(4-Pyridyl)butane-2,3-diol)-dithiocyanato-iron(ii))

Space Group: P4/ncc **Cell:** **a** 14.726(1) **b** 14.726(1) **c** 17.899(3)
Space Group No.: 130 **(Å, °)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 7.00 **Temperature(K):** 375 **Density(g/cm³):** 1.130



Search: search5 (Wed Aug 10 21:31:08 2011): Hit 4

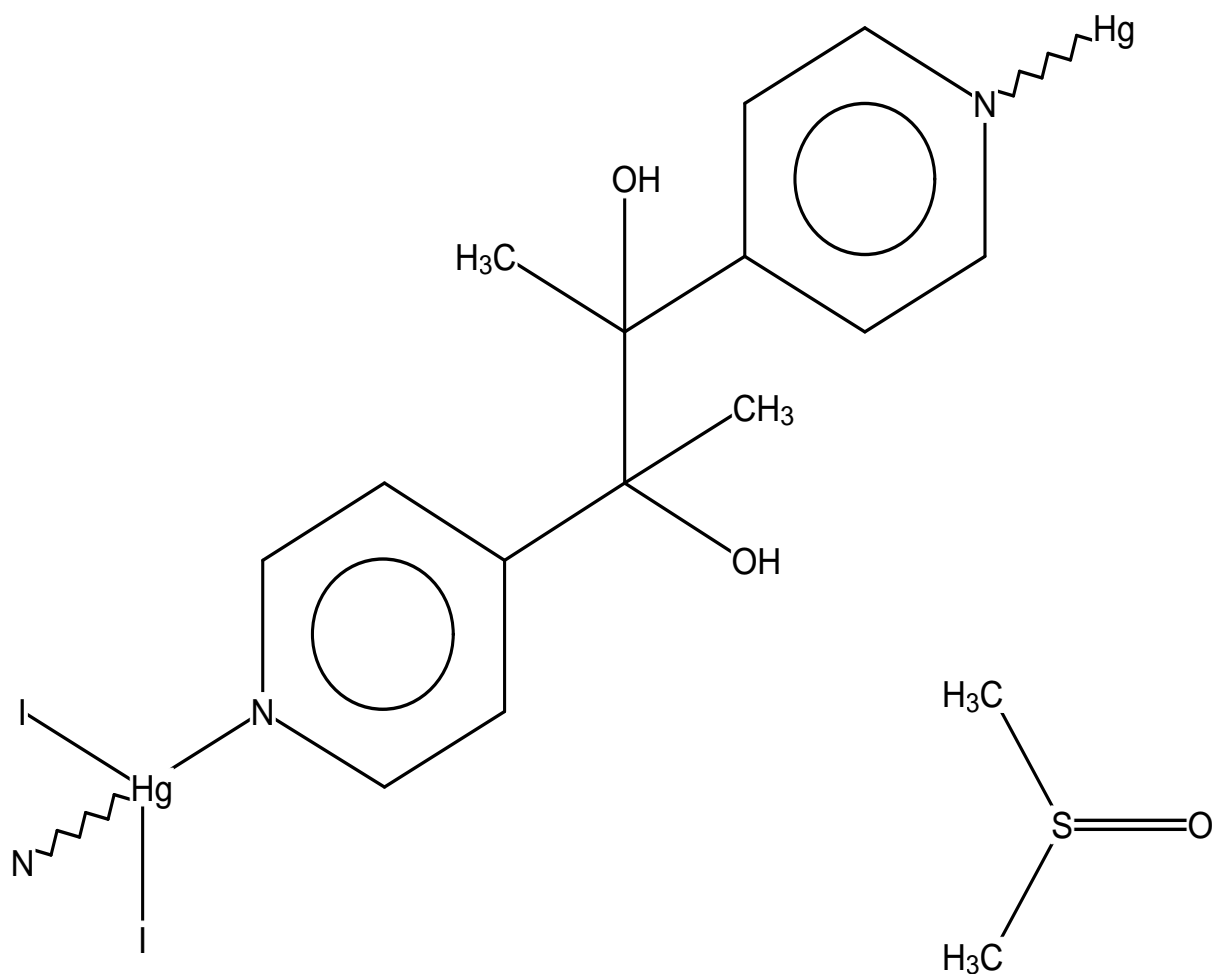
GEQCOV

Reference: Yunyin Niu, Xiaoling Guo, Xiucun Liu, Qingli Wang, Ning Zhang, Yu Zhu, Hongwei Hou, Yaoting Fan (2006) *J.Chem.Cryst.* ,**36**,643

Formula: (C₁₄ H₁₆ Hg₁ I₂ N₂ O₂)_n,2n(C₂ H₆ O₁ S₁)

Compound Name: catena-((μ₂-meso-2,3-bis(4-Pyridyl)-2,3-butanediol)-di-iodo-mercury dimethylsulfoxide solvate)

Space Group:	Pnma	Cell:	a 10.821(2)	b 25.196(5)	c 10.039(2)
Space Group No.:	62	(Å, °)	α 90.00	β 90.00	γ 90.00
R-Factor (%):	6.11	Temperature(K):	291	Density(g/cm³):	2.075



