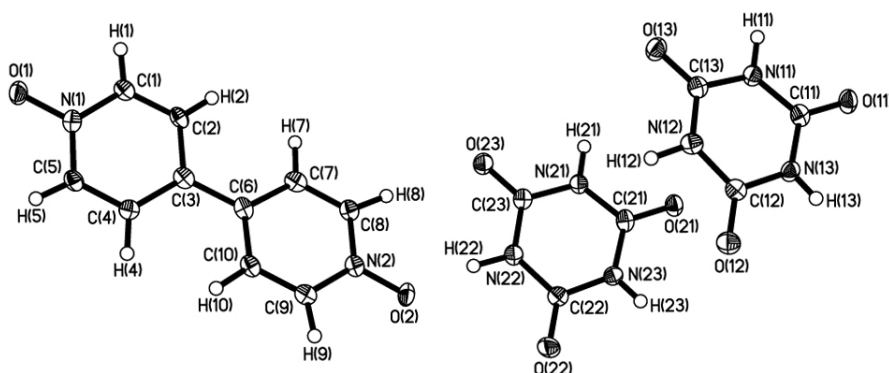


## Supramolecular Synthesis of Some Molecular Adducts of 4,4'-Bipyridine *N,N'*-Dioxide

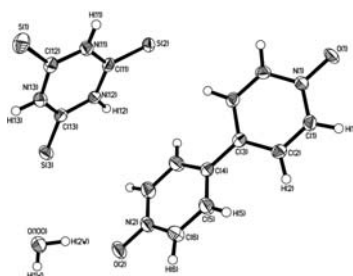
Kapildev K. Arora, Mayura S. Talwelkar and V. R. Pedireddi\*

*Solid State & Supramolecular Structural Chemistry Unit, Division of Organic Chemistry,  
National Chemical Laboratory, Dr. Homi Bhabha Road, Pune 411008, India. Fax: +91  
20 25892629; Tel: +91 20 25902097; Email: vr.pedireddi@ncl.res.in*

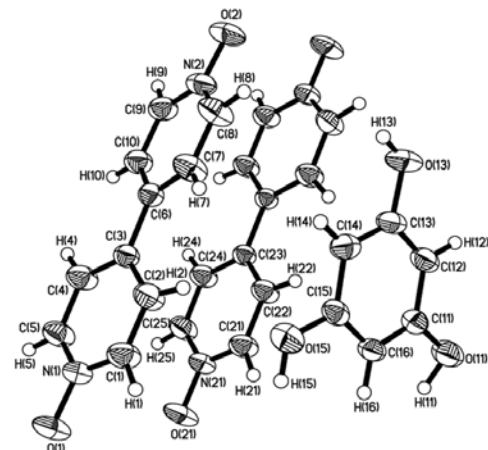
### Supporting Information



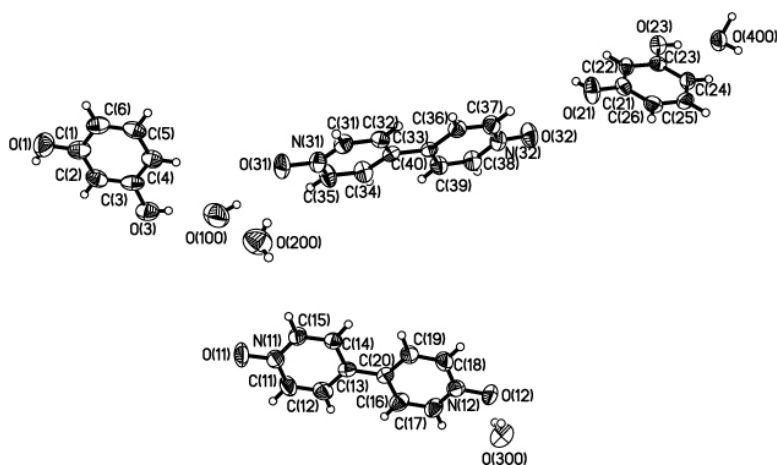
**Figure 1.** ORTEP of molecular complex, **1a**



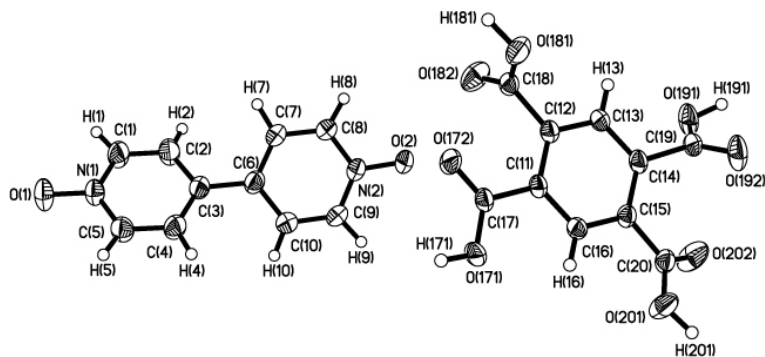
**Figure 2.** ORTEP of asymmetric unit in the crystal structure of **1b**.



**Figure 3.** Contents of asymmetric unit in the crystal structure of **1c**.



**Figure 4:** ORTEP of asymmetric unit in the crystal structure of molecular complex, **1d**.



**Figure 5:** ORTEP of asymmetric unit in the complex, **1e**

# Search Overview

Supplementary Material (ESI) for New Journal of Chemistry  
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**Search:** search3

**Date/Time done:** Wed Aug 20 11:52:28 2008

**Database(s):** CSD version 5.29 (November 2007)  
CSD version 5.29 updates (Jan 2008)

**Restriction Info:** No refcode restrictions applied

**Filters:** Only Organics

**Percentage Completed:** 100%

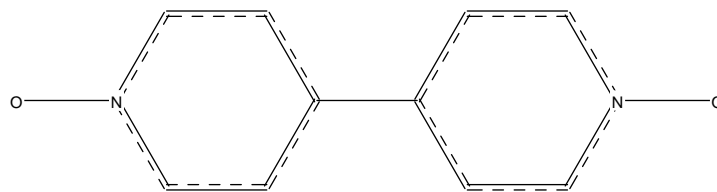
**Number of Hits:** 22

**Single query used. Search found structures that:**

match

**Query 1**

**Query 1**



# Search: search3 (Wed Aug 20 11:52:28 2008): Hits 1-4

Supplementary Material (ESI) for New Journal of Chemistry  
This journal is (c) The Royal Society of Chemistry and  
The Centre National de la Recherche Scientifique, 2008  
BAFTEH

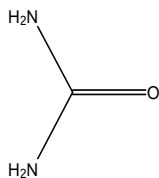
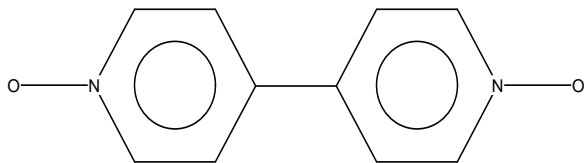
**Reference:** R.Thaimattam, D.S.Reddy, Feng Xue, T.C.W.Mak, A.Nangia, G.R.Desiraju (1998) *J.Chem.Soc.,Perkin Trans.2* ,1783

**Formula:** C<sub>10</sub> H<sub>8</sub> N<sub>2</sub> O<sub>2</sub>·C<sub>1</sub> H<sub>4</sub> N<sub>2</sub> O<sub>1</sub>

**Compound Name:** 4,4'-Bipyridine N,N'-dioxide urea clathrate

**Space Group:** P212121 **Cell:** a 7.162(2) b 10.221(2) c 15.255(3)  
**Space Group No.:** 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

**R-Factor (%):** 4.20 **Temperature(K):** 295 **Density(g/cm<sup>3</sup>):** 1.477



## BAFVEJ

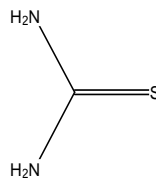
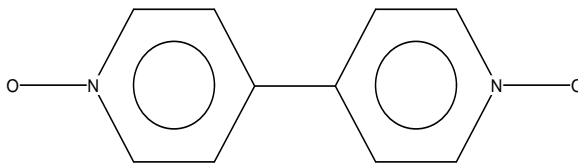
**Reference:** R.Thaimattam, D.S.Reddy, Feng Xue, T.C.W.Mak, A.Nangia, G.R.Desiraju (1998) *J.Chem.Soc.,Perkin Trans.2* ,1783

**Formula:** C<sub>10</sub> H<sub>8</sub> N<sub>2</sub> O<sub>2</sub>·C<sub>1</sub> H<sub>4</sub> N<sub>2</sub> S<sub>1</sub>

**Compound Name:** 4,4'-Bipyridine N,N'-dioxide thiourea clathrate

**Space Group:** C2/c **Cell:** a 18.197(2) b 6.826(2) c 20.100(3)  
**Space Group No.:** 15 **(Å, °)** α 90.00 β 104.21(1) γ 90.00

**R-Factor (%):** 5.49 **Temperature(K):** 295 **Density(g/cm<sup>3</sup>):** 1.451



## BAFVUZ

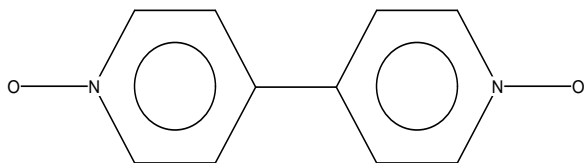
**Reference:** R.Thaimattam, D.S.Reddy, Feng Xue, T.C.W.Mak, A.Nangia, G.R.Desiraju (1998) *J.Chem.Soc.,Perkin Trans.2* ,1783

**Formula:** C<sub>10</sub> H<sub>8</sub> N<sub>2</sub> O<sub>2</sub>·2(H<sub>2</sub> O<sub>1</sub>)

**Compound Name:** 4,4'-Bipyridine-N,N'-dioxide dihydrate clathrate

**Space Group:** C2/m **Cell:** a 14.811(1) b 8.474(1) c 4.264(1)  
**Space Group No.:** 12 **(Å, °)** α 90.00 β 101.86(1) γ 90.00

**R-Factor (%):** 4.82 **Temperature(K):** 295 **Density(g/cm<sup>3</sup>):** 1.422



H<sub>2</sub>O

## BAXKER

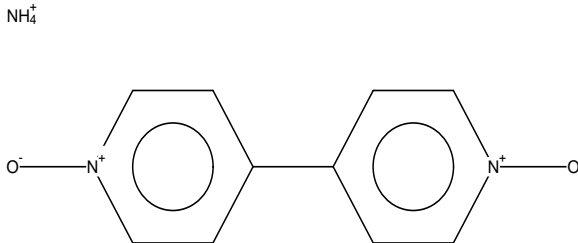
**Reference:** Bao-Qing Ma, Hao-Ling Sun, Song Gao (2003) *Chem.Commun.* ,2164

**Formula:** H<sub>4</sub> N<sub>1</sub><sup>1+</sup>·2(C<sub>10</sub> H<sub>8</sub> N<sub>2</sub> O<sub>2</sub>)·F<sub>6</sub> P<sub>1</sub><sup>1-</sup>·0.5(H<sub>2</sub> O<sub>1</sub>)

**Compound Name:** Ammonium bis(4,4'-bipyridyl 1,1'-dioxide) hexafluorophosphate hemihydrate

**Space Group:** P-4n2 **Cell:** a 17.994(1) b 17.994(1) c 7.255(0)  
**Space Group No.:** 118 **(Å, °)** α 90.00 β 90.00 γ 90.00

**R-Factor (%):** 6.49 **Temperature(K):** 90 **Density(g/cm<sup>3</sup>):** 1.551



NH<sub>4</sub><sup>+</sup>

H<sub>2</sub>O

P<sup>-</sup>—[F]<sub>6</sub>

# Search: search3 (Wed Aug 20 11:52:28 2008): Hits 5-8

Supplementary Material (ESI) for New Journal of Chemistry

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DAQZUR

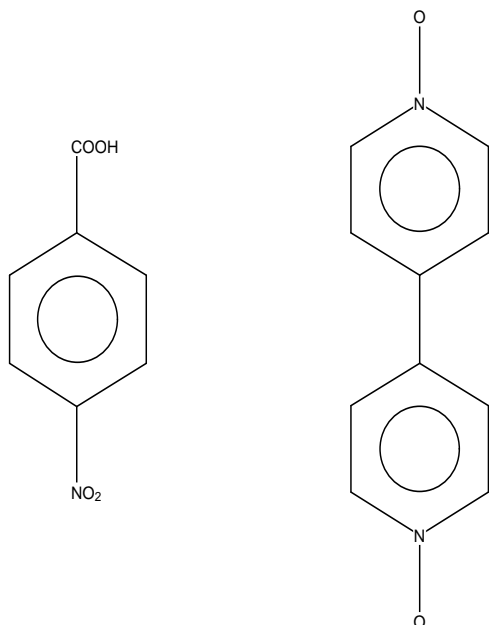
**Reference:** J.R.Bowers, G.W.Hopkins, G.P.A.Yap, K.A.Wheeler  
(2005) *Cryst.Growth Des.*, **5**,727

**Formula:** C<sub>7</sub>H<sub>5</sub>N<sub>1</sub>O<sub>4</sub>.0.5(C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>)

**Compound Name:** 4-Nitrobenzoic acid hemikis(4,4'-bipyridine-N,N'-dioxide)

**Space Group:** P-1 **Cell:** a 9.293(0) b 11.615(0) c 12.204(1)  
**Space Group No.:** 2 **(Å, °)** α 65.31(0) β 74.86(0) γ 75.30(0)

**R-Factor (%)**: 5.27 **Temperature(K)**: 298 **Density(g/cm<sup>3</sup>)**: 1.523



## DATQUL

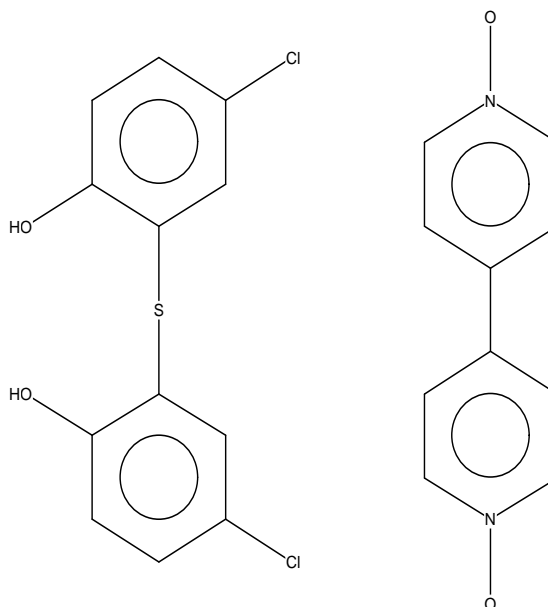
**Reference:** Qingdao Zeng, Dongxia Wu, Chen Wang, Hongwei Ma,  
Jun Lu, Caiming Liu, Shandong Xu, Yan Li, Chunli Bai (2005)  
*Cryst.Growth Des.*, **5**,1889

**Formula:** C<sub>12</sub>H<sub>8</sub>Cl<sub>2</sub>O<sub>2</sub>S<sub>1</sub>C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>

**Compound Name:** bis(2-Hydroxy-5-chlorophenyl)sulfide 4,4'-bipyridine N,N'-dioxide

**Space Group:** P-1 **Cell:** a 7.646(1) b 9.567(1) c 14.891(3)  
**Space Group No.:** 2 **(Å, °)** α 85.90(3) β 89.07(3) γ 70.81(3)

**R-Factor (%)**: 4.02 **Temperature(K)**: 293 **Density(g/cm<sup>3</sup>)**: 1.539



## DATREW

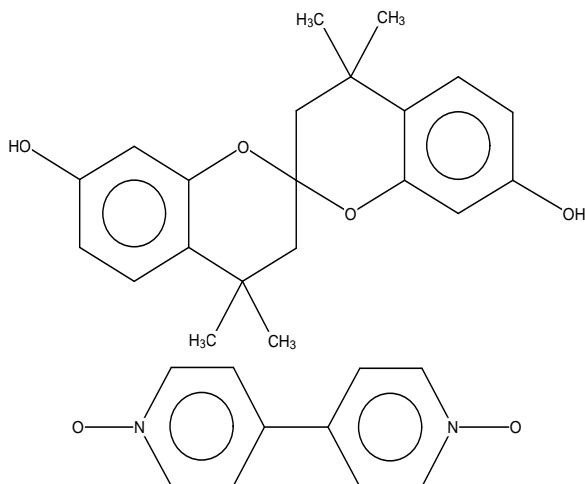
**Reference:** Qingdao Zeng, Dongxia Wu, Chen Wang, Hongwei Ma,  
Jun Lu, Caiming Liu, Shandong Xu, Yan Li, Chunli Bai (2005)  
*Cryst.Growth Des.*, **5**,1889

**Formula:** C<sub>21</sub>H<sub>24</sub>O<sub>4</sub>.C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>.H<sub>2</sub>O

**Compound Name:** Spirobichromane 4,4'-bipyridine N,N'-dioxide monohydrate

**Space Group:** P21/c **Cell:** a 16.274(3) b 10.564(2) c 16.094(3)  
**Space Group No.:** 14 **(Å, °)** α 90.00 β 92.52(3) γ 90.00