Search: search5 (Wed Aug 10 21:31:08 2011): Hit 5

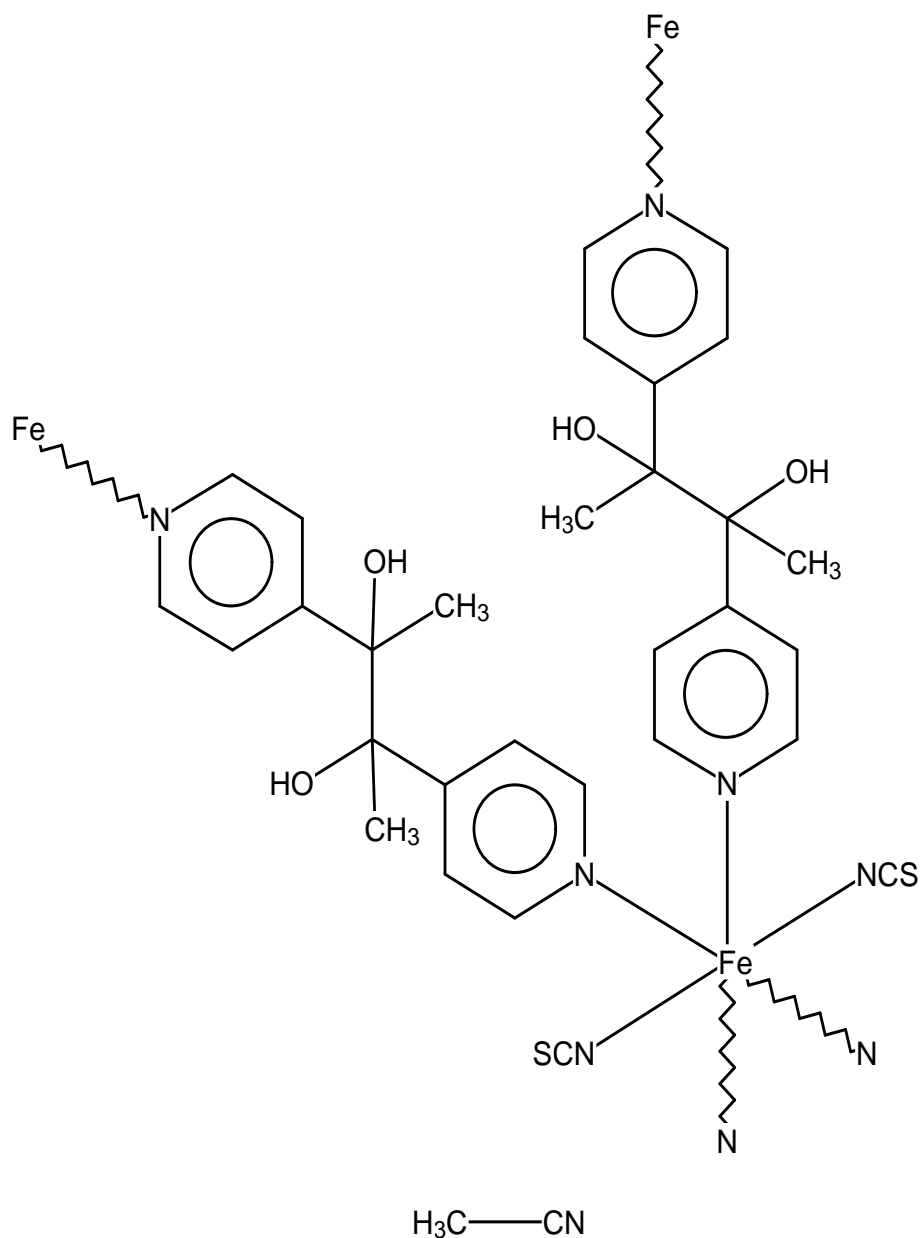
OHOSEK

Reference: S.M.Neville, G.J.Halder, K.W.Chapman, M.B.Duriska, B.Moubaraki, K.S.Murray, C.J.Kepert (2009) *J.Am.Chem.Soc.* ,**131**, 12106

Formula: $(C_{30} H_{32} Fe_1 N_6 O_4 S_2)_n, 2n(C_2 H_3 N_1)$

Compound Name: catena-(bis(μ_2 -2,3-bis(4-pyridyl)butane-2,3-diol)-bis(isothiocyanato)-iron acetonitrile solvate)

Space Group:	P4/ncc	Cell:	a 14.683(1)	b 14.683(1)	c 17.920(3)
Space Group No.:	130	(Å, °)	α 90.00	β 90.00	γ 90.00
R-Factor (%):	7.79	Temperature(K):	200	Density(g/cm³):	1.277



Search: search5 (Wed Aug 10 21:31:08 2011): Hit 6

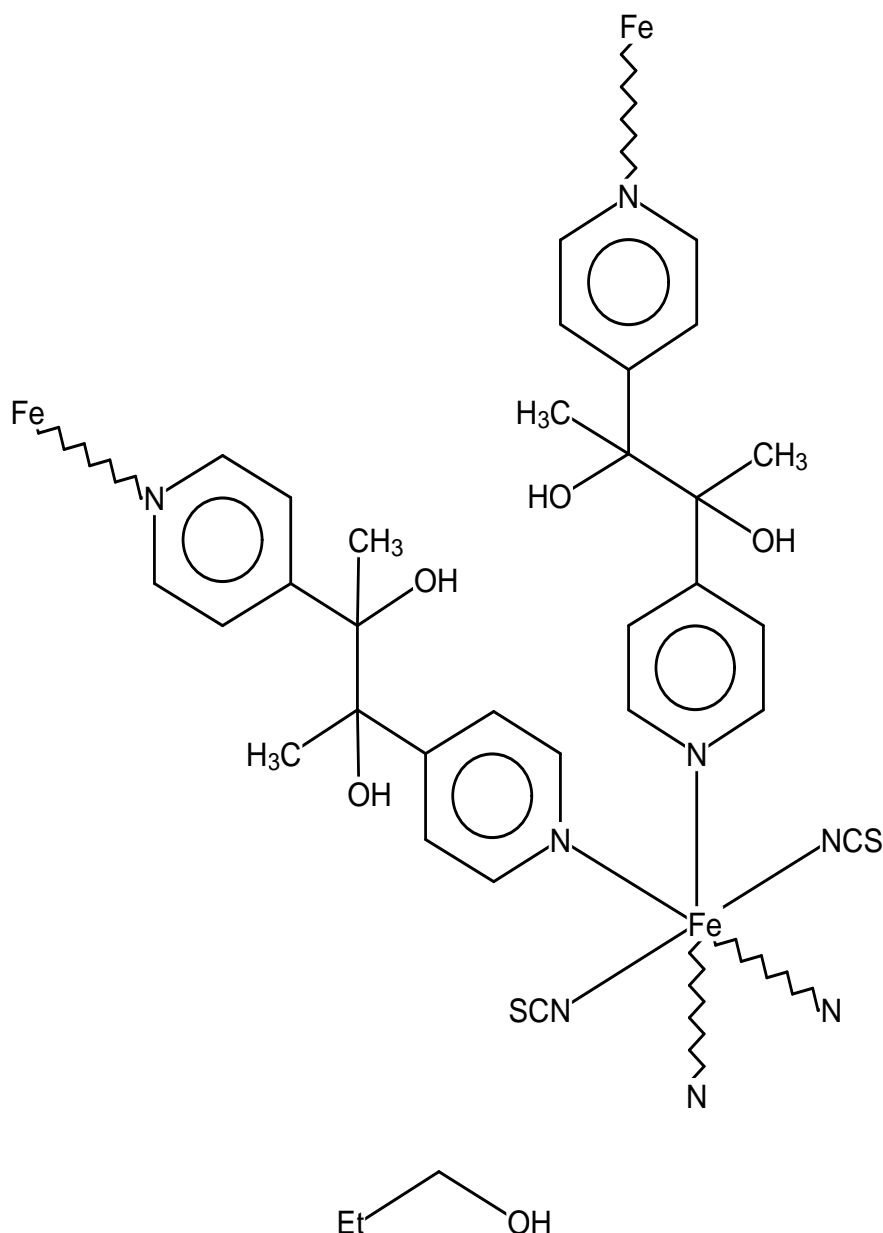
OHOSIO

Reference: S.M.Neville, G.J.Halder, K.W.Chapman, M.B.Duriska, B.Moubaraki, K.S.Murray, C.J.Kepert (2009) *J.Am.Chem.Soc.* ,**131**, 12106

Formula: (C₃₀ H₃₂ Fe₁ N₆ O₄ S₂)_n,n(C₃ H₈ O₁)

Compound Name: catena-(bis(μ₂-2,3-bis(4-pyridyl)butane-2,3-diol)-bis(isothiocyanato)-iron n-propanol solvate)

Space Group: P4/ncc **Cell:** **a** 14.726(1) **b** 14.726(1) **c** 17.899(3)
Space Group No.: 130 **(Å, °)** α 90.00 β 90.00 γ 90.00
R-Factor (%): 8.06 **Temperature(K):** 220 **Density(g/cm³):** 1.233