**R-Factor (%)**: 4.87 **Temperature(K)**: 296 **Density(g/cm<sup>3</sup>)**: 1.313



H<sub>2</sub>O

## HUZCUA

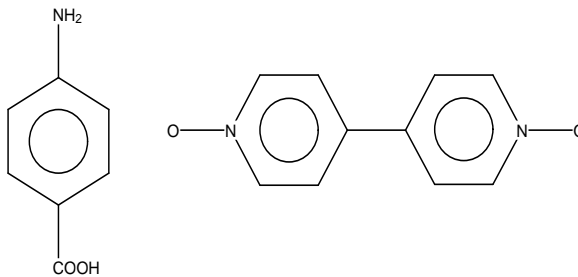
**Reference:** R.Moreno-Fuquen, M.Font i Carot, M.Garriga, F.Cano,  
M.Martinez-Ripoll, J.Valderrama-Naranjo, L.M.Serratto (2003)  
*Acta Crystallogr.,Sect.E:Struct.Rep.Online*, **59**,o495

**Formula:** 2(C<sub>7</sub>H<sub>7</sub>N<sub>1</sub>O<sub>2</sub>).C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>

**Compound Name:** bis(4-Aminobenzoic acid) 4,4'-bipyridyl N,N'-dioxide

**Space Group:** Pbca **Cell:** a 11.188(1) b 12.138(2) c 16.354(2)  
**Space Group No.:** 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

**R-Factor (%)**: 4.40 **Temperature(K)**: 293 **Density(g/cm<sup>3</sup>)**: 1.383



# Search: search3 (Wed Aug 20 11:52:28 2008): Hits 9-12

Supplementary Material (ESI) for the New Journal of Chemistry  
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JAWWUA

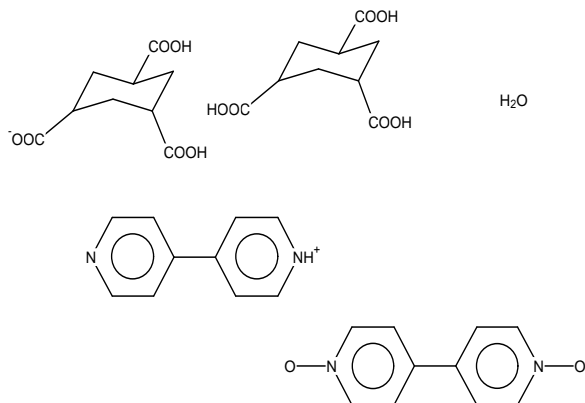
**Reference:** B.R.Bhogala, S.Basavoju, A.Nangia (2005)  
*CrystEngComm*, **7**,551

**Formula:**  $C_{10}H_9N_2^{1+}, C_9H_{11}O_6^{1-}; C_9H_{12}O_6, C_{10}H_8N_2O_2 \cdot 2(H_2O)$

**Compound Name:** 4,4'-Bipyridinium cis,cis-cyclohexane-1,3,5-tricarboxylic acid 4,4'-dipyridine-N,N'-dioxide cyclohexane-1-carboxylate-cis,cis-3,5-dicarboxylic acid dihydrate

**Space Group:** P21/c **Cell:** **a** 8.585(0) **b** 23.908(1) **c** 18.310(1)  
**Space Group No.:** 14 **(Å, °)** **α** 90.00 **β** 101.29(0) **γ** 90.00

**R-Factor (%):** 4.94 **Temperature(K):** 100 **Density(g/cm<sup>3</sup>):** 1.465



## LICJUD

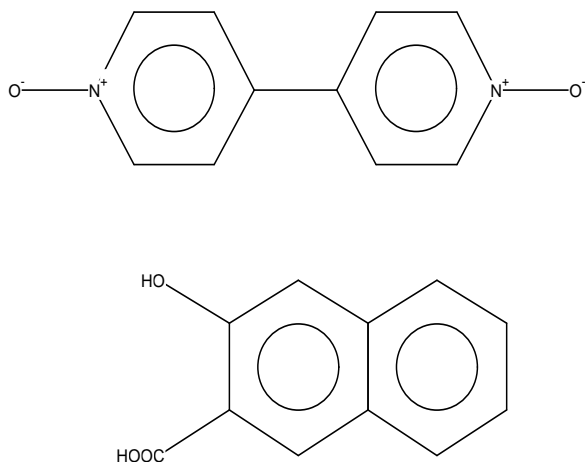
**Reference:** Ben-Yong Lou, Yan-Bin Huang (2007)  
*Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, **63**,o246

**Formula:**  $C_{10}H_8N_2O_2 \cdot 2(C_{11}H_8O_3)$

**Compound Name:** 4,4'-Bipyridyl N,N'-dioxide bis(3-hydroxy-2-naphthoic acid)

**Space Group:** P21/c **Cell:** **a** 10.780(1) **b** 11.880(1) **c** 11.470(1)  
**Space Group No.:** 14 **(Å, °)** **α** 90.00 **β** 114.82(0) **γ** 90.00

**R-Factor (%):** 5.14 **Temperature(K):** 293 **Density(g/cm<sup>3</sup>):** 1.406



## LAPLEU

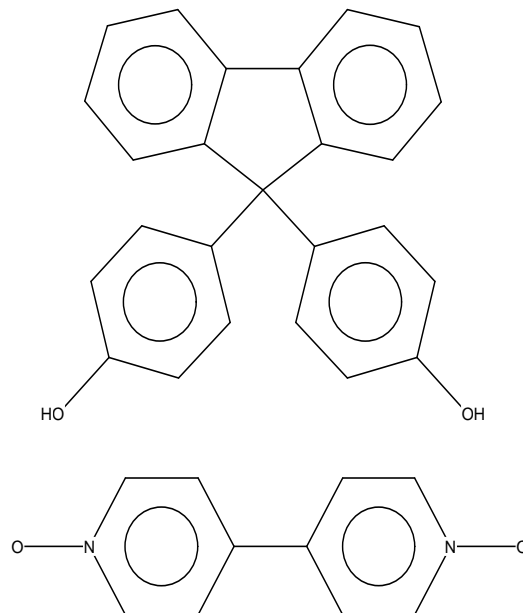
**Reference:** Qingdao Zeng, Dongxia Wu, Caiming Liu, Hongwei Ma, Jun Lu, Shandong Xu, Yan Li, Chen Wang, Chunli Bai (2005)  
*Cryst.Growth Des.*, **5**,1041

**Formula:**  $C_{25}H_{18}O_2 \cdot C_{10}H_8N_2O_2$

**Compound Name:** 4,4'-(9-Fluorenylidene)diphenol 4,4'-bipyridine N,N'-dioxide

**Space Group:** C2/c **Cell:** **a** 18.988(4) **b** 13.295(3) **c** 11.009(2)  
**Space Group No.:** 15 **(Å, °)** **α** 90.00 **β** 105.97(3) **γ** 90.00

**R-Factor (%):** 4.42 **Temperature(K):** 293 **Density(g/cm<sup>3</sup>):** 1.339



## MEGCUX

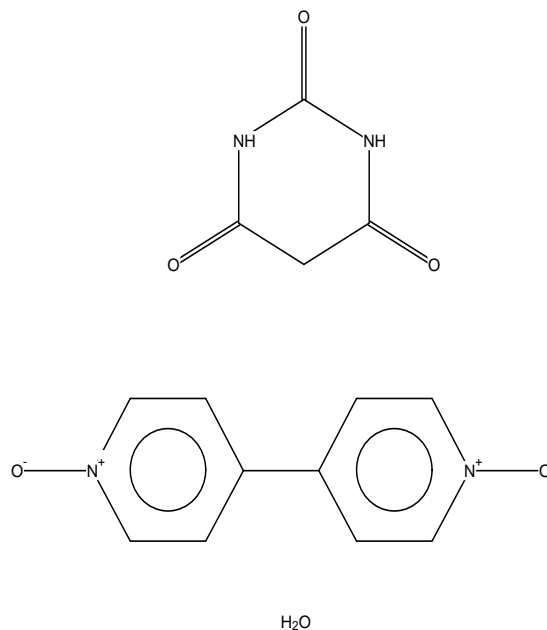
**Reference:** L.S.Reddy, N.J.Babu, A.Nangia (2006) *Chem. Commun.*, 1369

**Formula:**  $C_4H_4N_2O_3 \cdot C_{10}H_8N_2O_2 \cdot H_2O$

**Compound Name:** Barbituric acid 4,4'-bipyridine-N,N'-dioxide monohydrate

**Space Group:** Pbca **Cell:** **a** 16.221(1) **b** 6.597(0) **c** 27.069(1)  
**Space Group No.:** 61 **(Å, °)** **α** 90.00 **β** 90.00 **γ** 90.00

**R-Factor (%):** 5.10 **Temperature(K):** 100 **Density(g/cm<sup>3</sup>):** 1.533

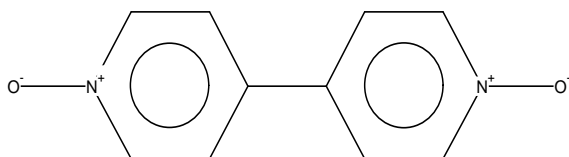
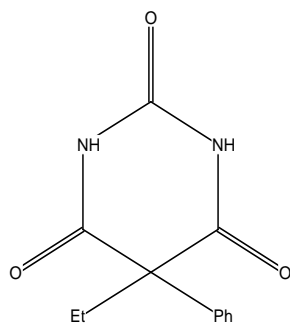


# Search: search3 (Wed Aug 20 11:52:28 2008): Hits 13-16

Supplementary Material (ESI) for New Journal of Chemistry  
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MEGDIM

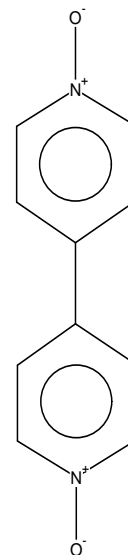
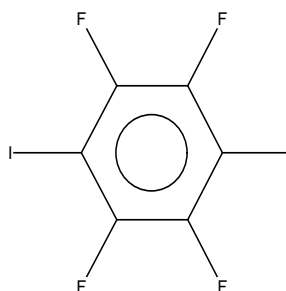
**Reference:** L.S.Reddy, N.J.Babu, A.Nangia (2006) *Chem. Commun.*, 1369  
**Formula:** C<sub>12</sub> H<sub>12</sub> N<sub>2</sub> O<sub>3</sub>.0.5(C<sub>10</sub> H<sub>8</sub> N<sub>2</sub> O<sub>2</sub>)  
**Compound Name:** 5-Ethyl-5-phenylbarbituric acid hemikis(4,4'-bipyridine-N,N'-dioxide)

**Space Group:** P21/c **Cell:** a 10.377(1) b 15.873(1) c 9.452(1)  
**Space Group No.:** 14 **(Å, °)** α 90.00 β 93.17(0) γ 90.00  
**R-Factor (%):** 4.58 **Temperature(K):** 100 **Density(g/cm<sup>3</sup>):** 1.394



**Reference:** M.T.Messina, P.Metrangolo, W.Panzeri, T.Pilati, G.Resnati (2001) *Tetrahedron*, 57,8543  
**Formula:** C<sub>10</sub> H<sub>8</sub> N<sub>2</sub> O<sub>2</sub>.C<sub>6</sub> F<sub>4</sub> I<sub>2</sub>  
**Compound Name:** 4,4'-Bipyridyl-N,N'-dioxide 1,4-di-iodotetrafluorobenzene

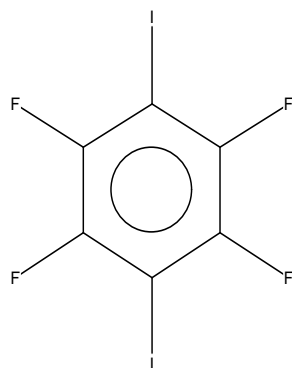
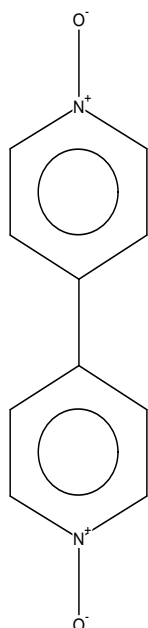
**Space Group:** P-1 **Cell:** a 4.295(0) b 8.129(0) c 13.647(1)  
**Space Group No.:** 2 **(Å, °)** α 100.73(0) β 98.82(0) γ 103.79(0)  
**R-Factor (%):** 2.96 **Temperature(K):** 291 **Density(g/cm<sup>3</sup>):** 2.203



## OCOMU001

**Reference:** A.Forni, P.Metrangolo, T.Pilati, G.Resnati (2004) *Cryst.Growth Des.*, 4,291  
**Formula:** C<sub>10</sub> H<sub>8</sub> N<sub>2</sub> O<sub>2</sub>.C<sub>6</sub> F<sub>4</sub> I<sub>2</sub>  
**Compound Name:** 4,4'-Bipyridyl-N,N'-dioxide 1,4-di-iodo-2,3,5,6-tetrafluorobenzene

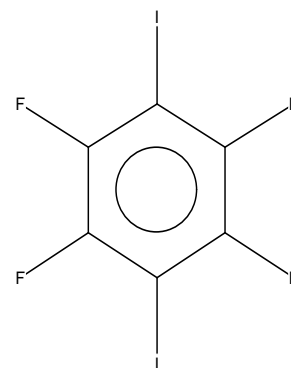
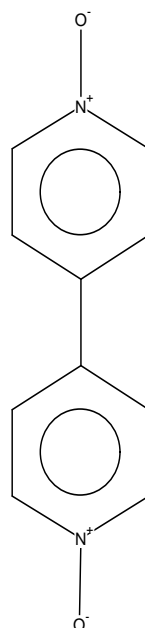
**Space Group:** P-1 **Cell:** a 4.294(1) b 8.123(3) c 13.638(5)  
**Space Group No.:** 2 **(Å, °)** α 100.75(1) β 98.82(1) γ 103.80(1)  
**R-Factor (%):** 3.67 **Temperature(K):** 292 **Density(g/cm<sup>3</sup>):** 2.207



## OCOMU002

**Reference:** A.Forni, P.Metrangolo, T.Pilati, G.Resnati (2004) *Cryst.Growth Des.*, 4,291  
**Formula:** C<sub>10</sub> H<sub>8</sub> N<sub>2</sub> O<sub>2</sub>.C<sub>6</sub> F<sub>4</sub> I<sub>2</sub>  
**Compound Name:** 4,4'-Bipyridyl-N,N'-dioxide 1,4-di-iodo-2,3,5,6-tetrafluorobenzene

**Space Group:** P-1 **Cell:** a 4.257(1) b 8.059(2) c 13.589(3)  
**Space Group No.:** 2 **(Å, °)** α 101.01(0) β 98.83(0) γ 103.08(0)  
**R-Factor (%):** 2.75 **Temperature(K):** 200 **Density(g/cm<sup>3</sup>):** 2.246



# Search: search3 (Wed Aug 20 11:52:28 2008): Hits 17-20

Supplementary Material (ESI) for New Journal of Chemistry  
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OCOMUO03

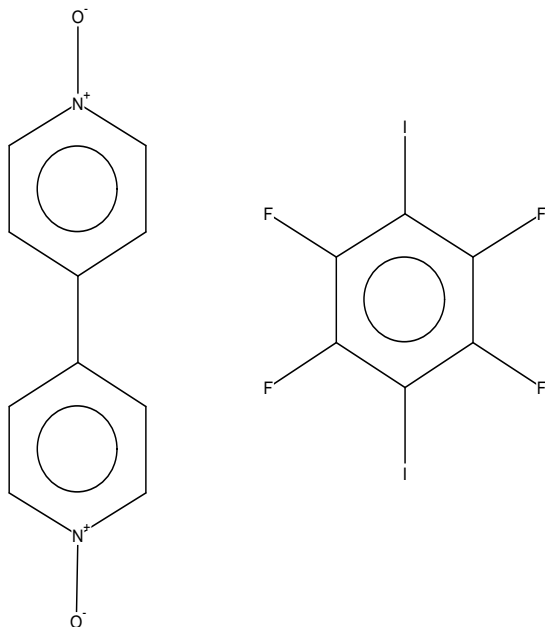
**Reference:** A.Forni, P.Metrangolo, T.Pilati, G.Resnati (2004)  
*Cryst.Growth Des.* ,4,291

**Formula:** C<sub>10</sub> H<sub>8</sub> N<sub>2</sub> O<sub>2</sub> C<sub>6</sub> F<sub>4</sub> I<sub>2</sub>

**Compound Name:** 4,4'-Bipyridyl-N,N'-dioxide 1,4-di-iodo-2,3,5,6-tetrafluorobenzene

**Space Group:** P-1 **Cell:** a 4.240(1) b 8.029(2) c 13.574(4)  
**Space Group No.:** 2 **(Å, °)** α 101.11(0) β 98.87(0) γ 102.72(0)

**R-Factor (%):** 2.33 **Temperature(K):** 145 **Density(g/cm<sup>3</sup>):** 2.263



OCOMUO04

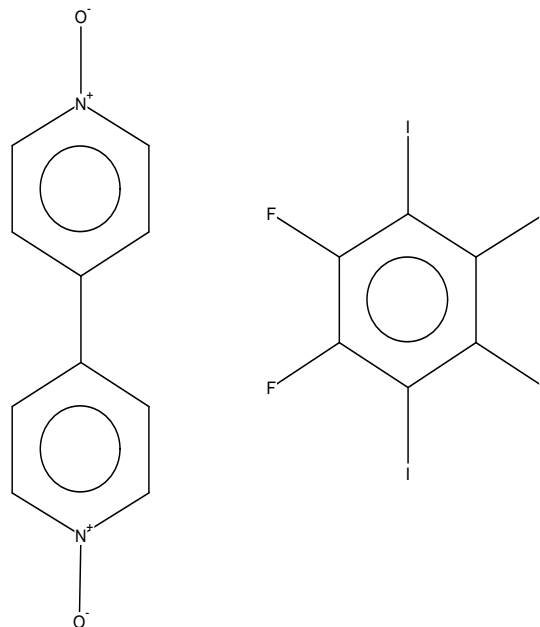
**Reference:** A.Forni, P.Metrangolo, T.Pilati, G.Resnati (2004)  
*Cryst.Growth Des.* ,4,291

**Formula:** C<sub>10</sub> H<sub>8</sub> N<sub>2</sub> O<sub>2</sub> C<sub>6</sub> F<sub>4</sub> I<sub>2</sub>

**Compound Name:** 4,4'-Bipyridyl-N,N'-dioxide 1,4-di-iodo-2,3,5,6-tetrafluorobenzene

**Space Group:** P-1 **Cell:** a 4.228(1) b 8.006(2) c 13.568(4)  
**Space Group No.:** 2 **(Å, °)** α 101.18(0) β 98.94(0) γ 102.37(0)

**R-Factor (%):** 2.04 **Temperature(K):** 90 **Density(g/cm<sup>3</sup>):** 2.275



OCOMUO05

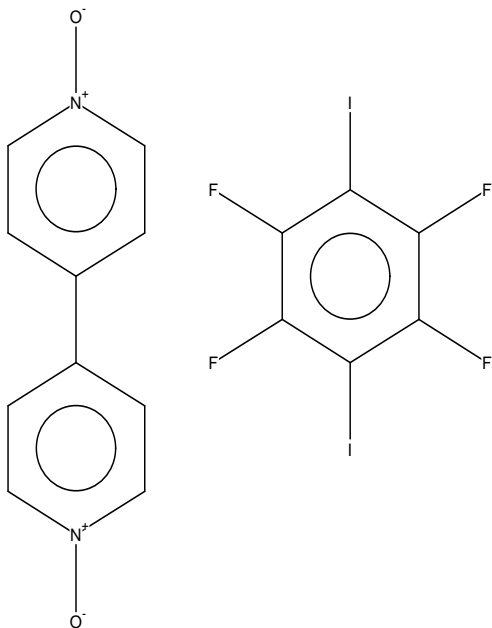
**Reference:** R.Bianchi, A.Forni, T.Pilati (2004)  
*Acta Crystallogr., Sect.B: Struct. Sci.* ,60,559

**Formula:** C<sub>10</sub> H<sub>8</sub> N<sub>2</sub> O<sub>2</sub> C<sub>6</sub> F<sub>4</sub> I<sub>2</sub>

**Compound Name:** 4,4'-Bipyridyl N,N'-dioxide 1,4-di-iodo-2,3,5,6-tetrafluorobenzene

**Space Group:** P-1 **Cell:** a 4.228(1) b 8.009(2) c 13.569(3)  
**Space Group No.:** 2 **(Å, °)** α 101.18(0) β 98.95(0) γ 102.35(0)

**R-Factor (%):** 2.72 **Temperature(K):** 90 **Density(g/cm<sup>3</sup>):** 2.274



TEFRUS

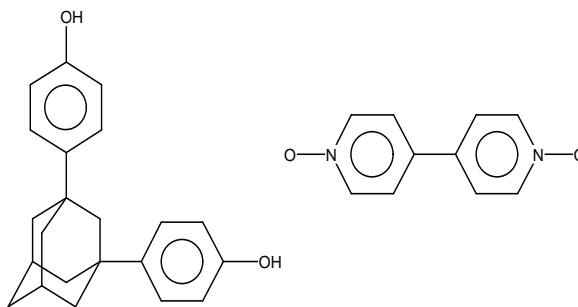
**Reference:** Qingdao Zeng, Dongxia Wu, Hongwei Ma, Chuyang Shu,  
Yan Li, Chen Wang (2006) *CrystEngComm* ,8,189

**Formula:** C<sub>22</sub> H<sub>24</sub> O<sub>2</sub> C<sub>10</sub> H<sub>8</sub> N<sub>2</sub> O<sub>2</sub>

**Compound Name:** 4,4'-(1,3-Adamantanediyl)diphenol 4,4'-dipyridyl N,N'-dioxide

**Space Group:** P21/c **Cell:** a 18.823(4) b 10.157(2) c 13.869(3)  
**Space Group No.:** 14 **(Å, °)** α 90.00 β 100.44(3) γ 90.00

**R-Factor (%):** 4.08 **Temperature(K):** 293 **Density(g/cm<sup>3</sup>):** 1.296





# Search: search3 (Wed Aug 20 11:52:28 2008): Hits 21-22

Supplemental Material (ESI) for New Journal of Chemistry

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VIGFOH

**Reference:** N.J.Babu, L.S.Reddy, A.Nangia (2007)  
*Mol.Pharmaceutics*, **4**,417

**Formula:** C<sub>7</sub> H<sub>5</sub> N<sub>1</sub> O<sub>3</sub> S<sub>1</sub>.0.5(C<sub>10</sub> H<sub>8</sub> N<sub>2</sub> O<sub>2</sub>)

**Compound Name:** Saccharin hemikis(4,4'-bipyridine-N,N'-oxide)

**Space Group:** P2<sub>1</sub>/n **Cell:** **a** 6.521(0) **b** 14.038(0) **c** 13.123(0)  
**Space Group No.:** 14 **(Å, °)** **α** 90.00 **β** 104.28(0) **γ** 90.00

**R-Factor (%)**: 3.62 **Temperature(K)**: 100 **Density(g/cm<sup>3</sup>)**: 1.582

VIGGEY

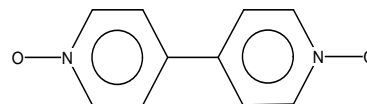
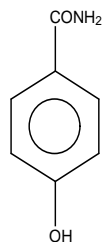
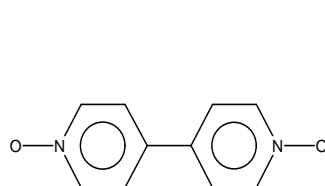
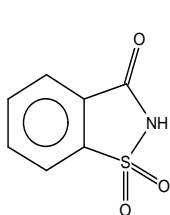
**Reference:** N.J.Babu, L.S.Reddy, A.Nangia (2007)  
*Mol.Pharmaceutics*, **4**,417

**Formula:** C<sub>7</sub> H<sub>7</sub> N<sub>1</sub> O<sub>2</sub>.0.5(C<sub>10</sub> H<sub>8</sub> N<sub>2</sub> O<sub>2</sub>)

**Compound Name:** 4-Hydroxybenzamide 4,4'-bipyridine-N,N'-dioxide

**Space Group:** P-1 **Cell:** **a** 5.692(4) **b** 9.482(6) **c** 10.751(7)  
**Space Group No.:** 2 **(Å, °)** **α** 69.89(1) **β** 84.23(1) **γ** 84.97(1)

**R-Factor (%)**: 4.55 **Temperature(K)**: 293 **Density(g/cm<sup>3</sup>)**: 1.419



# Search Overview

Supplementary Material (ESI) for New Journal of Chemistry  
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**Search:** search4

**Date/Time done:** Wed Aug 20 12:01:40 2008

**Database(s):** CSD version 5.29 (November 2007)  
CSD version 5.29 updates (Jan 2008)

**Restriction Info:** No refcode restrictions applied

**Filters:** Only Organometallic

**Percentage Completed:** 100%

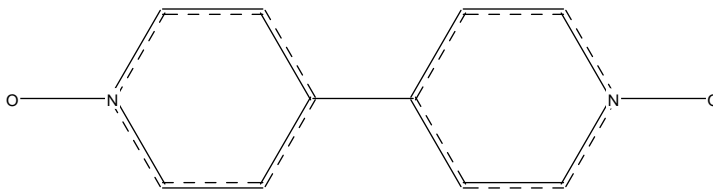
**Number of Hits:** 118

*Single query used. Search found structures that:*

match

**Query 1**

**Query 1**



# Search: search4 (Wed Aug 20 12:01:40 2008): Hits 1-4

Supplementary Material (ESI) for New Journal of Chemistry  
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 The Centre National de la Recherche Scientifique, 2008  
 BICVEP

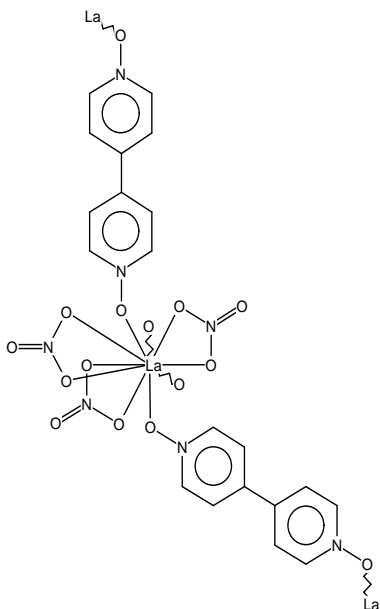
**Reference:** R.J.Hill, De-Liang Long, M.S.Turvey, A.J.Blake, N.R.Champness, P.Hubberstey, C.Wilson, M.Schroder (2004) *Chem.Commun.*, 1792

**Formula:** (C<sub>20</sub>H<sub>16</sub>La<sub>1</sub>N<sub>7</sub>O<sub>13</sub>)<sub>n</sub>

**Compound Name:** catena-(bis(μ<sub>2</sub>-4,4'-Bipyridine-N,N'-dioxide)-tris(nitrate)-lanthanum(iii))

**Space Group:** C2/c **Cell:** a 27.008(8) b 13.389(4) c 13.982(3)  
**Space Group No.:** 15 **(Å, °)** α 90.00 β 106.29(2) γ 90.00

**R-Factor (%):** 2.92 **Temperature(K):** 298 **Density(g/cm<sup>3</sup>):** 1.920



**BICVIT**

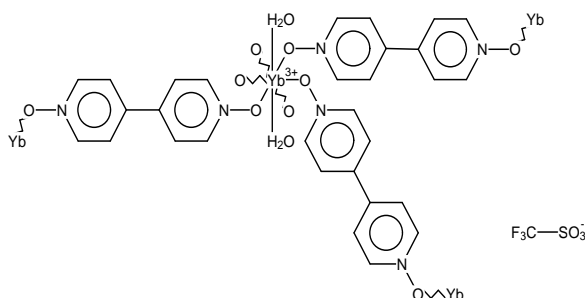
**Reference:** R.J.Hill, De-Liang Long, M.S.Turvey, A.J.Blake, N.R.Champness, P.Hubberstey, C.Wilson, M.Schroder (2004) *Chem.Commun.*, 1792

**Formula:** (C<sub>30</sub>H<sub>28</sub>N<sub>6</sub>O<sub>8</sub>Yb<sub>1</sub><sup>3+</sup>)<sub>n</sub>.3n(C<sub>1</sub>F<sub>3</sub>O<sub>3</sub>S<sub>1</sub><sup>1-</sup>)

**Compound Name:** catena-(tris(μ<sub>2</sub>-4,4'-Bipyridine-N,N'-dioxide)-diaqua-ytterbium(iii) tris(trifluoromethanesulfonate))

**Space Group:** Pcca **Cell:** a 16.794(3) b 13.764(3) c 20.044(4)  
**Space Group No.:** 54 **(Å, °)** α 90.00 β 90.00 γ 90.00

**R-Factor (%):** 9.65 **Temperature(K):** 150 **Density(g/cm<sup>3</sup>):** 1.750



**BICVOZ**

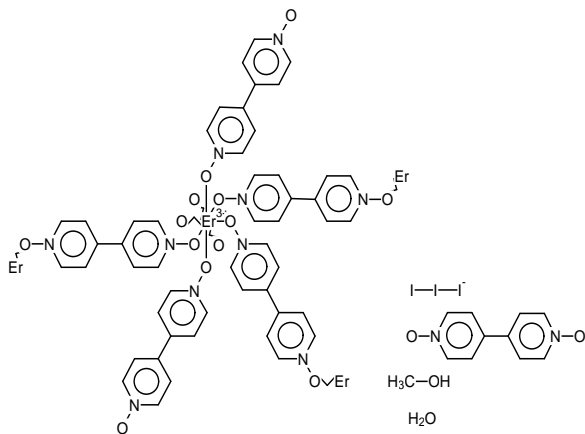
**Reference:** R.J.Hill, De-Liang Long, M.S.Turvey, A.J.Blake, N.R.Champness, P.Hubberstey, C.Wilson, M.Schroder (2004) *Chem.Commun.*, 1792

**Formula:** (C<sub>50</sub>H<sub>40</sub>Er<sub>1</sub>N<sub>10</sub>O<sub>10</sub><sup>3+</sup>)<sub>n</sub>.3n(Cl<sub>3</sub><sup>1-</sup>).0.5n(C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>).n(C<sub>1</sub>H<sub>4</sub>O<sub>1</sub>).0.5n(H<sub>2</sub>O)

**Compound Name:** catena-(tris(μ<sub>2</sub>-4,4'-Bipyridine-N,N'-dioxide)-bis(4,4'-bipyridine-N,N'-dioxide)-erbium(iii) tris(triiodide) 4,4'-bipyridine-N,N'-dioxide methanol solvate hemihydrate)

**Space Group:** Pbcn **Cell:** a 43.203(8) b 19.245(4) c 17.168(3)  
**Space Group No.:** 60 **(Å, °)** α 90.00 β 90.00 γ 90.00

**R-Factor (%):** 7.88 **Temperature(K):** 150 **Density(g/cm<sup>3</sup>):** 2.220



**BICVUF**

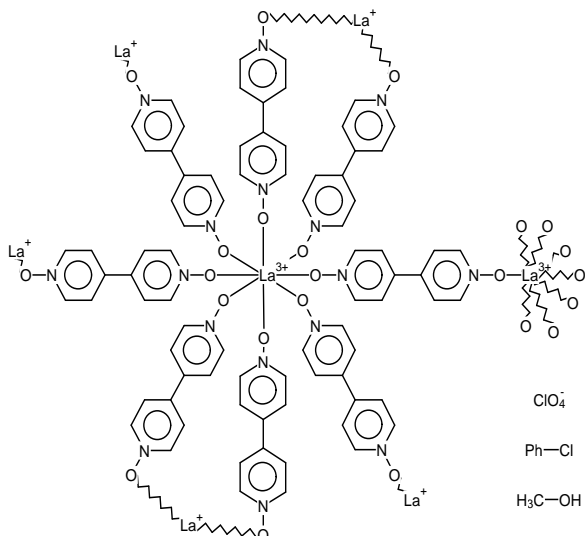
**Reference:** R.J.Hill, De-Liang Long, M.S.Turvey, A.J.Blake, N.R.Champness, P.Hubberstey, C.Wilson, M.Schroder (2004) *Chem.Commun.*, 1792

**Formula:** (C<sub>80</sub>H<sub>64</sub>La<sub>2</sub>N<sub>16</sub>O<sub>16</sub><sup>6+</sup>)<sub>n</sub>.6n(Cl<sub>1</sub>O<sub>4</sub><sup>1-</sup>).2n(C<sub>6</sub>H<sub>5</sub>Cl<sub>1</sub>).2n(C<sub>1</sub>H<sub>4</sub>O<sub>1</sub>)

**Compound Name:** catena-(octakis(μ<sub>2</sub>-4,4'-Bipyridin-N,N'-dioxide)-di-lanthanum hexaperchlorate chlorobenzene methanol solvate)

**Space Group:** P21/n **Cell:** a 16.685(0) b 19.875(0) c 32.669(2)  
**Space Group No.:** 14 **(Å, °)** α 90.00 β 100.66(0) γ 90.00

**R-Factor (%):** 5.85 **Temperature(K):** 150 **Density(g/cm<sup>3</sup>):** 1.665



# Search: search4 (Wed Aug 20 12:01:40 2008): Hits 5-8

Supplementary Material (ESI) for New Journal of Chemistry  
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 BICWAM

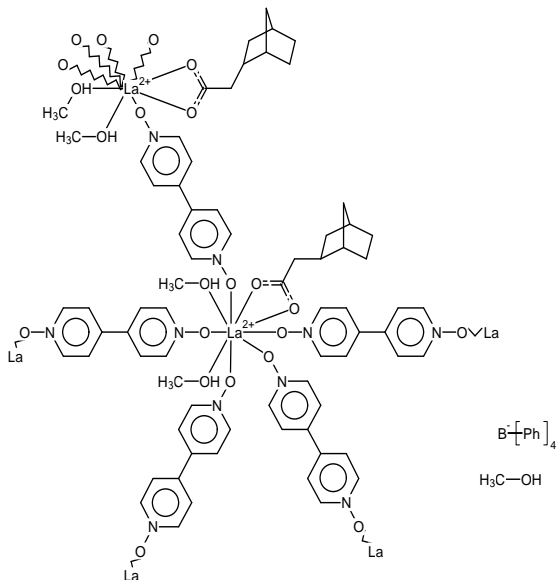
**Reference:** R.J.Hill, De-Liang Long, M.S.Turvey, A.J.Blake, N.R.Champness, P.Hubberstey, C.Wilson, M.Schroder (2004) *Chem.Commun.*, 1792

**Formula:**  $(C_{72}H_{82}La_2N_{10}O_{18}^{4+})_n, 4n(C_{24}H_{20}B_1^{-1}), 5.4n(C_1H_4O_1)$

**Compound Name:** catena-(pentakis( $\mu_2$ -4,4'-Bipyridine-N,N'-dioxide)-bis(2-norbornane acetato)-tetrakis(methanol)-di-lanthanum tetrakis(tetraphenylborate) methanol solvate)

**Space Group:** C2/c **Cell:** a 49.269(7) b 17.698(3) c 18.718(3)  
**Space Group No.:** 15 **(Å, °)**  $\alpha$  90.00  $\beta$  105.95(0)  $\gamma$  90.00