Search: search5 (Wed Aug 10 21:31:08 2011): Hit 7

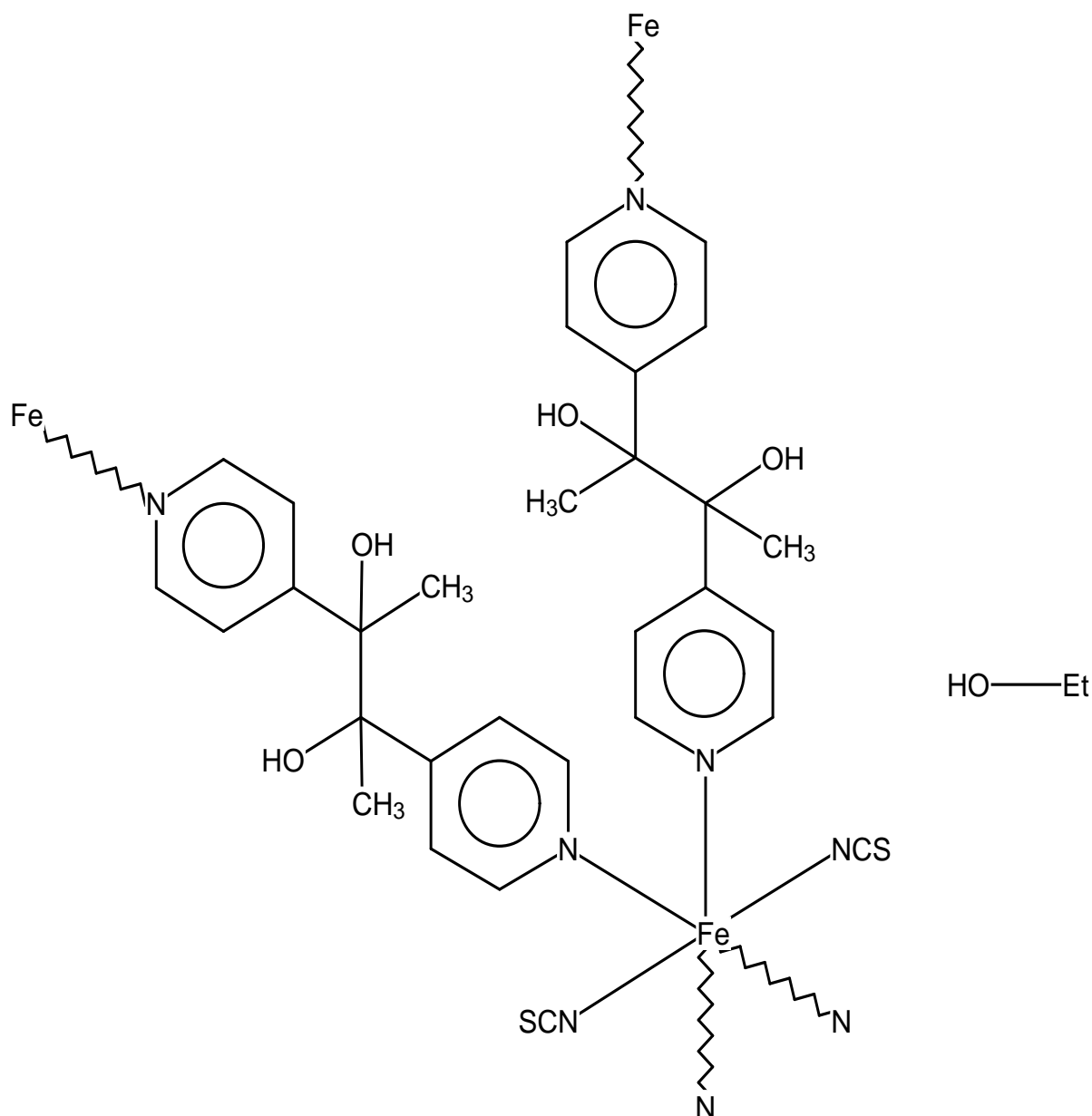
OHOSOU

Reference: S.M.Neville, G.J.Halder, K.W.Chapman, M.B.Duriska, B.Moubaraki, K.S.Murray, C.J.Kepert (2009) *J.Am.Chem.Soc.*, **131**, 12106

Formula: $(C_{30}H_{32}Fe_1N_6O_4S_2)_n \cdot 3n(C_2H_6O_1)$

Compound Name: catena-(bis(μ_2 -2,3-bis(4-pyridyl)butane-2,3-diol)-bis(isothiocyanato)-iron ethanol solvate)

Space Group:	P4/ncc	Cell:	a 14.639(5)	b 14.639(5)	c 17.851(12)
Space Group No.:	130	(Å, °)	α 90.00	β 90.00	γ 90.00
R-Factor (%):	8.80	Temperature(K):	200	Density(g/cm³):	1.387