**R-Factor (%):** 6.80 **Temperature(K):** 150 **Density(g/cm<sup>3</sup>):** 1.313



## ECAJIB

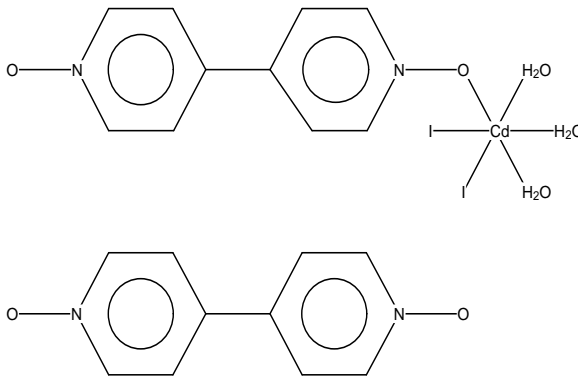
**Reference:** Bao-Qing Ma, Song Gao, Hao-Ling Sun, Guang-Xian Xu (2001) *CrystEngComm*, 3,147

**Formula:**  $C_{10}H_{14}Cd_1N_2O_5, 0.5(C_{10}H_8N_2O_2)$

**Compound Name:** bis(Triaqua-(4,4'-bipyridine dioxide)-diiodo-cadmium) 4,4'-bipyridine dioxide

**Space Group:** P21/c **Cell:** a 10.325(0) b 10.389(0) c 19.101(0)  
**Space Group No.:** 14 **(Å, °)**  $\alpha$  90.00  $\beta$  96.03(0)  $\gamma$  90.00

**R-Factor (%):** 3.01 **Temperature(K):** 293 **Density(g/cm<sup>3</sup>):** 2.290



## ECAJOH

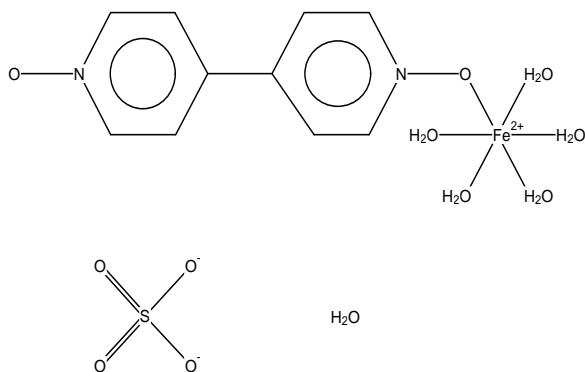
**Reference:** Bao-Qing Ma, Song Gao, Hao-Ling Sun, Guang-Xian Xu (2001) *CrystEngComm*, 3,147

**Formula:**  $C_{10}H_{18}Fe_1N_2O_7, 2, 4(H_2O_1)$

**Compound Name:** Penta-aqua-(4,4'-bipyridine dioxide)-iron sulfate tetrahydrate

**Space Group:** P21/c **Cell:** a 14.310(0) b 6.979(0) c 20.880(0)  
**Space Group No.:** 14 **(Å, °)**  $\alpha$  90.00  $\beta$  104.69(0)  $\gamma$  90.00

**R-Factor (%):** 5.90 **Temperature(K):** 293 **Density(g/cm<sup>3</sup>):** 1.654



## EFOKUF

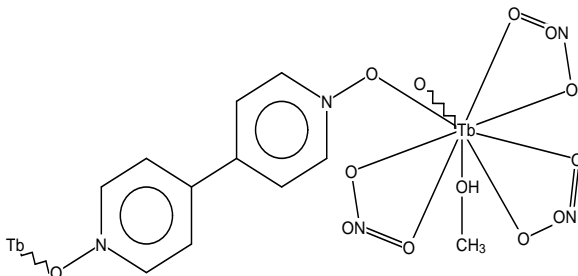
**Reference:** De-Liang Long, A.J.Blake, N.R.Champness, C.Wilson, M.Schroder (2002) *Chem.-Eur.J.*, 8,2026

**Formula:**  $(C_{11}H_{12}N_5O_{12}Tb_1)_n$

**Compound Name:** catena-(( $\mu_2$ -4,4'-bipyridine-N,N'-dioxide)-(methanol)-tris(nitrate)-terbium(III))

**Space Group:** C2/c **Cell:** a 15.228(2) b 8.300(0) c 13.996(2)  
**Space Group No.:** 15 **(Å, °)**  $\alpha$  90.00  $\beta$  92.70(0)  $\gamma$  90.00

**R-Factor (%):** 2.70 **Temperature(K):** 150 **Density(g/cm<sup>3</sup>):** 2.124



# Search: search4 (Wed Aug 20 12:01:40 2008): Hits 9-12

Supplementary Material (ESI) for New Journal of Chemistry

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EFOLAM

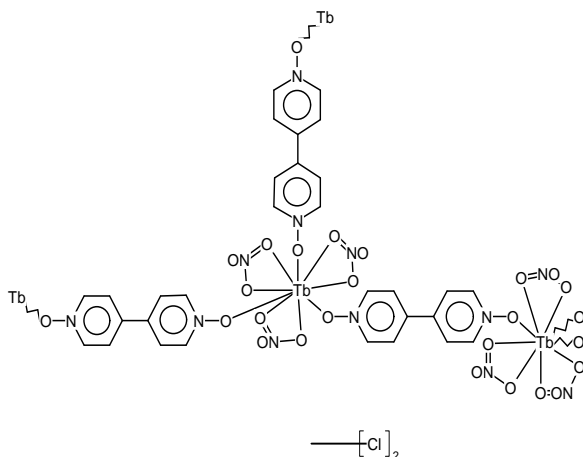
**Reference:** De-Liang Long, A.J.Blake, N.R.Champness, C.Wilson, M.Schroder (2002) *Chem.-Eur.J.*, **8**,2026

**Formula:** (C<sub>30</sub> H<sub>24</sub> N<sub>12</sub> O<sub>24</sub> Tb<sub>2</sub>)n,2n(C<sub>1</sub> H<sub>2</sub> Cl<sub>2</sub>)

**Compound Name:** catena-(tris(μ<sub>2</sub>-4,4'-bipyridine-N,N'-dioxide)-hexakis(nitrate)-diterbium(iii)) dichloromethane clathrate

**Space Group:** P-1 **Cell:** a 8.086(2) b 11.769(3) c 13.078(2)  
**Space Group No.:** 2 **(Å, °)** α 86.80(2) β 79.52(2) γ 78.79(2)

**R-Factor (%):** 5.30 **Temperature(K):** 298 **Density(g/cm<sup>3</sup>):** 1.971



## EFOLEQ

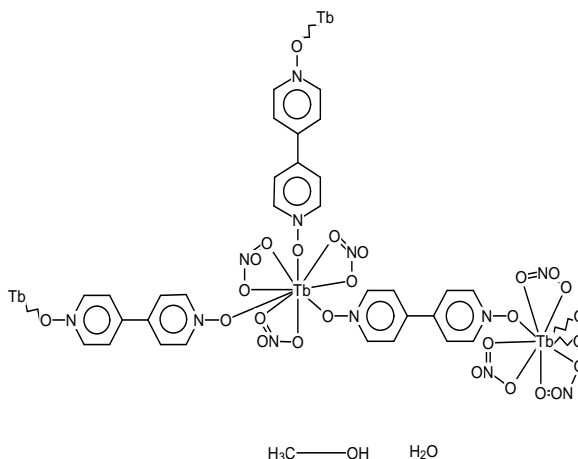
**Reference:** De-Liang Long, A.J.Blake, N.R.Champness, C.Wilson, M.Schroder (2002) *Chem.-Eur.J.*, **8**,2026

**Formula:** (C<sub>30</sub> H<sub>24</sub> N<sub>12</sub> O<sub>24</sub> Tb<sub>2</sub>)n,2n(C<sub>1</sub> H<sub>4</sub> O<sub>1</sub>),1.6n(H<sub>2</sub> O<sub>1</sub>)

**Compound Name:** catena-(tris(μ<sub>2</sub>-4,4'-bipyridine-N,N'-dioxide)-hexakis(nitrate)-diterbium(iii)) methanol solvate hydrate

**Space Group:** P-421c **Cell:** a 26.304(6) b 26.304(6) c 7.580(2)  
**Space Group No.:** 114 **(Å, °)** α 90.00 β 90.00 γ 90.00

**R-Factor (%):** 8.80 **Temperature(K):** 150 **Density(g/cm<sup>3</sup>):** 1.706



## EFOLIU

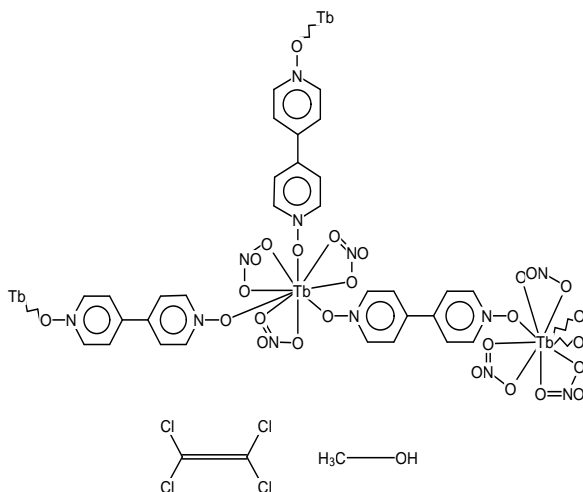
**Reference:** De-Liang Long, A.J.Blake, N.R.Champness, C.Wilson, M.Schroder (2002) *Chem.-Eur.J.*, **8**,2026

**Formula:** (C<sub>30</sub> H<sub>24</sub> N<sub>12</sub> O<sub>24</sub> Tb<sub>2</sub>)n,0.8n(C<sub>2</sub> Cl<sub>4</sub>),1.6n(C<sub>1</sub> H<sub>4</sub> O<sub>1</sub>)

**Compound Name:** catena-(tris(μ<sub>2</sub>-4,4'-bipyridine-N,N'-dioxide)-hexakis(nitrate)-diterbium(iii)) tetrachloroethylene methanol solvate

**Space Group:** P-421c **Cell:** a 26.154(4) b 26.154(4) c 7.583(1)  
**Space Group No.:** 114 **(Å, °)** α 90.00 β 90.00 γ 90.00

**R-Factor (%):** 4.30 **Temperature(K):** 150 **Density(g/cm<sup>3</sup>):** 1.842



## EFOLOA

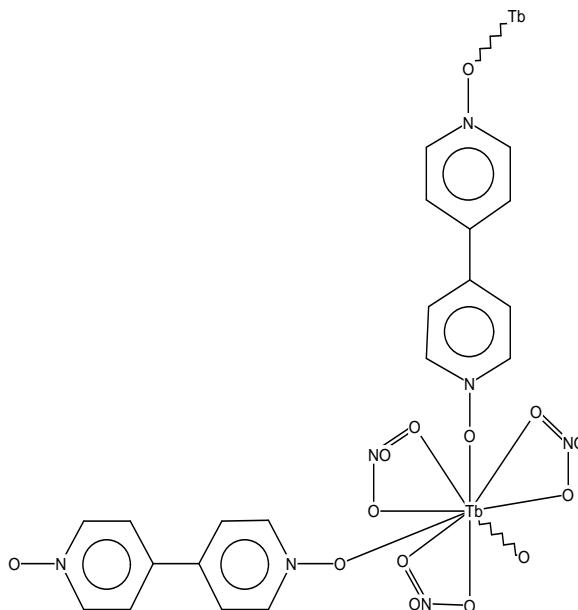
**Reference:** De-Liang Long, A.J.Blake, N.R.Champness, C.Wilson, M.Schroder (2002) *Chem.-Eur.J.*, **8**,2026

**Formula:** (C<sub>20</sub> H<sub>16</sub> N<sub>7</sub> O<sub>13</sub> Tb<sub>1</sub>)n

**Compound Name:** catena-(bis(μ<sub>2</sub>-4,4'-bipyridine-N,N'-dioxide)-tris(nitrate)-terbium(iii))

**Space Group:** P21/c **Cell:** a 9.394(0) b 14.650(0) c 17.287(1)  
**Space Group No.:** 14 **(Å, °)** α 90.00 β 90.58(0) γ 90.00

**R-Factor (%):** 2.10 **Temperature(K):** 150 **Density(g/cm<sup>3</sup>):** 2.014



# Search: search4 (Wed Aug 20 12:01:40 2008): Hits 13-16

Supplementary Material (ESI) for New Journal of Chemistry

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FARJEO

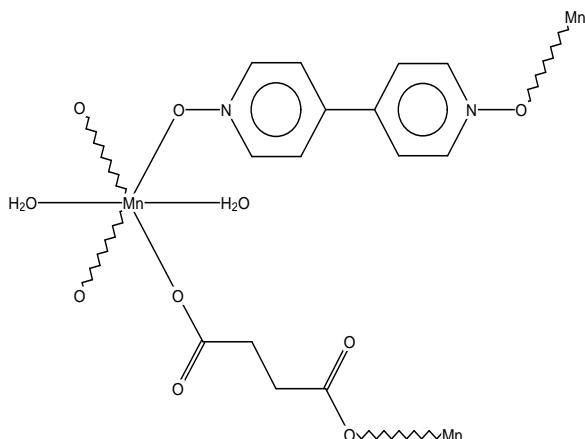
**Reference:** Siau Gek Ang, Bai Wang Sun (2005) *Cryst.Growth Des.* ,5, 383

**Formula:** (C<sub>14</sub> H<sub>16</sub> Mn<sub>1</sub> N<sub>2</sub> O<sub>8</sub>)<sub>n</sub>

**Compound Name:** catena-((μ<sub>2</sub>-4,4'-Bipyridyl-N,N'-dioxido)-(μ<sub>2</sub>-succinato)-diaqua-manganese(ii))

**Space Group:** P-1 **Cell:** a 5.406(0) b 7.294(0) c 9.985(0)  
**Space Group No.:** 2 **(Å, °)** α 86.55(0) β 84.75(0) γ 73.43(0)

**R-Factor (%):** 2.99 **Temperature(K):** 223 **Density(g/cm<sup>3</sup>):** 1.748



## FARJOY

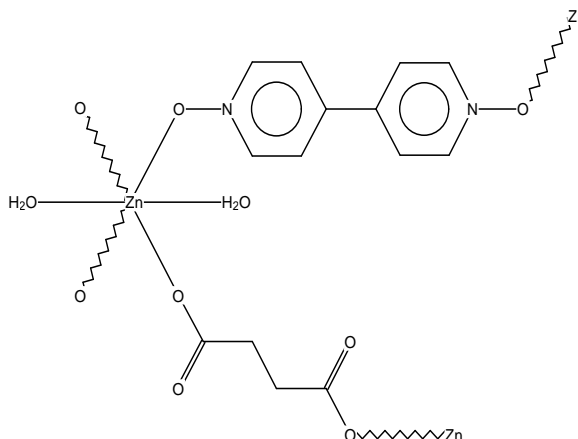
**Reference:** Siau Gek Ang, Bai Wang Sun (2005) *Cryst.Growth Des.* ,5, 383

**Formula:** (C<sub>14</sub> H<sub>16</sub> N<sub>2</sub> O<sub>8</sub> Zn<sub>1</sub>)<sub>n</sub>

**Compound Name:** catena-((μ<sub>2</sub>-4,4'-Bipyridyl-N,N'-dioxido)-(μ<sub>2</sub>-succinato)-diaqua-zinc(ii))

**Space Group:** P-1 **Cell:** a 5.402(1) b 7.371(1) c 9.823(2)  
**Space Group No.:** 2 **(Å, °)** α 86.41(0) β 84.11(0) γ 72.99(0)

**R-Factor (%):** 2.59 **Temperature(K):** 223 **Density(g/cm<sup>3</sup>):** 1.812



## FITGUL

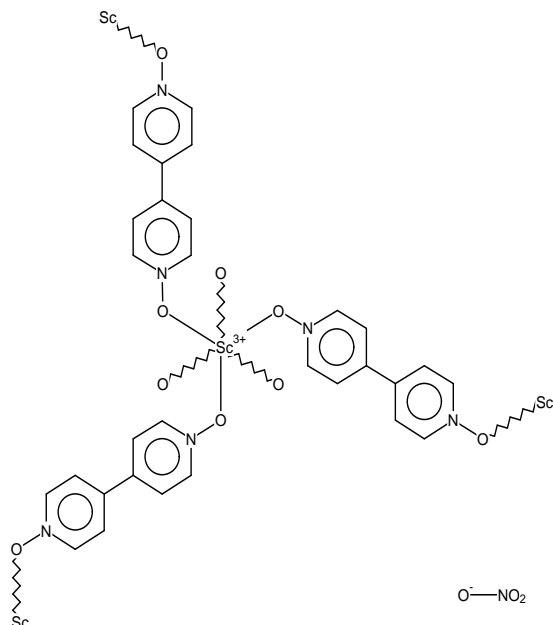
**Reference:** De-Liang Long, R.J.Hill, A.J.Blake, N.R.Champness, P.Hubberstey, C.Wilson, M.Schroder (2005) *Chem.-Eur.J.* ,11,1384

**Formula:** (C<sub>30</sub> H<sub>24</sub> N<sub>6</sub> O<sub>6</sub> Sc<sub>1</sub><sup>3+</sup>)<sub>n</sub>.3n(N<sub>1</sub> O<sub>3</sub><sup>1-</sup>)

**Compound Name:** catena-(tris(μ<sub>2</sub>-4,4'-Bipyridine-N,N'-dioxide)-scandium(iii) trinitrate)

**Space Group:** R-3c **Cell:** a 20.852(3) b 20.852(3) c 12.972(2)  
**Space Group No.:** 167 **(Å, °)** α 90.00 β 90.00 γ 120.00