Search: search5 (Wed Aug 10 21:31:08 2011): Hit 8

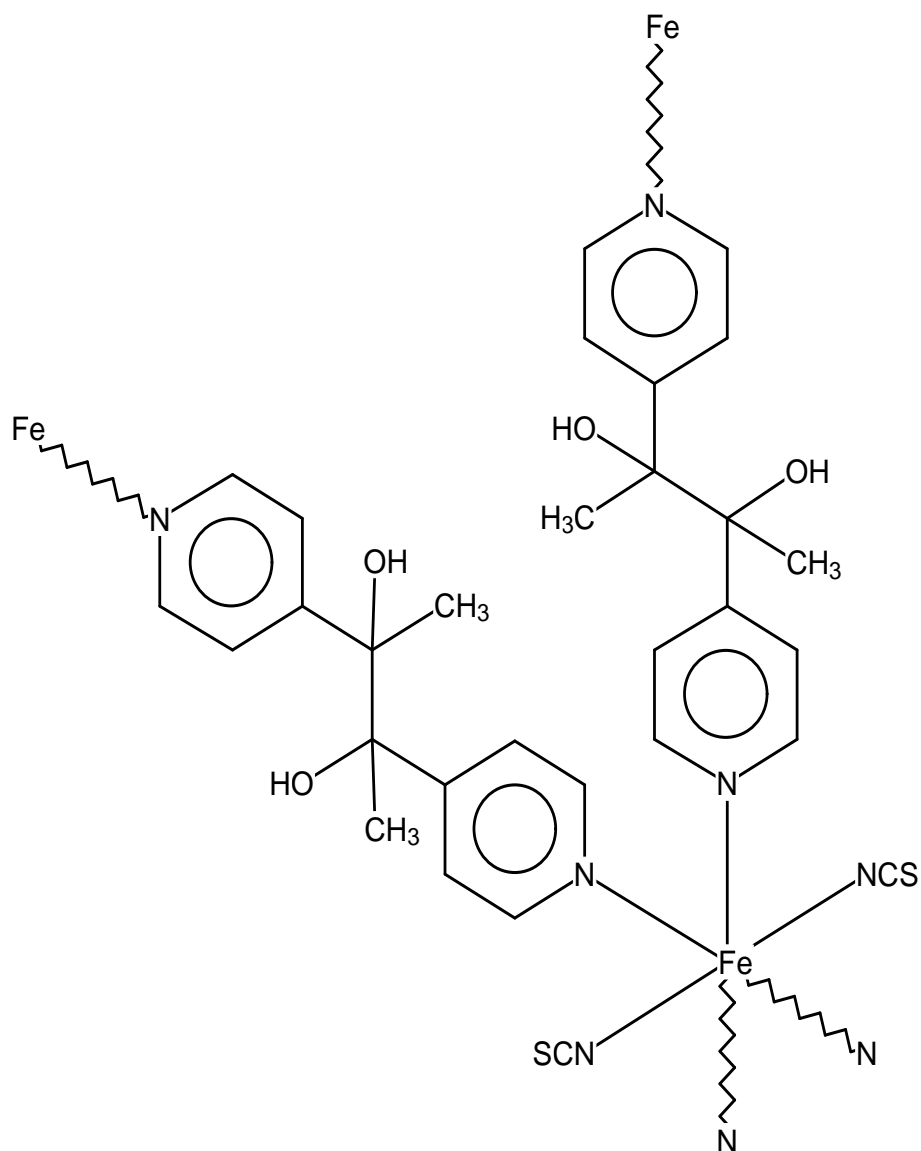
OHOSOU01

Reference: S.M.Neville, G.J.Halder, K.W.Chapman, M.B.Duriska, B.Moubaraki, K.S.Murray, C.J.Kepert (2009) *J.Am.Chem.Soc.* ,**131**, 12106

Formula: $(C_{30} H_{32} Fe_1 N_6 O_4 S_2)_n, 3n(C_2 H_6 O_1)$

Compound Name: catena-(bis(μ_2 -2,3-bis(4-pyridyl)butane-2,3-diol)-bis(isothiocyanato)-iron ethanol solvate)

Space Group:	Pccn	Cell:	a 14.493(0)	b 14.512(0)	c 17.887(0)
Space Group No.:	56	(Å, °)	α 90.00	β 90.00	γ 90.00
R-Factor (%):	10.88	Temperature(K):	100	Density(g/cm³):	1.410



HO—Et

Search: search5 (Wed Aug 10 21:31:08 2011): Hit 9

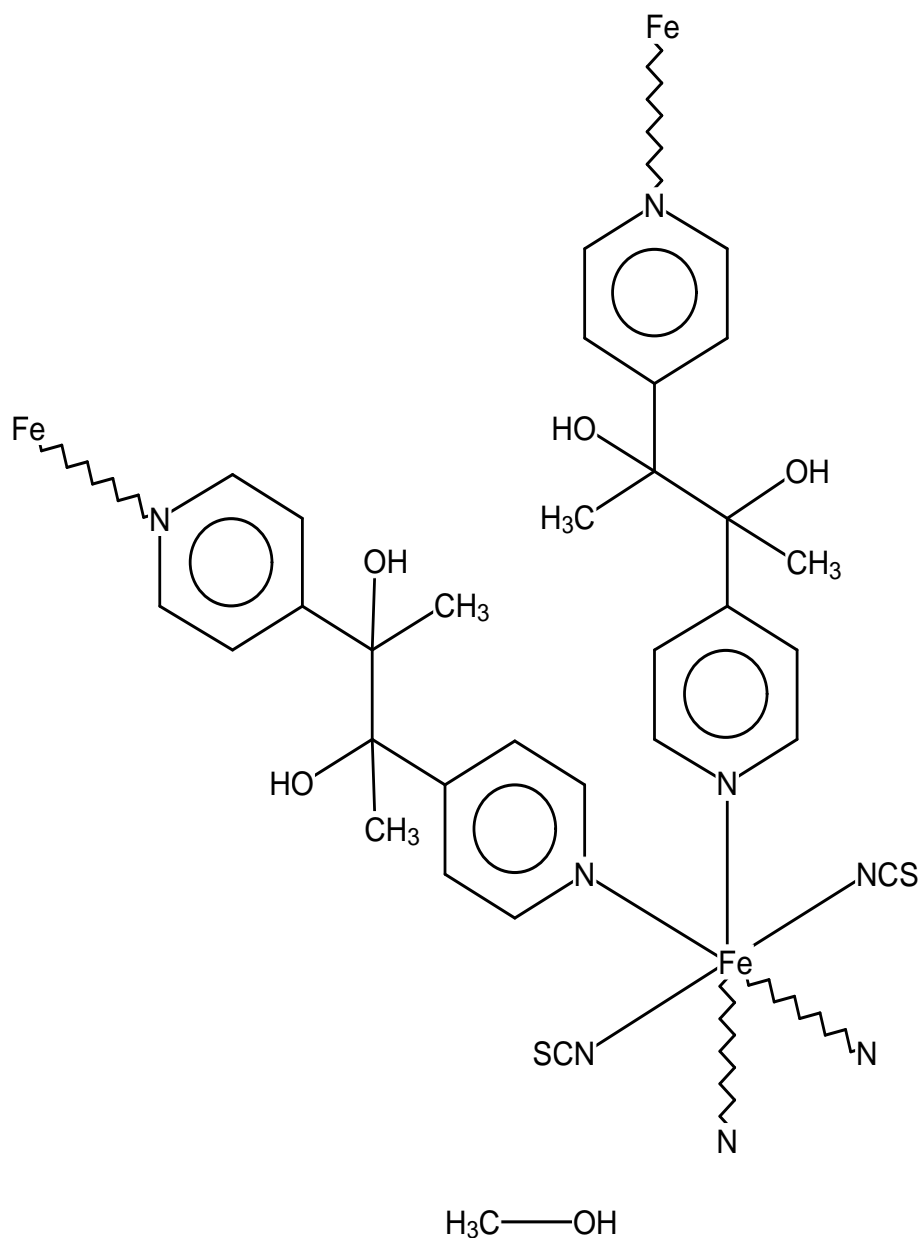
OHOSUA

Reference: S.M.Neville, G.J.Halder, K.W.Chapman, M.B.Duriska, B.Moubaraki, K.S.Murray, C.J.Kepert (2009) *J.Am.Chem.Soc.* ,**131**, 12106

Formula: $(C_{30}H_{32}Fe_1N_6O_4S_2)_n, 3n(C_1H_4O_1)$

Compound Name: catena-(bis(μ_2 -2,3-bis(4-pyridyl)butane-2,3-diol)-bis(isothiocyanato)-iron methanol solvate)

Space Group: P4/ncc **Cell:** **a** 14.675(3) **b** 14.675(3) **c** 17.984(7)
Space Group No.: 130 **(Å, °)** α 90.00 β 90.00 γ 90.00
R-Factor (%): 7.90 **Temperature(K):** 200 **Density(g/cm³):** 1.298



Search: search5 (Wed Aug 10 21:31:08 2011): Hit 10

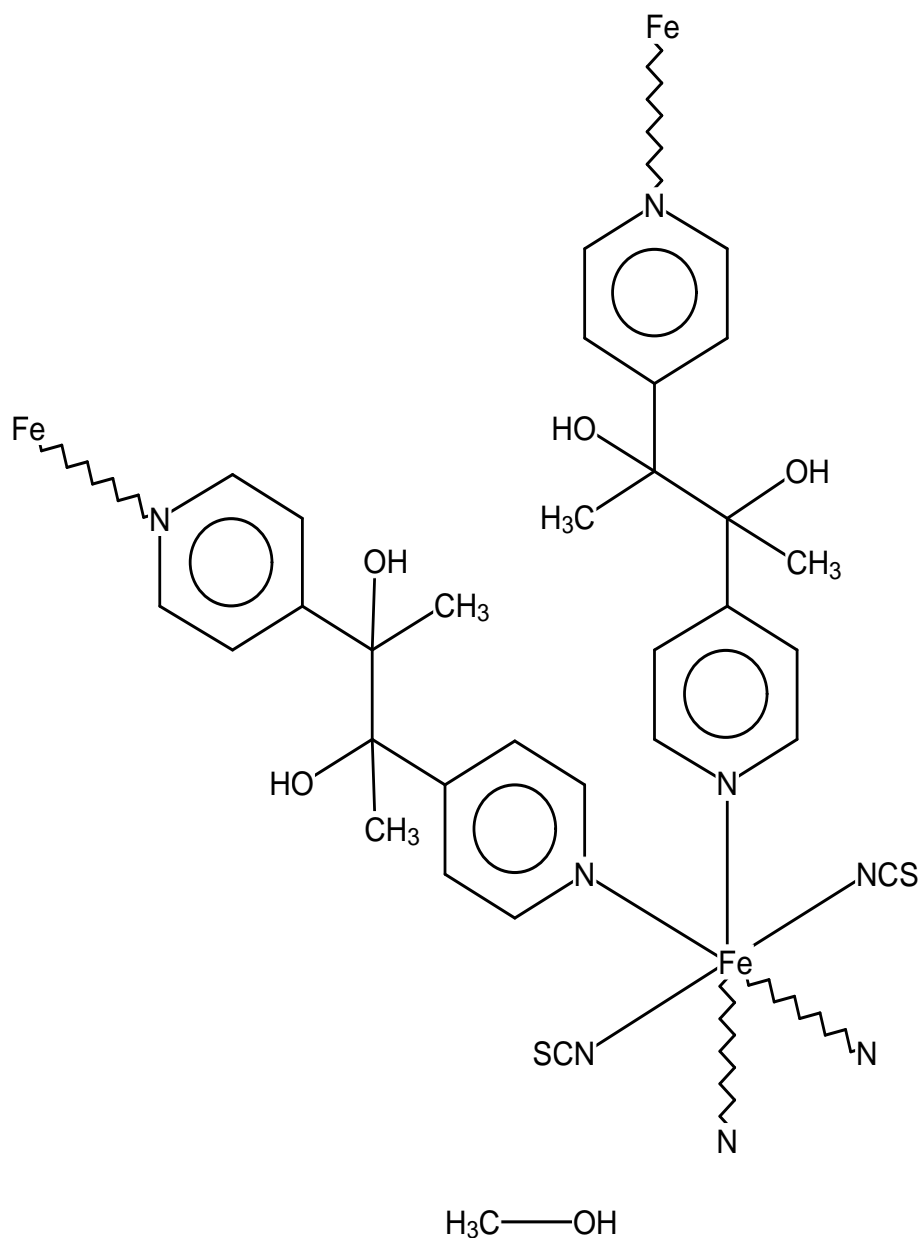
OHOSUA01

Reference: S.M.Neville, G.J.Halder, K.W.Chapman, M.B.Duriska, B.Moubaraki, K.S.Murray, C.J.Kepert (2009) *J.Am.Chem.Soc.* ,**131**, 12106

Formula: $(C_{30}H_{32}Fe_1N_6O_4S_2)_n, 3n(C_1H_4O_1)$

Compound Name: catena-(bis(μ_2 -2,3-bis(4-pyridyl)butane-2,3-diol)-bis(isothiocyanato)-iron methanol solvate)

Space Group:	Pccn	Cell:	a 14.358(0)	b 14.390(0)	c 17.881(0)
Space Group No.:	56	(Å, °)	α 90.00	β 90.00	γ 90.00
R-Factor (%):	6.31	Temperature(K):	100	Density(g/cm³):	1.360



Search: search5 (Wed Aug 10 21:31:08 2011): Hit 11

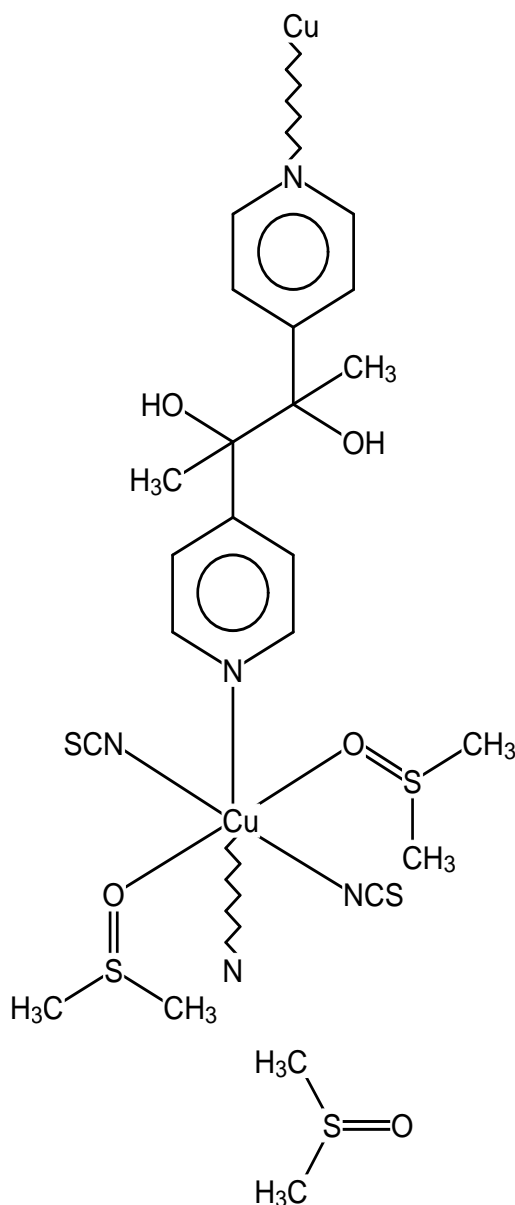
SOTRID

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: (C₂₀ H₂₈ Cu₁ N₄ O₄ S₄)_n,2n(C₂ H₆ O₁ S₁)

Compound Name: catena-((μ₂-meso-2,3-bis(4-Pyridyl)-2,3-butanediol-N,N')-bis(dimethylsulfoxide-O)-bis(isothiocyanato)-copper(ii) dimethylsulfoxide solvate)

Space Group:	P-1	Cell:	a 7.548(1)	b 10.822(3)	c 10.930(3)
Space Group No.:	2	(Å, °)	α 96.75(0)	β 91.45(0)	γ 105.34(0)
R-Factor (%):	4.13	Temperature(K):	291	Density(g/cm³):	1.433