**R-Factor (%):** 5.80 **Temperature(K):** 150 **Density(g/cm<sup>3</sup>):** 1.623



## FITHAS

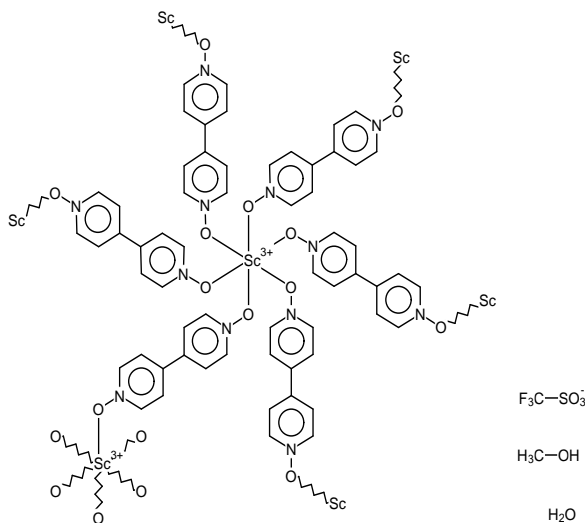
**Reference:** De-Liang Long, R.J.Hill, A.J.Blake, N.R.Champness, P.Hubberstey, C.Wilson, M.Schroder (2005) *Chem.-Eur.J.* ,11,1384

**Formula:** (C<sub>60</sub> H<sub>48</sub> N<sub>12</sub> O<sub>12</sub> Sc<sub>2</sub><sup>6+</sup>)<sub>n</sub>.6n(C<sub>1</sub> F<sub>3</sub> O<sub>3</sub> S<sub>1</sub><sup>1-</sup>).5.4n(C<sub>1</sub> H<sub>4</sub> O<sub>1</sub>).6n(H<sub>2</sub> O<sub>1</sub>)

**Compound Name:** catena-(hexakis(μ<sub>2</sub>-4,4'-Bipyridine-N,N'-dioxide)-di-scandium(iii) hexakis(trifluoromethanesulfonate) methanol solvate hexahydrate clathrate)

**Space Group:** P21/n **Cell:** a 20.787(0) b 12.806(0) c 21.625(1)  
**Space Group No.:** 14 **(Å, °)** α 90.00 β 103.25(0) γ 90.00

**R-Factor (%):** 12.40 **Temperature(K):** 120 **Density(g/cm<sup>3</sup>):** 1.419



# Search: search4 (Wed Aug 20 12:01:40 2008): Hits 17-20

Supplementary Material (ESI) for New Journal of Chemistry  
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 The Centre National de la Recherche Scientifique, 2008  
 FITHEW

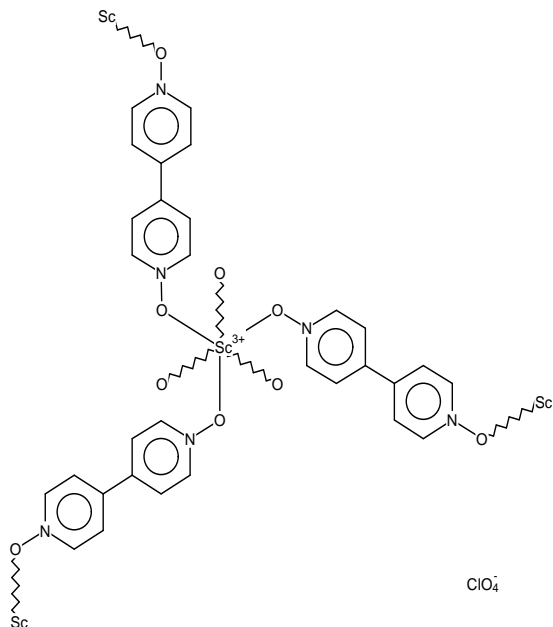
**Reference:** De-Liang Long, R.J.Hill, A.J.Blake, N.R.Champness, P.Hubberstey, C.Wilson, M.Schroder (2005) *Chem.-Eur.J.*, **11**,1384

**Formula:** (C<sub>30</sub>H<sub>24</sub>N<sub>6</sub>O<sub>6</sub>Sc<sub>1</sub><sup>3+</sup>)<sub>n</sub>.3n(Cl<sub>1</sub>O<sub>4</sub><sup>1-</sup>)

**Compound Name:** catena-(tris(μ<sub>2</sub>-4,4'-Bipyridine-N,N'-dioxide)-scandium(iii) triperchlorate)

**Space Group:** R-3c      **Cell:**    **a** 20.495(1)    **b** 20.495(1)    **c** 15.818(2)  
**Space Group No.:** 167      **(Å, °)**    α 90.00      β 90.00      γ 120.00

**R-Factor (%):** 4.64      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.572



**FITHIA**

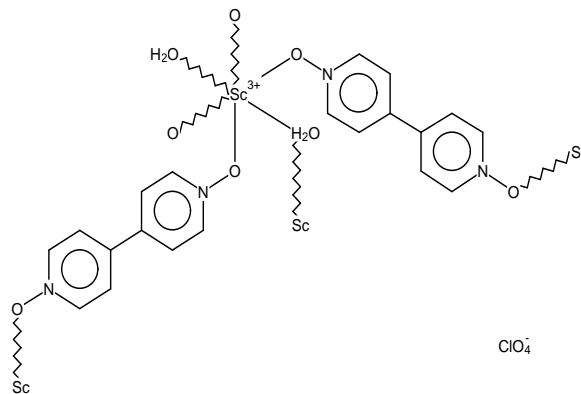
**Reference:** De-Liang Long, R.J.Hill, A.J.Blake, N.R.Champness, P.Hubberstey, C.Wilson, M.Schroder (2005) *Chem.-Eur.J.*, **11**,1384

**Formula:** (C<sub>20</sub>H<sub>18</sub>N<sub>4</sub>O<sub>5</sub>Sc<sub>1</sub><sup>3+</sup>)<sub>n</sub>.3n(Cl<sub>1</sub>O<sub>4</sub><sup>1-</sup>)

**Compound Name:** catena-((μ<sub>2</sub>-Aqua)-bis(μ<sub>2</sub>-4,4'-bipyridine-N,N'-dioxide)-scandium(iii) triperchlorate)

**Space Group:** I-42d      **Cell:**    **a** 23.995(4)    **b** 23.995(4)    **c** 3.950(0)  
**Space Group No.:** 122      **(Å, °)**    α 90.00      β 90.00      γ 90.00

**R-Factor (%):** 7.26      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.077



**FIVGUN**

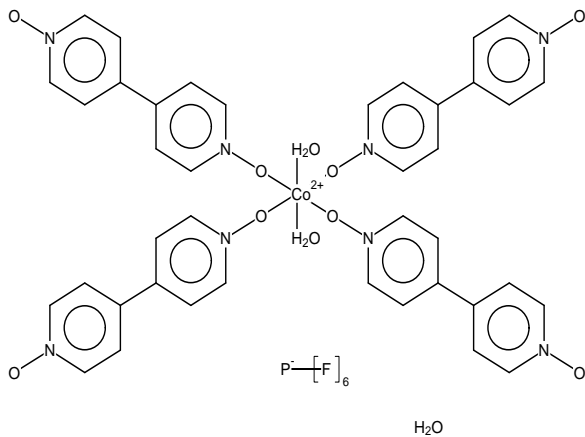
**Reference:** Bao-Qing Ma, Hao-Ling Sun, Song Gao (2005) *Inorg.Chem.*, **44**,837

**Formula:** C<sub>40</sub>H<sub>36</sub>Co<sub>1</sub>N<sub>8</sub>O<sub>10</sub><sup>2+</sup>.2(F<sub>6</sub>P<sub>1</sub><sup>1-</sup>).2(H<sub>2</sub>O<sub>1</sub>)

**Compound Name:** Diaqua-tetrakis(4,4'-dipyridine-N,N'-dioxide)-cobalt(ii) bis(hexafluorophosphate) dihydrate

**Space Group:** I-4      **Cell:**    **a** 23.169(3)    **b** 23.169(3)    **c** 8.220(1)  
**Space Group No.:** 82      **(Å, °)**    α 90.00      β 90.00      γ 90.00

**R-Factor (%):** 7.25      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.767



**FIVHAU**

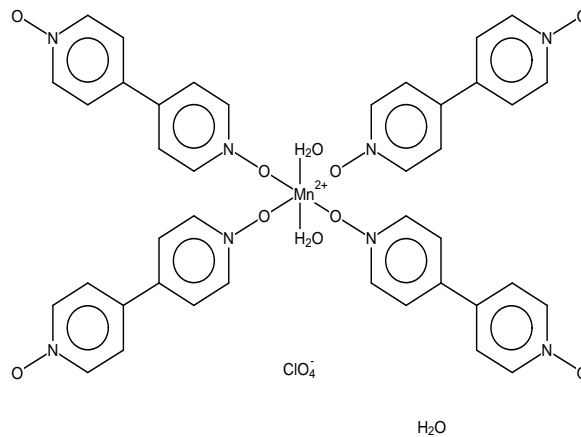
**Reference:** Bao-Qing Ma, Hao-Ling Sun, Song Gao (2005) *Inorg.Chem.*, **44**,837

**Formula:** C<sub>40</sub>H<sub>36</sub>Mn<sub>1</sub>N<sub>8</sub>O<sub>10</sub><sup>2+</sup>.2(Cl<sub>1</sub>O<sub>4</sub><sup>1-</sup>).2(H<sub>2</sub>O<sub>1</sub>)

**Compound Name:** Diaqua-tetrakis(4,4'-dipyridine-N,N'-dioxide)-manganese(ii) diperchlorate dihydrate

**Space Group:** I-4      **Cell:**    **a** 23.150(3)    **b** 23.150(3)    **c** 8.150(1)  
**Space Group No.:** 82      **(Å, °)**    α 90.00      β 90.00      γ 90.00

**R-Factor (%):** 4.18      **Temperature(K):** 297      **Density(g/cm<sup>3</sup>):** 1.640



# Search: search4 (Wed Aug 20 12:01:40 2008): Hits 21-24

Supplementary Material (ESI) for New Journal of Chemistry  
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FIVHEY

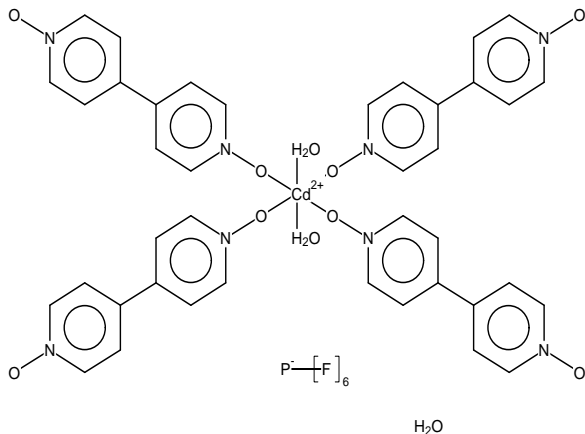
**Reference:** Bao-Qing Ma, Hao-Ling Sun, Song Gao (2005)  
*Inorg.Chem.*, **44**,837

**Formula:**  $C_{40}H_{36}Cd_1N_8O_{10}^{2+} \cdot 2(F_6P_1^{-1}) \cdot 2(H_2O_1)$

**Compound Name:** Diaqua-tetrakis(4,4'-dipyridine-N,N'-dioxide)-cadmium(ii) bis(hexafluorophosphate) dihydrate

**Space Group:** I-4      **Cell:**    **a** 23.523(3)    **b** 23.523(3)    **c** 8.145(2)  
**Space Group No.:** 82      **(Å, °)**     $\alpha$  90.00       $\beta$  90.00       $\gamma$  90.00

**R-Factor (%):** 0.00      **Temperature(K):** 295      **Density(g/cm<sup>3</sup>):** 1.809



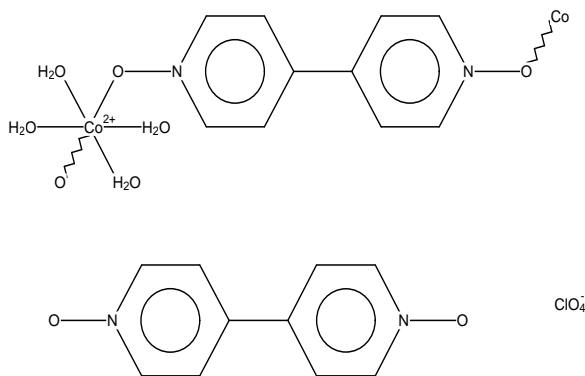
**Reference:** Bao-Qing Ma, Song Gao, Hao-Ling Sun, Guang-Xian Xu (2001) *J.Chem.Soc.,Dalton Trans.*, 130

**Formula:**  $(C_{10}H_{16}Co_1N_2O_6^{2+})_n \cdot 2n(Cl_1O_4^{1-}) \cdot 2n(C_{10}H_8N_2O_2)$

**Compound Name:** catena-((μ<sub>2</sub>-4,4'-Bipyridine-N,N'-dioxide-O,O')-tetra-aqua-cobalt diperchlorate 4,4'-bipyridine-N,N'-dioxide solvate)

**Space Group:** P-1      **Cell:**    **a** 5.521(0)    **b** 11.831(0)    **c** 14.981(0)  
**Space Group No.:** 2      **(Å, °)**     $\alpha$  107.81(0)     $\beta$  96.00(0)     $\gamma$  100.59(0)

**R-Factor (%):** 4.55      **Temperature(K):** 295      **Density(g/cm<sup>3</sup>):** 1.646



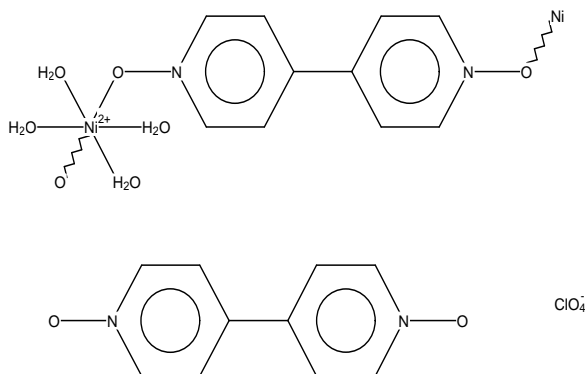
**Reference:** Bao-Qing Ma, Song Gao, Hao-Ling Sun, Guang-Xian Xu (2001) *J.Chem.Soc.,Dalton Trans.*, 130

**Formula:**  $(C_{10}H_{16}Ni_1N_2O_6^{2+})_n \cdot 2n(Cl_1O_4^{1-}) \cdot 2n(C_{10}H_8N_2O_2)$

**Compound Name:** catena-((μ<sub>2</sub>-4,4'-Bipyridine-N,N'-dioxide-O,O')-tetra-aqua-nickel diperchlorate 4,4'-bipyridine-N,N'-dioxide solvate)

**Space Group:** P-1      **Cell:**    **a** 5.465(0)    **b** 11.817(0)    **c** 15.089(0)  
**Space Group No.:** 2      **(Å, °)**     $\alpha$  108.76(0)     $\beta$  95.40(0)     $\gamma$  100.16(0)

**R-Factor (%):** 8.59      **Temperature(K):** 295      **Density(g/cm<sup>3</sup>):** 1.657



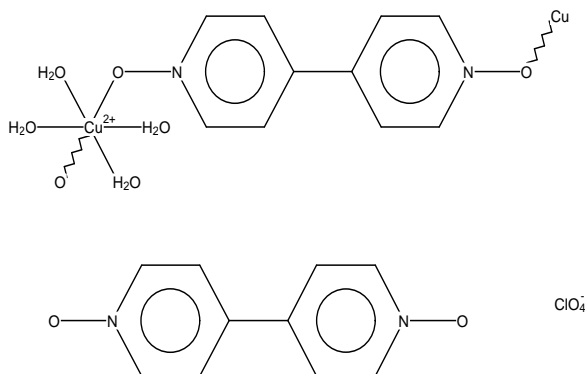
**Reference:** Bao-Qing Ma, Song Gao, Hao-Ling Sun, Guang-Xian Xu (2001) *J.Chem.Soc.,Dalton Trans.*, 130

**Formula:**  $(C_{10}H_{16}Cu_1N_2O_6^{2+})_n \cdot 2n(Cl_1O_4^{1-}) \cdot 2n(C_{10}H_8N_2O_2)$

**Compound Name:** catena-((μ<sub>2</sub>-4,4'-Bipyridine-N,N'-dioxide-O,O')-tetra-aqua-copper diperchlorate 4,4'-bipyridine-N,N'-dioxide solvate)

**Space Group:** P-1      **Cell:**    **a** 5.354(0)    **b** 11.892(0)    **c** 15.271(0)  
**Space Group No.:** 2      **(Å, °)**     $\alpha$  110.74(0)     $\beta$  94.04(0)     $\gamma$  99.23(0)

**R-Factor (%):** 4.21      **Temperature(K):** 295      **Density(g/cm<sup>3</sup>):** 1.680





# Search: search4 (Wed Aug 20 12:01:40 2008): Hits 25-28

Supplementary Material (ESI) for New Journal of Chemistry

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HAYYOF

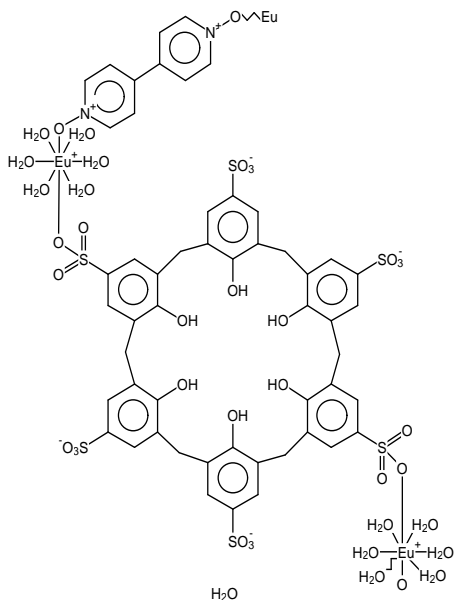
**Reference:** S.J.Dalgarno, M.J.Hardie, J.L.Atwood, C.L.Raston (2004)  
*Inorg.Chem.* **43**,6351