Search: search5 (Wed Aug 10 21:31:08 2011): Hit 12

WIHYAO

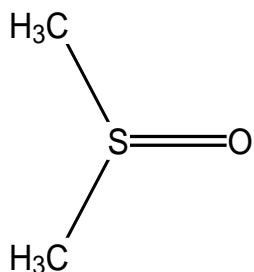
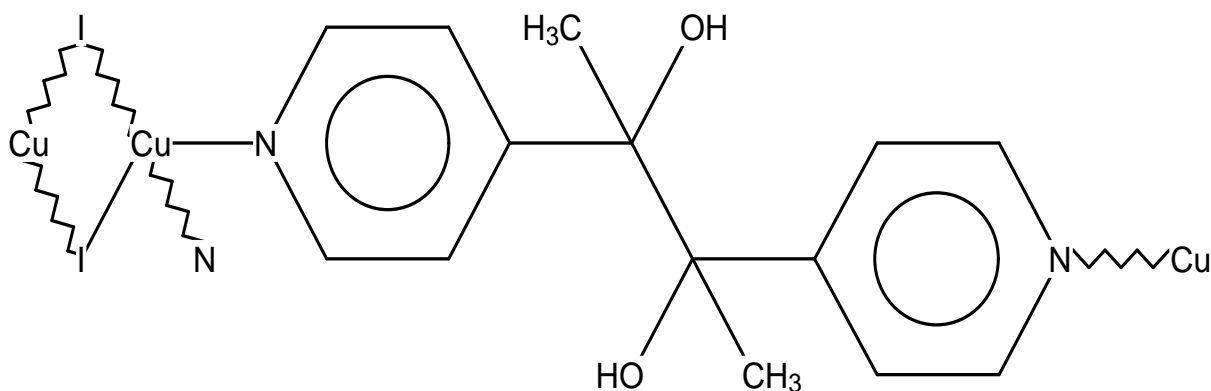
Reference: S.W.Ng (2007) *Acta Crystallogr., Sect. E: Struct. Rep. Online*, **63**,m2003

Formula: (C₁₄ H₁₆ Cu₁ I₁ N₂ O₂)_n,n(C₂ H₆ O₁ S₁)

Compound Name: catena-((μ₂-2,3-bis(4-Pyridyl)-2,3-butanediol-N,N')-(μ₂-iodo)-copper(i) dimethylsulfoxide solvate)

Space Group: C2/m **Cell:** **a** 19.122(1) **b** 18.499(1) **c** 7.254(0)
Space Group No.: 12 (**Å, °**) **α** 90.00 **β** 91.42(0) **γ** 90.00

R-Factor (%): 4.60 **Temperature(K):** 291 **Density(g/cm³):** 1.328



Search: search5 (Wed Aug 10 21:31:08 2011): Hit 13

YEJPUZ

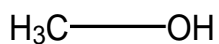
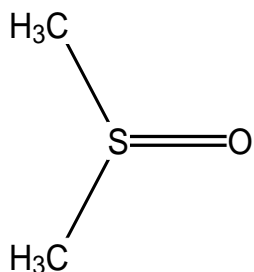
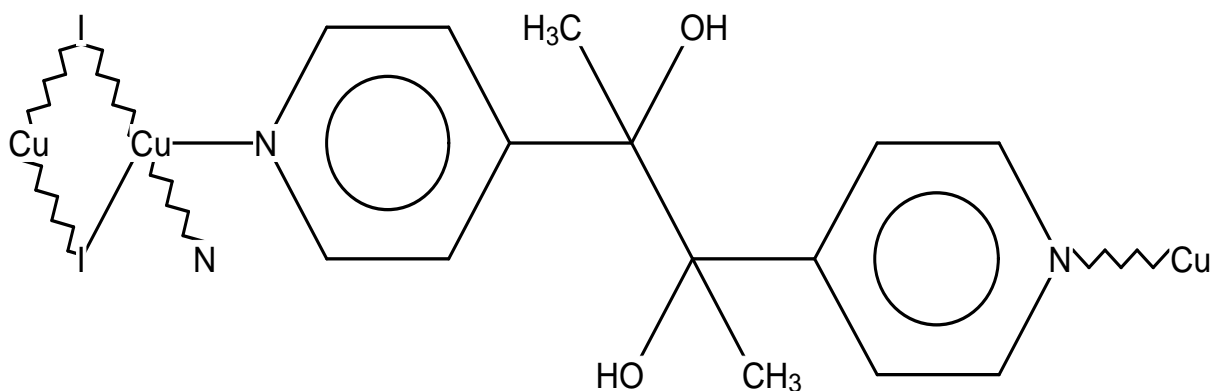
Reference: Yunyin Niu, Yinglin Song, Qingli Wang, Xiaoling Guo, Yu Zhu, Hongwei Hou (2006) *Chem.Lett.* ,**35**,650

Formula: (C₁₄ H₁₆ Cu₁ I₁ N₂ O₂)_n,n(C₂ H₆ O₁ S₁),n(C₁ H₄ O₁),0.25n(H₂ O₁)

Compound Name: catena-((μ₂-2,3-bis(4-Pyridyl)-2,3-butanediol-N,N')-(μ₂-iodo)-copper(i) dimethylsulfoxide methanol solvate hydrate)

Space Group: C2/m **Cell:** **a** 19.122(2) **b** 18.499(2) **c** 7.254(0)
Space Group No.: 12 **(Å, °)** **α** 90.00 **β** 91.42(0) **γ** 90.00

R-Factor (%): 4.01 **Temperature(K):** 291 **Density(g/cm³):** 1.423



Search Overview

Search: search9
Date/Time done: Wed Aug 10 21:52:59 2011
Database(s): CSD version 5.32 (November 2010)
CSD version 5.32 updates (Nov 2010)
Restriction Info: No refcode restrictions applied
Filters: None
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Number of Hits: 4

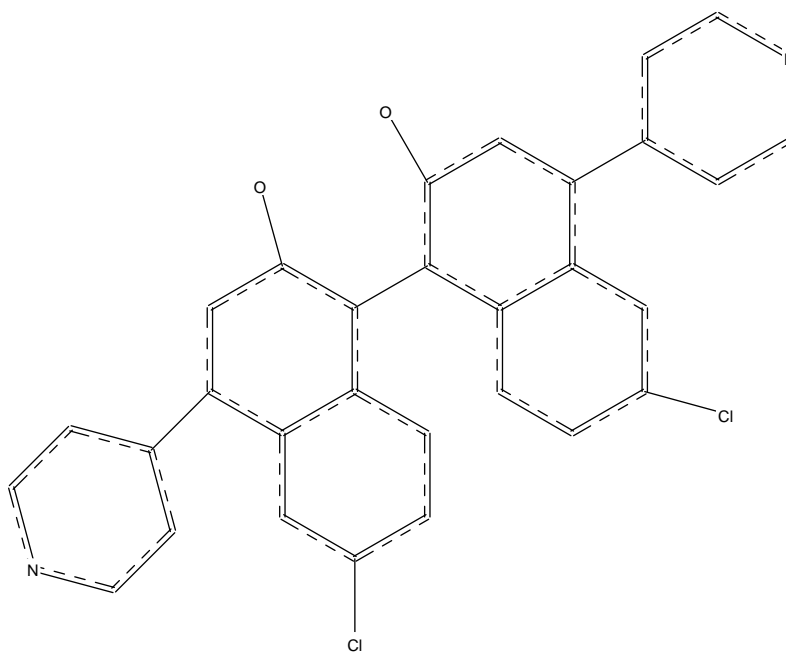
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