**Formula:** (C<sub>52</sub>H<sub>60</sub>Eu<sub>2</sub>N<sub>2</sub>O<sub>38</sub>S<sub>6</sub>)n.8n(H<sub>2</sub>O)<sub>1</sub>

**Compound Name:** catena-((μ<sub>2</sub>-37,38,39,40,41,42-Hexahydroxycalix(6)arene-17,35-bis(sulfonato-O)-5,11,23,29-tetrakisulfonato)-(μ<sub>2</sub>-4,4'-bipyridine-N,N'-dioxide-O,O)-dodeca-aqua-di-europium(iii) octahydrate)

**Space Group:** P2<sub>1</sub>/c **Cell:** a 13.817(0) b 12.229(0) c 22.356(0)  
**Space Group No.:** 14 **(Å, °)** α 90.00 β 107.86(0) γ 90.00

**R-Factor (%)**: 3.62 **Temperature(K)**: 150 **Density(g/cm<sup>3</sup>)**: 1.812



## IBOTEY

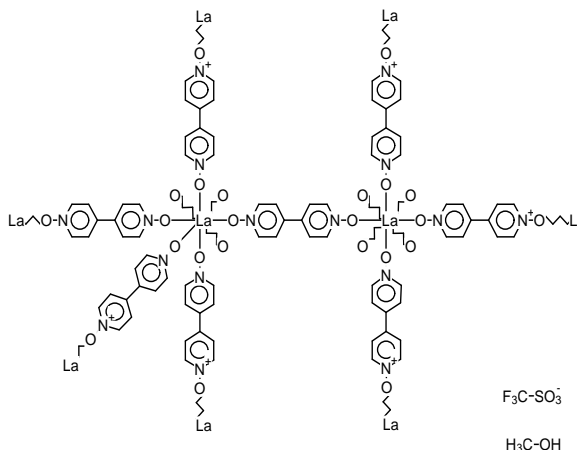
**Reference:** De-Liang Long, A.J.Blake, N.R.Champness, C.Wilson,  
M.Schroder (2001) *Angew.Chem.,Int.Ed.* **40**,2444

**Formula:** (C<sub>80</sub>H<sub>64</sub>La<sub>2</sub>N<sub>16</sub>O<sub>16</sub>6+)n.6n(C<sub>1</sub>F<sub>3</sub>O<sub>3</sub>S<sub>1</sub><sup>-1</sup>).8.4n(C<sub>1</sub>H<sub>4</sub>O<sub>1</sub>)

**Compound Name:** catena-(octakis(μ<sub>2</sub>-4,4'-Bipyridine-N,N'-dioxido)-di-lanthanum(iii) hexakis(trifluoromethanesulfonate) methanol solvate)

**Space Group:** P-4c2 **Cell:** a 25.997(0) b 25.997(0) c 26.785(0)  
**Space Group No.:** 116 **(Å, °)** α 90.00 β 90.00 γ 90.00

**R-Factor (%)**: 13.20 **Temperature(K)**: 150 **Density(g/cm<sup>3</sup>)**: 1.622



F<sub>3</sub>C-SO<sub>3</sub><sup>-</sup>

H<sub>3</sub>C-OH

## IBOTIC

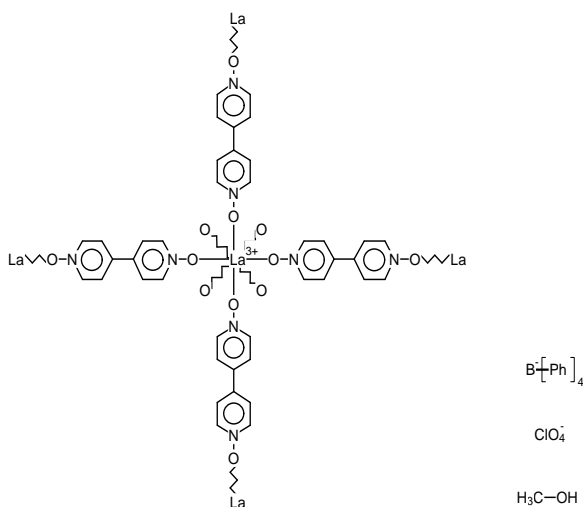
**Reference:** De-Liang Long, A.J.Blake, N.R.Champness, C.Wilson,  
M.Schroder (2001) *Angew.Chem.,Int.Ed.* **40**,2444

**Formula:** (C<sub>40</sub>H<sub>32</sub>La<sub>1</sub>N<sub>8</sub>O<sub>8</sub><sup>3+</sup>)n.n(C<sub>24</sub>H<sub>20</sub>B<sub>1</sub><sup>-1</sup>).2n(Cl<sub>1</sub>O<sub>4</sub><sup>-1</sup>).2.75n(C<sub>1</sub>H<sub>4</sub>O<sub>1</sub>)

**Compound Name:** catena-(tetrakis(μ<sub>2</sub>-4,4'-Bipyridine-N,N'-dioxido)-lanthanum(iii) tetraphenylborate diperchlorate methanol solvate clathrate)

**Space Group:** P2<sub>1</sub>/n **Cell:** a 13.224(1) b 38.366(3) c 13.252(1)  
**Space Group No.:** 14 **(Å, °)** α 90.00 β 99.75(0) γ 90.00

**R-Factor (%)**: 6.20 **Temperature(K)**: 150 **Density(g/cm<sup>3</sup>)**: 1.502



B[Ph]<sub>4</sub><sup>-</sup>

ClO<sub>4</sub><sup>-</sup>

H<sub>3</sub>C-OH

## IBOTOI

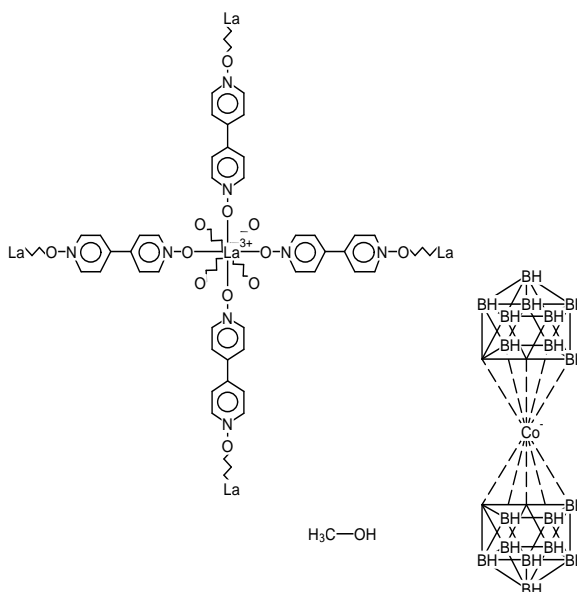
**Reference:** De-Liang Long, A.J.Blake, N.R.Champness, C.Wilson,  
M.Schroder (2001) *Angew.Chem.,Int.Ed.* **40**,2444

**Formula:** (C<sub>40</sub>H<sub>32</sub>La<sub>1</sub>N<sub>8</sub>O<sub>8</sub><sup>3+</sup>)n.3n(C<sub>4</sub>H<sub>22</sub>B<sub>18</sub>Co<sub>1</sub><sup>-1</sup>).0.5n(C<sub>1</sub>H<sub>4</sub>O<sub>1</sub>)

**Compound Name:** catena-(tetrakis(μ<sub>2</sub>-4,4'-Bipyridine-N,N'-dioxido)-lanthanum(iii) tris(bis(η<sup>5</sup>-7,8-dicarba-nido-undecaborate(11))-cobalt) methanol solvate clathrate)

**Space Group:** P2<sub>1</sub>2<sub>1</sub>2 **Cell:** a 17.570(1) b 18.571(2) c 13.336(1)  
**Space Group No.:** 18 **(Å, °)** α 90.00 β 90.00 γ 90.00

**R-Factor (%)**: 4.40 **Temperature(K)**: 150 **Density(g/cm<sup>3</sup>)**: 1.434



H<sub>3</sub>C-OH

# Search: search4 (Wed Aug 20 12:01:40 2008): Hits 29-32

Supplementary Material (ESI) for New Journal of Chemistry  
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IBOTUO

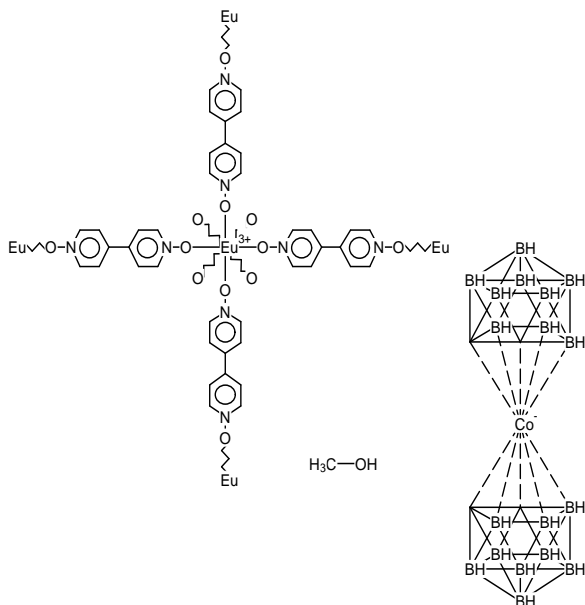
**Reference:** De-Liang Long, A.J.Blake, N.R.Champness, C.Wilson, M.Schroder (2001) *Angew.Chem.,Int.Ed.* **40**,2444

**Formula:** (C<sub>40</sub> H<sub>32</sub> Eu<sub>1</sub> N<sub>8</sub> O<sub>8</sub><sup>3+</sup>)n,3n(C<sub>4</sub> H<sub>22</sub> B<sub>18</sub> Co<sub>1</sub><sup>1-</sup>),0.5n(C<sub>1</sub> H<sub>4</sub> O<sub>1</sub>)

**Compound Name:** catena-(tetrakis(μ<sub>2</sub>-4,4'-Bipyridine-N,N'-dioxido)-europium(iii) tris(bis(η<sup>5</sup>-7,8-dicarba-nido-undecaborate(11))-cobalt) methanol solvate clathrate)

**Space Group:** P21212 **Cell:** a 17.425(0) b 18.635(0) c 13.202(0)  
**Space Group No.:** 18 **(Å, °)** α 90.00 β 90.00 γ 90.00

**R-Factor (%):** 0.00 **Temperature(K):** 295 **Density(g/cm<sup>3</sup>):** 1.466



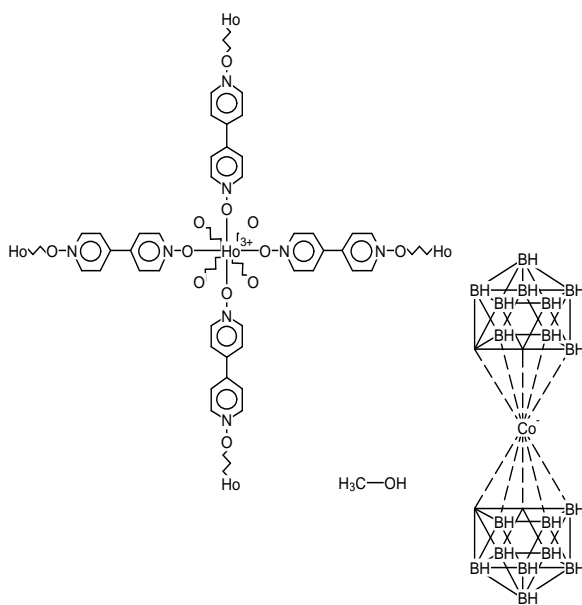
**Reference:** De-Liang Long, A.J.Blake, N.R.Champness, C.Wilson, M.Schroder (2001) *Angew.Chem.,Int.Ed.* **40**,2444

**Formula:** (C<sub>40</sub> H<sub>32</sub> Ho<sub>1</sub> N<sub>8</sub> O<sub>8</sub><sup>3+</sup>)n,3n(C<sub>4</sub> H<sub>22</sub> B<sub>18</sub> Co<sub>1</sub><sup>1-</sup>),0.5n(C<sub>1</sub> H<sub>4</sub> O<sub>1</sub>)

**Compound Name:** catena-(tetrakis(μ<sub>2</sub>-4,4'-Bipyridine-N,N'-dioxido)-holmium(iii) tris(bis(η<sup>5</sup>-7,8-dicarba-nido-undecaborate(11))-cobalt) methanol solvate clathrate)

**Space Group:** P21212 **Cell:** a 17.363(7) b 18.715(5) c 13.184(5)  
**Space Group No.:** 18 **(Å, °)** α 90.00 β 90.00 γ 90.00

**R-Factor (%):** 0.00 **Temperature(K):** 295 **Density(g/cm<sup>3</sup>):** 1.477



## ICIFEF

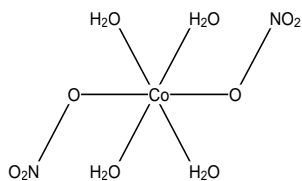
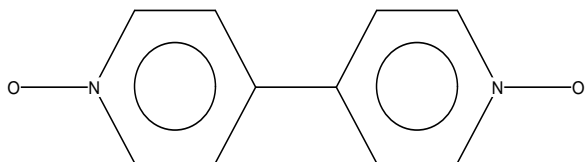
**Reference:** A.J.Blake, M.T.Brett, N.R.Champness, A.N.Khlobystov, De-Liang Long, C.Wilson, M.Schroder (2001) *Chem.Comm.* ,2258

**Formula:** 2(C<sub>10</sub> H<sub>8</sub> N<sub>2</sub> O<sub>2</sub>),H<sub>8</sub> Co<sub>1</sub> N<sub>4</sub> O<sub>10</sub>

**Compound Name:** bis(4,4'-Bipyridine N,N'-dioxide) tetra-aqua-bis(nitrato-O)-cobalt(ii)

**Space Group:** I41/a **Cell:** a 19.331(1) b 19.331(1) c 13.469(0)  
**Space Group No.:** 88 **(Å, °)** α 90.00 β 90.00 γ 90.00

**R-Factor (%):** 2.76 **Temperature(K):** 150 **Density(g/cm<sup>3</sup>):** 1.666



## ICIFUJ

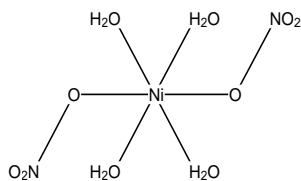
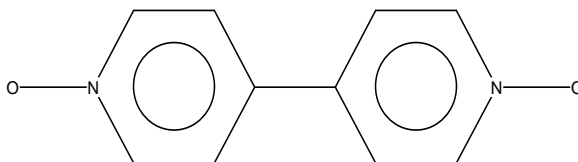
**Reference:** A.J.Blake, M.T.Brett, N.R.Champness, A.N.Khlobystov, De-Liang Long, C.Wilson, M.Schroder (2001) *Chem.Comm.* ,2258

**Formula:** 2(C<sub>10</sub> H<sub>8</sub> N<sub>2</sub> O<sub>2</sub>),H<sub>8</sub> Ni<sub>1</sub> O<sub>10</sub>

**Compound Name:** bis(4,4'-Bipyridine N,N'-dioxide) tetra-aqua-bis(nitrato-O)-nickel(ii)

**Space Group:** I41cd **Cell:** a 19.309(1) b 19.309(1) c 13.427(0)  
**Space Group No.:** 110 **(Å, °)** α 90.00 β 90.00 γ 90.00

**R-Factor (%):** 2.46 **Temperature(K):** 150 **Density(g/cm<sup>3</sup>):** 1.675



# Search: search4 (Wed Aug 20 12:01:40 2008): Hits 33-36

Supplementary Material (ESI) for New Journal of Chemistry  
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ICIFOP

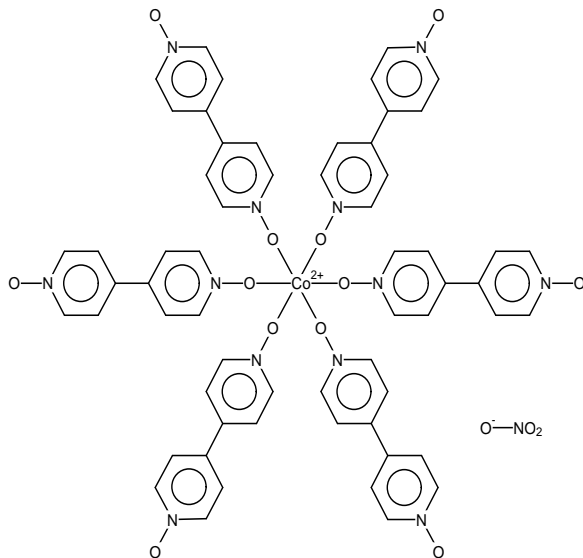
**Reference:** A.J.Blake, M.T.Brett, N.R.Champness, A.N.Khlobystov, De-Liang Long, C.Wilson, M.Schroder (2001) *Chem.Commun.* ,2258