4M

Search: search9 (Wed Aug 10 21:52:59 2011): Hit 1

DARSEV

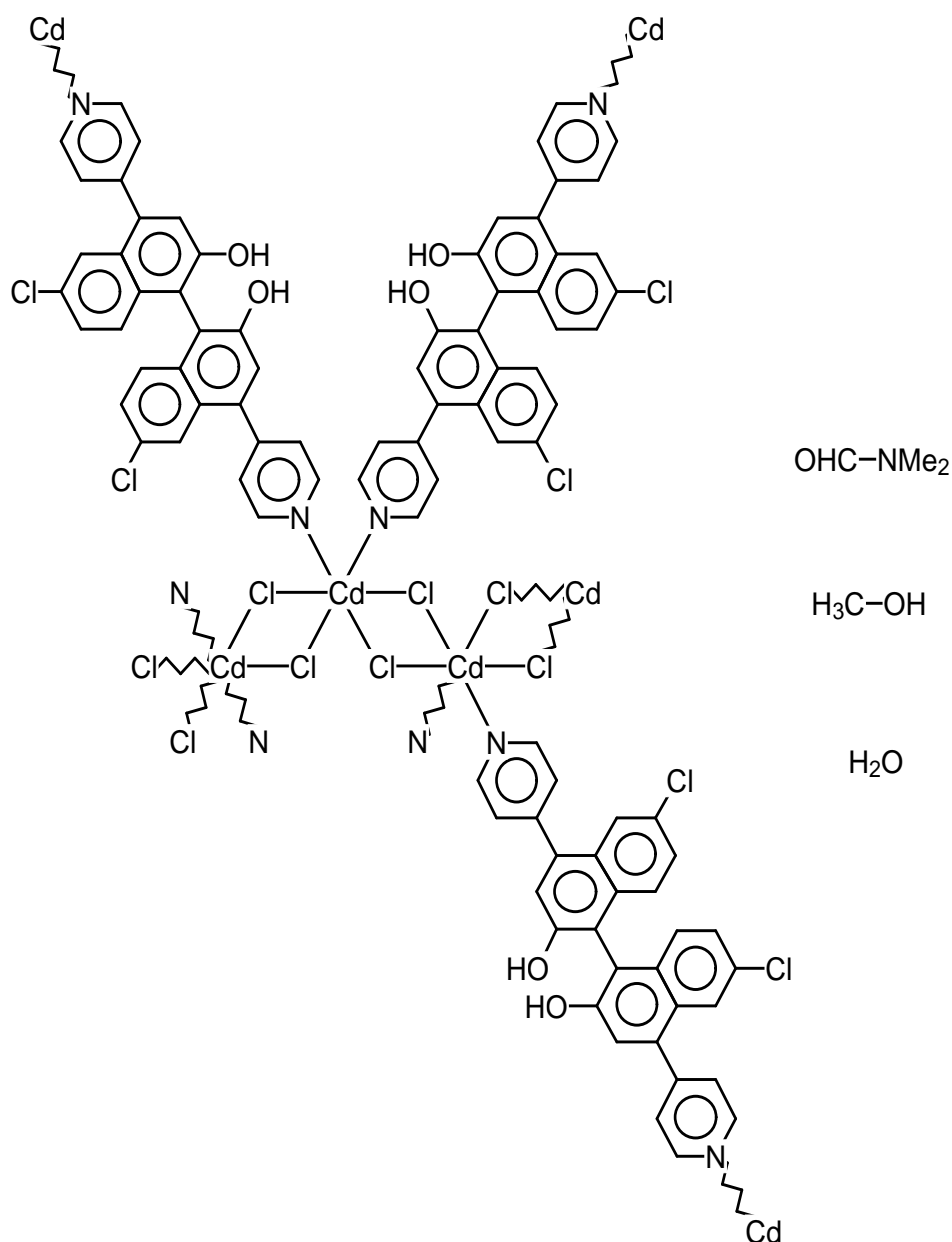
Reference: Chuan-De Wu, Aiguo Hu, Lin Zhang, Wenbin Lin (2005)
J.Am.Chem.Soc. ,**127**,8940

Formula: $(C_{90} H_{54} Cd_3 Cl_{12} N_6 O_6)_n, 4n(C_3 H_7 N_1 O_1), 6n(C_1 H_4 O_1), 3n(H_2 O_1)$

Compound Name: catena-(hexakis(μ_2 -Chloro)-tris(μ_2 -(R)-6,6'-dichloro-2,2'-dihydroxy-4,4'-bis(4-pyridyl)-1,1'-binaphthyl-N,N')-tri-cadmium(ii) N,N-dimethylformamide methanol solvate trihydrate)

Space Group: P1 **Cell:** **a** 10.234(0) **b** 19.118(1) **c** 20.929(1)
Space Group No.: 1 **(Å, °)** α 67.55(0) β 86.75(0) γ 83.63(0)

R-Factor (%): 8.27 **Temperature(K):** 173 **Density(g/cm³):** 1.155



Search: search9 (Wed Aug 10 21:52:59 2011): Hit 2

DARSIZ

Reference: Chuan-De Wu, Aiguo Hu, Lin Zhang, Wenbin Lin (2005)
J.Am.Chem.Soc. ,**127**,8940

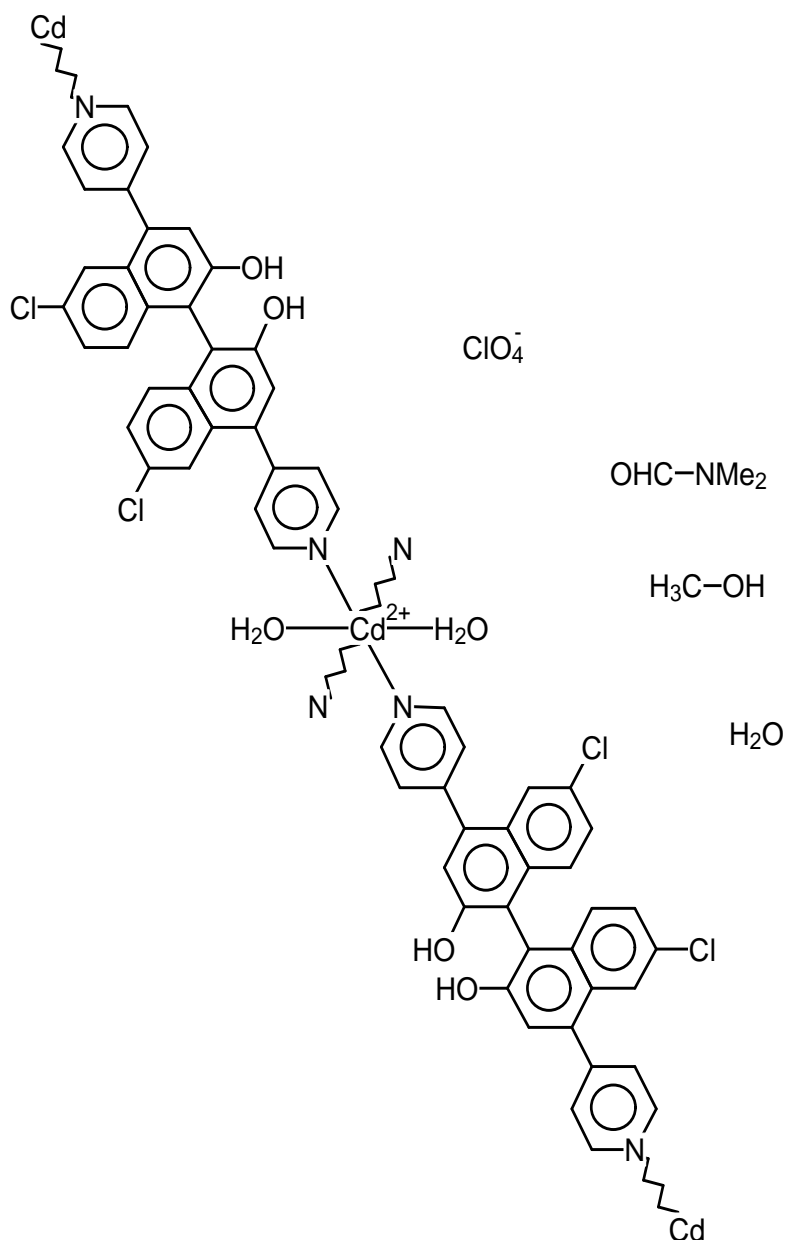
Formula: $(C_{60}H_{40}Cd_1Cl_4N_4O_6^{2+})_n, 2n(Cl_1O_4^{1-}), n(C_3H_7N_1O_1), 4n(C_1H_4O_1), n(H_2O_1)$