**Formula:** C<sub>60</sub> H<sub>48</sub> Co<sub>1</sub> N<sub>12</sub> O<sub>12</sub> 2<sup>+</sup>, 2(N<sub>1</sub> O<sub>3</sub> 1<sup>-</sup>)

**Compound Name:** hexakis(4,4'-Bipyridine N,N'-dioxide-O)-cobalt(ii) dinitrate

**Space Group:** P-1 **Cell:** a 8.945(0) b 11.716(1) c 14.073(1)  
**Space Group No.:** 2 **(Å, °)** α 104.71(0) β 96.80(0) γ 98.23(0)

**R-Factor (%):** 4.20 **Temperature(K):** 298 **Density(g/cm<sup>3</sup>):** 1.564



## IXEDIY

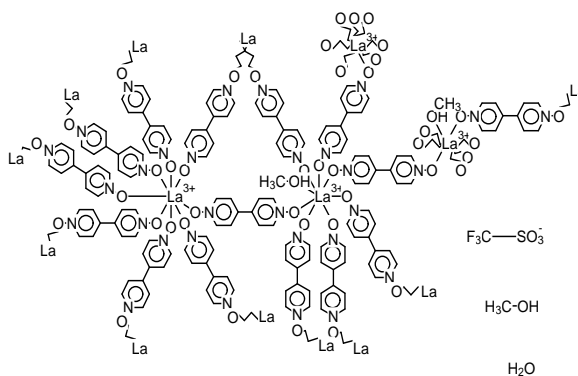
**Reference:** De-Liang Long, R.J.Hill, A.J.Blake, N.R.Champness, P.Hubberstey, D.M.Proserpio, C.Wilson, M.Schroder (2004) *Angew.Chem.,Int.Ed.* ,43,1851

**Formula:** (C<sub>152</sub> H<sub>128</sub> La<sub>4</sub> N<sub>30</sub> O<sub>32</sub> 12<sup>+</sup>)n, 12n(C<sub>1</sub> F<sub>3</sub> O<sub>3</sub> S<sub>1</sub> 1<sup>-</sup>), 4n(C<sub>1</sub> H<sub>4</sub> O<sub>1</sub>), 7.2n(H<sub>2</sub> O)

**Compound Name:** catena-(pentadecakis(μ<sub>2</sub>-4,4'-Bipyridine N,N'-dioxide-O,O')-bis(methanol)-tetra-lanthanum(iii) dodecakis(trifluoromethanesulfonate) methanol solvate hydrate)

**Space Group:** P-1 **Cell:** a 16.932(1) b 18.509(1) c 18.771(1)  
**Space Group No.:** 2 **(Å, °)** α 90.06(0) β 111.53(0) γ 102.21(0)

**R-Factor (%):** 6.20 **Temperature(K):** 150 **Density(g/cm<sup>3</sup>):** 1.711



## IXEDOE

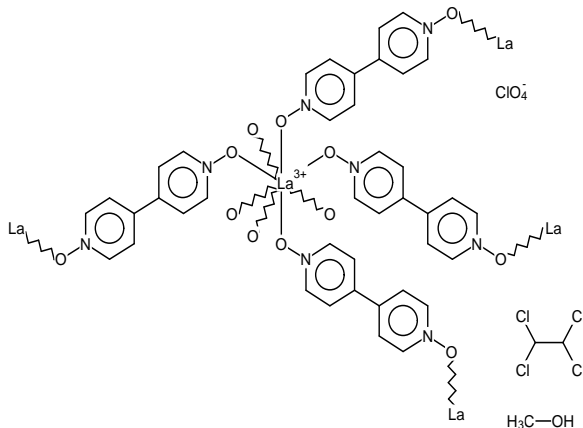
**Reference:** De-Liang Long, R.J.Hill, A.J.Blake, N.R.Champness, P.Hubberstey, D.M.Proserpio, C.Wilson, M.Schroder (2004) *Angew.Chem.,Int.Ed.* ,43,1851

**Formula:** (C<sub>40</sub> H<sub>32</sub> La<sub>1</sub> N<sub>8</sub> O<sub>8</sub> 3<sup>+</sup>)n, 3n(Cl<sub>1</sub> O<sub>4</sub> 1<sup>-</sup>), 4n(C<sub>2</sub> H<sub>2</sub> Cl<sub>4</sub>), n(C<sub>1</sub> H<sub>4</sub> O<sub>1</sub>)

**Compound Name:** catena-(tetrakis(μ<sub>2</sub>-4,4'-Bipyridine N,N'-dioxide-O,O')-lanthanum(iii) triperchlorate 1,1,2,2-tetrachloroethane methanol solvate)

**Space Group:** Cc **Cell:** a 13.520(2) b 22.575(3) c 23.688(3)  
**Space Group No.:** 9 **(Å, °)** α 90.00 β 103.92(0) γ 90.00

**R-Factor (%):** 4.40 **Temperature(K):** 150 **Density(g/cm<sup>3</sup>):** 1.792



## IXEDUK

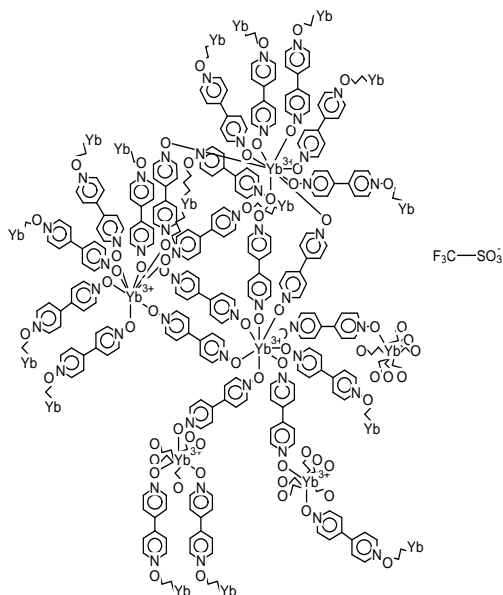
**Reference:** De-Liang Long, R.J.Hill, A.J.Blake, N.R.Champness, P.Hubberstey, D.M.Proserpio, C.Wilson, M.Schroder (2004) *Angew.Chem.,Int.Ed.* ,43,1851

**Formula:** (C<sub>240</sub> H<sub>192</sub> N<sub>48</sub> O<sub>48</sub> Yb<sub>6</sub> 18<sup>+</sup>)n, 18n(C<sub>1</sub> F<sub>3</sub> O<sub>3</sub> S<sub>1</sub> 1<sup>-</sup>)

**Compound Name:** catena-(tetracosakis(μ<sub>2</sub>-4,4'-Bipyridine N,N'-dioxide-O,O')-hexa-ytterbium(iii) octadecakis(trifluoromethanesulfonate) unknown solvate)

**Space Group:** P-1 **Cell:** a 24.046(0) b 24.157(0) c 24.383(0)  
**Space Group No.:** 2 **(Å, °)** α 83.86(0) β 61.84(0) γ 61.70(0)

**R-Factor (%):** 10.30 **Temperature(K):** 150 **Density(g/cm<sup>3</sup>):** 1.258



# Search: search4 (Wed Aug 20 12:01:40 2008): Hits 37-40

Supplementary Material (ESI) for New Journal of Chemistry  
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The Centre National de la Recherche Scientifique, 2008  
IXEFAS

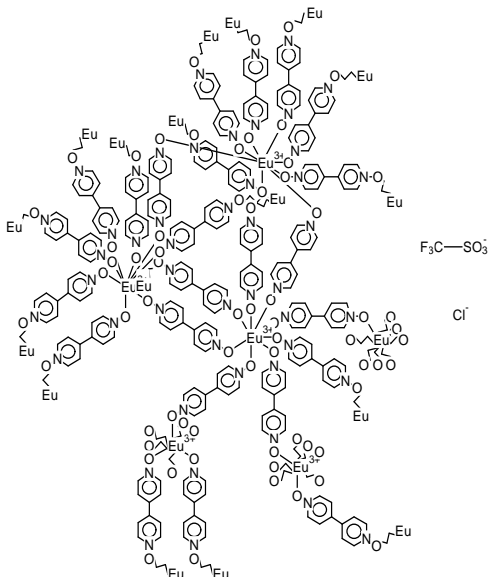
**Reference:** De-Liang Long, R.J.Hill, A.J.Blake, N.R.Champness, P.Hubberstey, D.M.Proserpio, C.Wilson, M.Schroder (2004) *Angew.Chem.,Int.Ed.*, **43**,1851

**Formula:** (C<sub>240</sub> H<sub>192</sub> Eu<sub>6</sub> N<sub>48</sub> O<sub>48</sub><sup>18+</sup>)<sub>n</sub>.8n(C<sub>1</sub> F<sub>3</sub> O<sub>3</sub> S<sub>1</sub><sup>1-</sup>).10n(Cl<sub>1</sub><sup>1-</sup>)

**Compound Name:** catena-(tetracosakis(μ<sub>2</sub>-4,4'-Bipyridine N,N'-dioxide-O,O')-hexa-europium(iii) octakis(trifluoromethanesulfonate) decachloride unknown solvate)

**Space Group:** P-1 **Cell:** a 24.141(1) b 24.303(1) c 24.471(1)  
**Space Group No.:** 2 **(Å, °)** α 84.43(0) β 61.74(0) γ 61.49(0)

**R-Factor (%):** 10.70 **Temperature(K):** 150 **Density(g/cm<sup>3</sup>):** 1.057



## JAPQIB

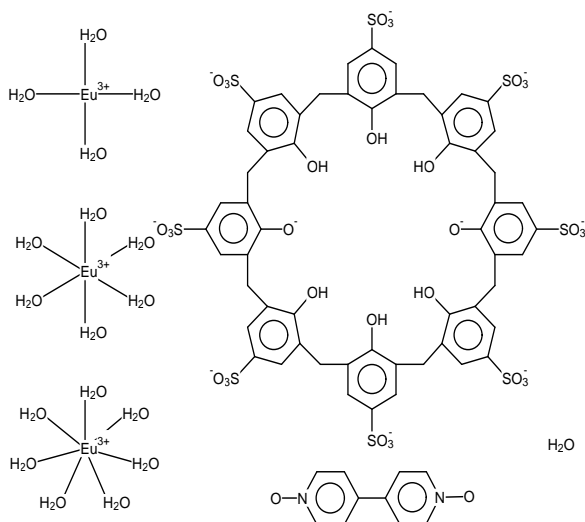
**Reference:** S.J.Dalgarno, M.J.Hardie, J.L.Atwood, J.E.Warren, C.L.Raston (2005) *New J.Chem.*, **29**,649

**Formula:** (H<sub>8</sub> Eu<sub>1</sub> O<sub>4</sub><sup>3+</sup>)<sub>2n</sub>.n(H<sub>12</sub> Eu<sub>1</sub> O<sub>6</sub><sup>3+</sup>).0.33n(H<sub>14</sub> Eu<sub>1</sub> O<sub>7</sub><sup>3+</sup>).n(C<sub>56</sub> H<sub>38</sub> O<sub>32</sub> S<sub>8</sub><sup>10-</sup>).6n(C<sub>10</sub> H<sub>8</sub> N<sub>2</sub> O<sub>2</sub>).8n(H<sub>2</sub>O)

**Compound Name:** catena-(bis(Tetra-aqua-europium) hexa-aqua-europium hepta-aqua-europium 50,51,52,54,55,56-hexahydroxy-49,53-dioxycalix(8)arene-5,11,17,23,29,35,41,47-octasulfonate hexakis(4,4'-bipyridine-N,N'-dioxide) octahydrate)

**Space Group:** P-1 **Cell:** a 16.994(0) b 22.113(1) c 23.009(1)  
**Space Group No.:** 2 **(Å, °)** α 69.12(0) β 69.42(0) γ 71.42(0)

**R-Factor (%):** 6.99 **Temperature(K):** 123 **Density(g/cm<sup>3</sup>):** 1.600



## LAWLAX

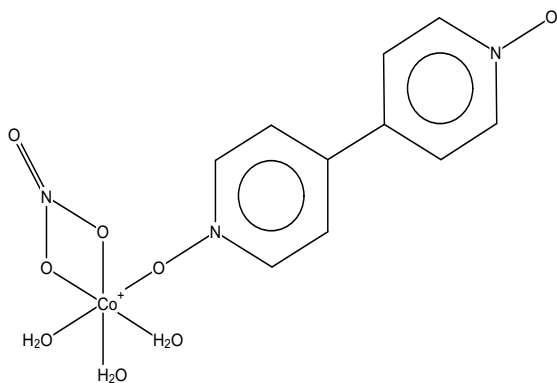
**Reference:** S.A.Bourne, L.J.Moitsheki (2005) *CrystEngComm*, **7**,674

**Formula:** C<sub>10</sub> H<sub>8</sub> N<sub>2</sub> O<sub>2</sub>.C<sub>10</sub> H<sub>14</sub> Co<sub>1</sub> N<sub>3</sub> O<sub>8</sub><sup>1+</sup>.N<sub>1</sub> O<sub>3</sub><sup>1-</sup>.H<sub>2</sub> O<sub>1</sub>

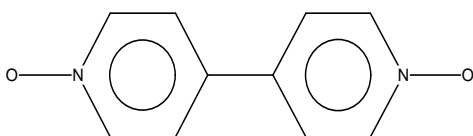
**Compound Name:** (4,4'-bipyridine-N,N'-dioxide-O)-triaqua-(nitrate-O,O')-cobalt(ii) nitrate (4,4'-bipyridine-N,N'-dioxide) monohydrate

**Space Group:** P-1 **Cell:** a 7.814(0) b 9.913(0) c 17.186(0)  
**Space Group No.:** 2 **(Å, °)** α 78.61(0) β 83.46(0) γ 85.61(0)

**R-Factor (%):** 7.04 **Temperature(K):** 298 **Density(g/cm<sup>3</sup>):** 1.620



O<sub>2</sub>N—O<sup>-</sup> H<sub>2</sub>O



## LAWLAX01

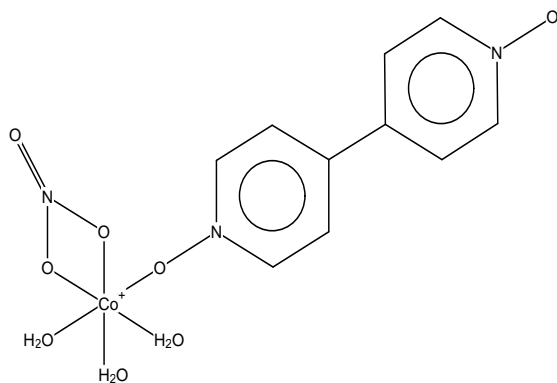
**Reference:** S.A.Bourne, L.J.Moitsheki (2005) *CrystEngComm*, **7**,674

**Formula:** C<sub>10</sub> H<sub>8</sub> N<sub>2</sub> O<sub>2</sub>.C<sub>10</sub> H<sub>14</sub> Co<sub>1</sub> N<sub>3</sub> O<sub>8</sub><sup>1+</sup>.N<sub>1</sub> O<sub>3</sub><sup>1-</sup>.H<sub>2</sub> O<sub>1</sub>

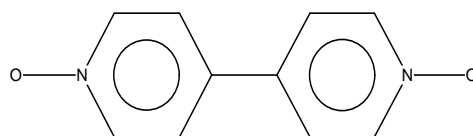
**Compound Name:** (4,4'-bipyridine-N,N'-dioxide-O)-triaqua-(nitrate-O,O')-cobalt(ii) nitrate (4,4'-bipyridine-N,N'-dioxide) monohydrate

**Space Group:** P-1 **Cell:** a 12.129(2) b 12.907(3) c 17.896(4)  
**Space Group No.:** 2 **(Å, °)** α 77.49(3) β 70.25(3) γ 76.28(3)

**R-Factor (%):** 4.12 **Temperature(K):** 113 **Density(g/cm<sup>3</sup>):** 1.656



O<sub>2</sub>N—O<sup>-</sup> H<sub>2</sub>O



# Search: search4 (Wed Aug 20 12:01:40 2008): Hits 41-44

Supplementary Material (ESI) for New Journal of Chemistry  
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LEQVUZ

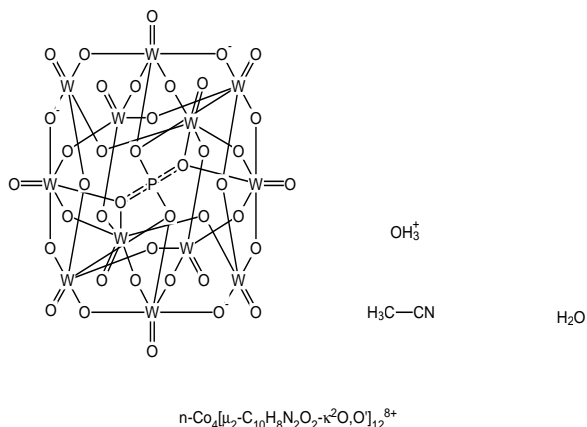
**Reference:** Meilin Wei, Cheng He, Weijie Hua, Chunying Duan, Shuhua Li, Qingjin Meng (2006) *J. Am. Chem. Soc.*, **128**, 13318

**Formula:**  $(C_{120}H_{96}Co_4N_{24}O_{24}^{8+})n, 3n(O_{40}P_1W_{12}^{3-}), n(H_3O_1^{1+}), 26n(H_2O_1), 12n(C_2H_4N_2O_2)$

**Compound Name:** catena-(docosakis( $\mu_2$ -4,4'-bipyridine-N,N'-dioxide)-tetra-cobalt hydroxonium tris( $\mu_2$ -phosphato)-tetracosakis( $\mu_2$ -oxo)-dodecaoxo-dodeca-tungsten) acetonitrile solvate hydrate