Compound Name: catena-(bis(μ_2 -6,6'-Dichloro-2,2'-dihydroxy-4,4'-bis(4-pyridyl)-1,1'-binaphthyl-N,N')-diaqua-cadmium diperchlorate N,N-dimethylformamide methanol solvate monohydrate)

Space Group: P43212 **Cell:** **a** 17.962(0) **b** 17.962(0) **c** 31.649(1)

Space Group No.: 96 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 12.40 **Temperature(K):** 173 **Density(g/cm³):** 1.031



Search: search9 (Wed Aug 10 21:52:59 2011): Hit 3

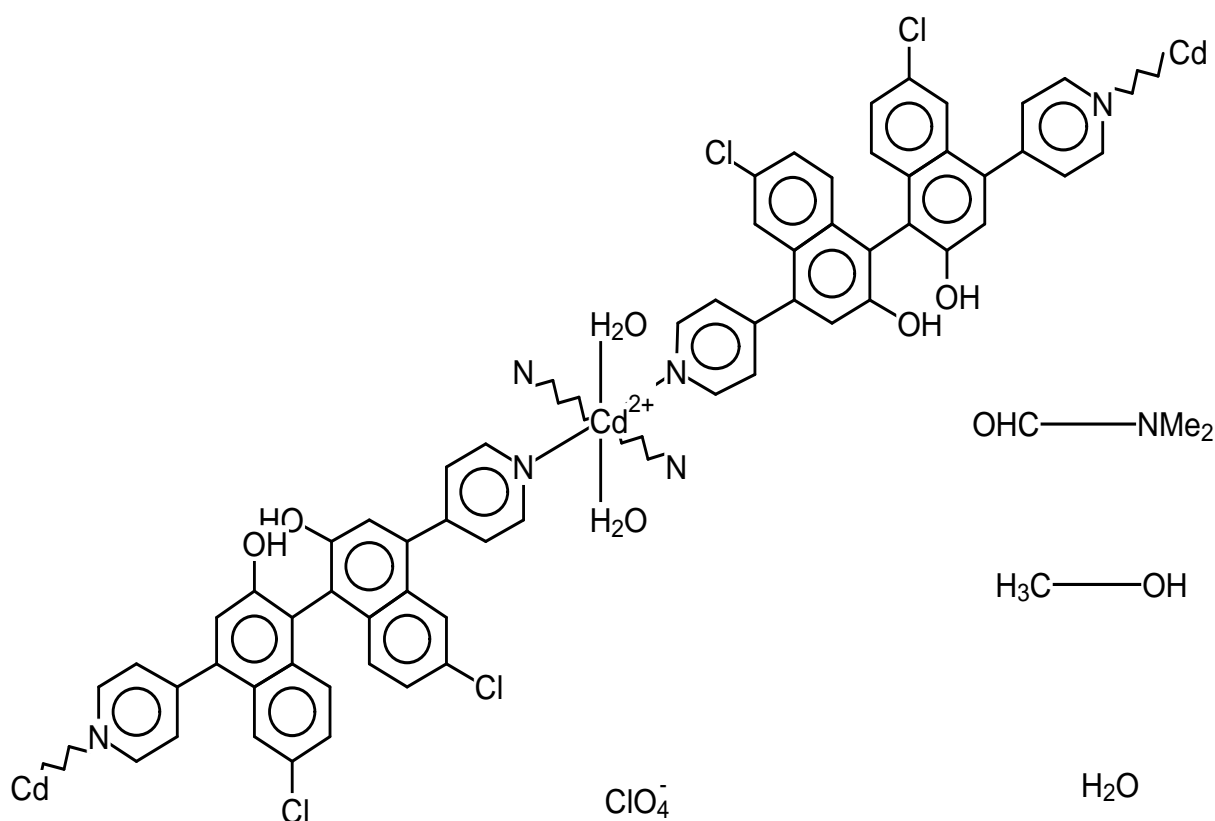
DARSIZ01

Reference: Chuan-De Wu, Wenbin Lin (2007) *Angew.Chem.,Int.Ed.* ,
46,1075

Formula: $(C_{60} H_{40} Cd_1 Cl_4 N_4 O_6^{2+})_n, 2n(Cl_1 O_4^{1-}), n(C_3 H_7 N_1 O_1), 4n(C_1 H_4 O_1), n(H_2 O_1)$

Compound Name: catena-(bis(μ_2 -(R)-6,6'-Dichloro-2,2'-dihydroxy-4,4'-bis(4-pyridyl)-1,1'-binaphthyl-N,N')-diaqua-cadmium(ii) diperchlorate N,N-dimethylformamide methanol solvate monohydrate)

Space Group:	P43212	Cell:	a 17.962(0)	b 17.962(0)	c 31.649(1)
Space Group No.:	96	(Å, °)	α 90.00	β 90.00	γ 90.00
R-Factor (%):	12.40	Temperature(K):	173	Density(g/cm³):	1.031



Search: search9 (Wed Aug 10 21:52:59 2011): Hit 4

SEWCED

Reference: Chuan-De Wu, Wenbin Lin (2007) *Angew.Chem.,Int.Ed.* , 46,1075

Formula: $(C_{120} H_{72} Cd_3 Cl_8 N_{14} O_{26})n, 7n(C_1 H_4 O_1), 5n(H_2 O_1)$

Compound Name: catena-(tetrakis(μ_2 -(R)-6,6'-Dichloro-2,2'-dihydroxy-4,4'-bis(4-pyridyl)-1,1'-binaphthyl-N,N')-bis(μ_2 -nitrate-O,O')-tetrakis(nitrate-O,O')-tri-cadmium(ii) methanol solvate pentahydrate)

Space Group:	P4122	Cell:	a 20.305(1)	b 20.305(1)	c 49.641(4)
Space Group No.:	91	(Å, °)	α 90.00	β 90.00	γ 90.00
R-Factor (%):	6.39	Temperature(K):	173	Density(g/cm³):	0.993