**Space Group:** Im-3 **Cell:** a 23.162(2) b 23.162(2) c 23.162(2)  
**Space Group No.:** 204 **(Å, °)**  $\alpha$  90.00  $\beta$  90.00  $\gamma$  90.00

**R-Factor (%):** 4.30 **Temperature(K):** 123 **Density(g/cm<sup>3</sup>):** 3.235



## LICQOE

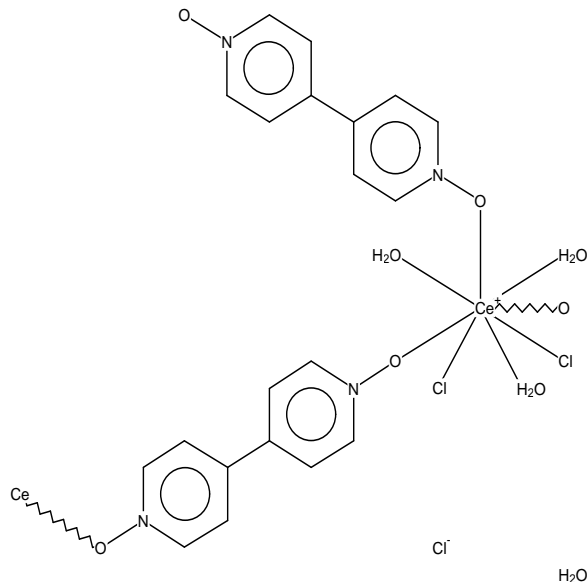
**Reference:** Da-Qiang Yuan, Fen-Yan Lian, Mao-Chun Hong (2007) *Acta Crystallogr., Sect. E: Struct. Rep. Online*, **63**, m1430

**Formula:**  $(C_{20}H_{22}Ce_1Cl_2N_4O_7^{1+})n, n(Cl_1^{1-}), n(H_2O_1)$

**Compound Name:** catena-[( $\mu_2$ -4,4'-Bipyridine N,N'-dioxide- $x^2O:O$ )-triaqua-(4,4'-bipyridine N,N'-dioxide- $xO$ )-dichloro-cerium(iii) chloride monohydrate]

**Space Group:** P-1 **Cell:** a 8.668(0) b 10.458(0) c 14.786(0)  
**Space Group No.:** 2 **(Å, °)**  $\alpha$  83.36(0)  $\beta$  73.03(0)  $\gamma$  86.19(0)

**R-Factor (%):** 3.26 **Temperature(K):** 293 **Density(g/cm<sup>3</sup>):** 1.813



## PALYEH

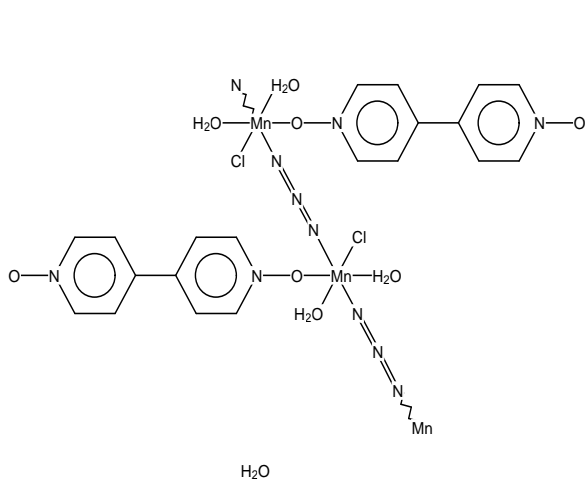
**Reference:** A.K.Ghosh, D.Ghoshal, E.Zangrando, J.Ribas, N.R.Chaudhuri (2005) *Inorg. Chem.*, **44**, 1786

**Formula:**  $(C_{20}H_{24}Cl_2Mn_2N_{10}O_8)n, 2n(H_2O_1)$

**Compound Name:** catena-(bis( $\mu_2$ -1,3-Azido)-bis(4,4'-bipyridine-N,N'-dioxide)-dichloro-tetraaqua-di-manganese(ii) dihydrate)

**Space Group:** P-1 **Cell:** a 7.060(3) b 10.345(3) c 11.697(4)  
**Space Group No.:** 2 **(Å, °)**  $\alpha$  106.86(2)  $\beta$  113.33(2)  $\gamma$  96.39(3)

**R-Factor (%):** 6.17 **Temperature(K):** 293 **Density(g/cm<sup>3</sup>):** 1.715



## QEHFEO

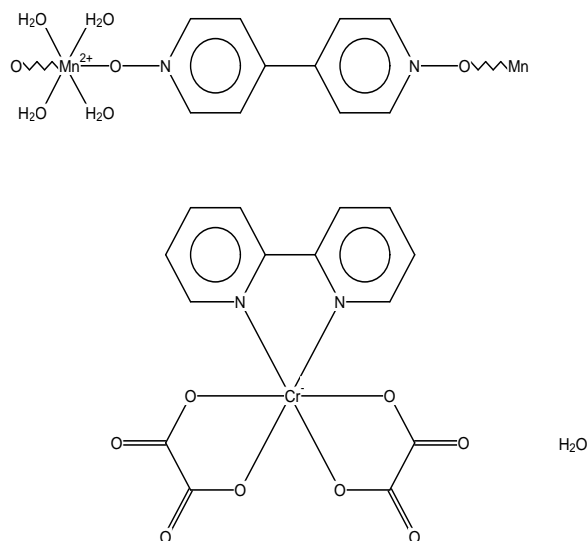
**Reference:** S.Bruda, M.Andruh, H.W.Roesky, Y.Journaux, M.Noltemeyer, E.Riviere (2001) *Inorg. Chem. Commun.*, **4**, 1111

**Formula:**  $(C_{10}H_{16}Mn_1N_2O_6^{2+})n, 2n(C_{14}H_8Cr_1N_2O_8^{1-}), 8n(H_2O_1)$

**Compound Name:** catena-( $\mu_2$ -4,4'-Bipyridyl-N,N'-dioxide)-tetraaqua-manganese(ii) bis((2,2'-bipyridyl)-bis(oxalato)-chromium(iii) octahydrate)

**Space Group:** P21 **Cell:** a 10.870(2) b 13.248(4) c 17.804(6)  
**Space Group No.:** 4 **(Å, °)**  $\alpha$  90.00  $\beta$  102.91(3)  $\gamma$  90.00

**R-Factor (%):** 3.94 **Temperature(K):** 295 **Density(g/cm<sup>3</sup>):** 1.632



# Search: search4 (Wed Aug 20 12:01:40 2008): Hits 45-48

Supplementary Material (ESI) for New Journal of Chemistry  
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QIBTAW

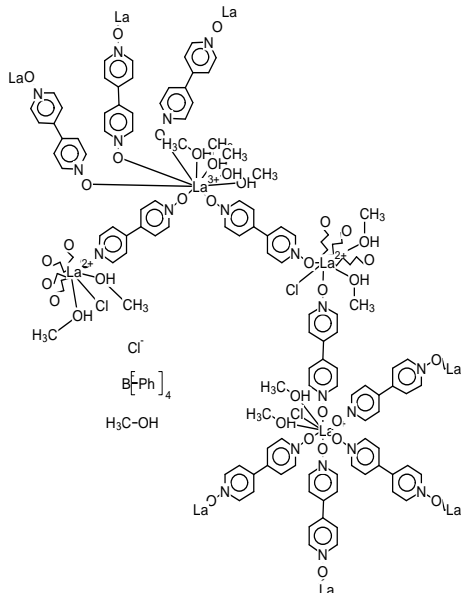
**Reference:** D.-L.Long, A.J.Blake, N.R.Champness, C.Wilson, M.Schroder (2001) *J.Am.Chem.Soc.*, **123**,3401

**Formula:** (C<sub>110</sub> H<sub>120</sub> Cl<sub>3</sub> La<sub>4</sub> N<sub>20</sub> O<sub>30</sub> 9<sup>+</sup>)n,n(C<sub>1</sub> 1<sup>-</sup>),8n(C<sub>24</sub> H<sub>20</sub> B<sub>1</sub> 1<sup>-</sup>),22n(C<sub>1</sub> H<sub>4</sub> O<sub>1</sub>)

**Compound Name:** catena-(decakis(μ<sub>2</sub>-4,4'-Bipyridine-N,N'-dioxide)-decakis(methanol)-trichloro-tetra-lanthanum(iii) chloride octakis(tetraphenylborate) methanol solvate)

**Space Group:** Pc **Cell:** a 15.134(3) b 47.621(8) c 22.431(4)  
**Space Group No.:** 7 **(Å, °)** α 90.00 β 91.95(0) γ 90.00

**R-Factor (%):** 9.10 **Temperature(K):** 150 **Density(g/cm<sup>3</sup>):** 1.266



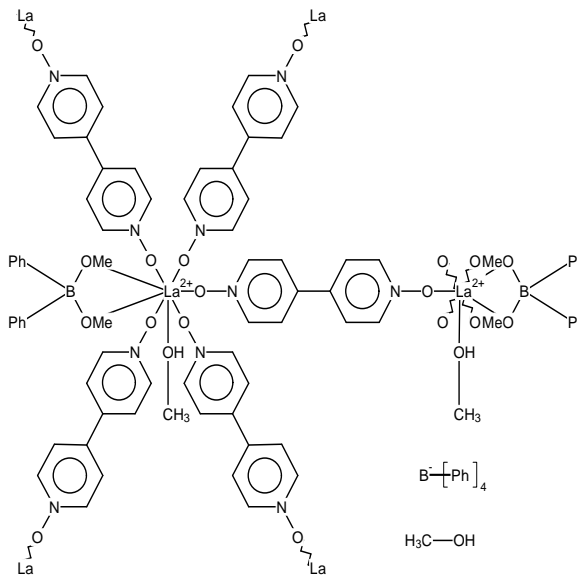
**Reference:** D.-L.Long, A.J.Blake, N.R.Champness, C.Wilson, M.Schroder (2001) *J.Am.Chem.Soc.*, **123**,3401

**Formula:** (C<sub>80</sub> H<sub>80</sub> B<sub>2</sub> La<sub>2</sub> N<sub>10</sub> O<sub>16</sub> 4<sup>+</sup>)n,4n(C<sub>24</sub> H<sub>20</sub> B<sub>1</sub> 1<sup>-</sup>),9n(C<sub>1</sub> H<sub>4</sub> O<sub>1</sub>)

**Compound Name:** catena-(pentakis(μ<sub>2</sub>-4,4'-Bipyridine-N,N'-dioxide)-bis(diphenyldimethoxyborate)-bis(methanol)-di-lanthanum(iii) tetrakis(tetraphenylborate) methanol solvate)

**Space Group:** Pbcn **Cell:** a 48.422(7) b 21.958(3) c 15.814(2)  
**Space Group No.:** 60 **(Å, °)** α 90.00 β 90.00 γ 90.00

**R-Factor (%):** 8.10 **Temperature(K):** 150 **Density(g/cm<sup>3</sup>):** 1.305



**QOZKEV**

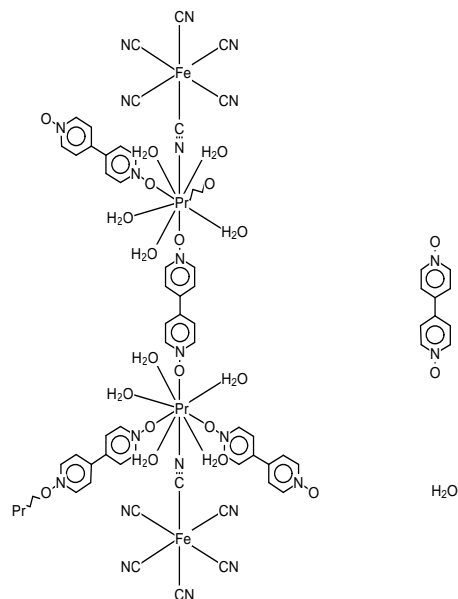
**Reference:** S.Tanase, M.Andruh, A.Muller, M.Schmidtman, C.Mathoniere, G.Rombaut (2001) *Chem.Comm.*, 1084

**Formula:** (C<sub>52</sub> H<sub>52</sub> Fe<sub>2</sub> N<sub>20</sub> O<sub>18</sub> Pr<sub>2</sub>)n,n(C<sub>10</sub> H<sub>8</sub> N<sub>2</sub> O<sub>2</sub>),8n(H<sub>2</sub> O<sub>1</sub>)

**Compound Name:** catena-(bis((μ<sub>2</sub>-4,4'-Bipyridyl N,N'-dioxide)-(μ<sub>2</sub>-cyanido)-penta-aqua-(4,4'-bipyridyl N,N'-dioxide)-pentacyano-iron(iii)-praseodymium(iii)) 4,4'-bipyridyl N,N'-dioxide octahydrate)

**Space Group:** P-1 **Cell:** a 8.361(0) b 15.439(0) c 15.492(0)  
**Space Group No.:** 2 **(Å, °)** α 84.78(0) β 80.67(0) γ 85.66(0)

**R-Factor (%):** 2.36 **Temperature(K):** 183 **Density(g/cm<sup>3</sup>):** 1.669



**QOZKIZ**

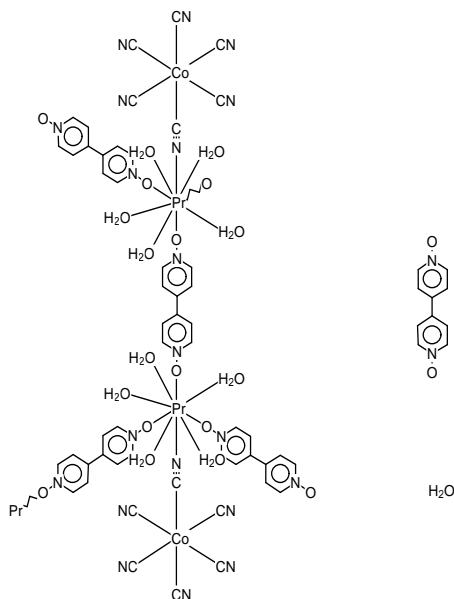
**Reference:** S.Tanase, M.Andruh, A.Muller, M.Schmidtman, C.Mathoniere, G.Rombaut (2001) *Chem.Comm.*, 1084

**Formula:** (C<sub>52</sub> H<sub>52</sub> Co<sub>2</sub> N<sub>20</sub> O<sub>18</sub> Pr<sub>2</sub>)n,n(C<sub>10</sub> H<sub>8</sub> N<sub>2</sub> O<sub>2</sub>),8n(H<sub>2</sub> O<sub>1</sub>)

**Compound Name:** catena-(bis((μ<sub>2</sub>-4,4'-Bipyridyl N,N'-dioxide)-(μ<sub>2</sub>-cyanido)-penta-aqua-(4,4'-bipyridyl N,N'-dioxide)-pentacyano-cobalt(iii)-praseodymium(iii)) 4,4'-bipyridyl N,N'-dioxide octahydrate)

**Space Group:** P-1 **Cell:** a 8.375 b 15.410 c 15.420  
**Space Group No.:** 2 **(Å, °)** α 84.88 β 80.66 γ 85.63

**R-Factor (%):** 0.00 **Temperature(K):** 295 **Density(g/cm<sup>3</sup>):** 1.682



# Search: search4 (Wed Aug 20 12:01:40 2008): Hits 49-52

Supplementary Material (ESI) for New Journal of Chemistry  
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RAXMUZ01

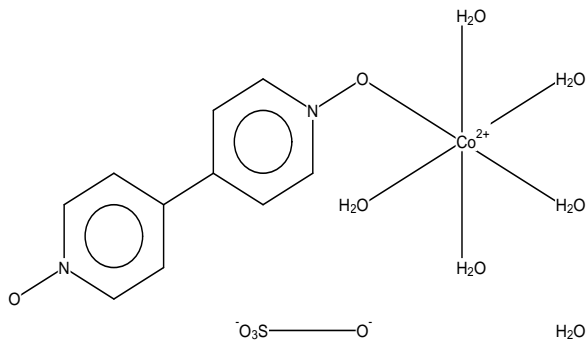
**Reference:** D.G.Mantero, A.Neels, H.Stoeckli-Evans (2006)  
*Inorg.Chem.* **45**,3287

**Formula:**  $C_{10}H_{18}Co_1N_2O_7^{2+} \cdot O_4S_1^{2-} \cdot 2(H_2O_1)$

**Compound Name:** penta-aqua-(4,4'-bipyridine-N,N'-dioxide-O)-cobalt(II) sulfate dihydrate

**Space Group:** P21/n **Cell:** a 7.137(1) b 25.432(2) c 10.226(1)  
**Space Group No.:** 14 **(Å, °)** α 90.00 β 92.59(1) γ 90.00

**R-Factor (%):** 3.32 **Temperature(K):** 253 **Density(g/cm³):** 1.681



## WEHPEF

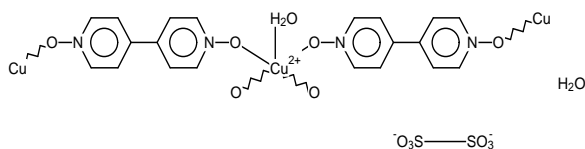
**Reference:** D.G.Mantero, A.Neels, H.Stoeckli-Evans (2006)  
*Inorg.Chem.* **45**,3287

**Formula:**  $(C_{20}H_{18}Cu_1N_4O_5^{2+})_n \cdot n(H_2O_1) \cdot n(O_6S_2^{2-})$

**Compound Name:** catena-(bis(μ₂-4,4'-bipyridine-N,N'-dioxide-O,O')-aqua-copper(II) dithionate monohydrate)

**Space Group:** P21/n **Cell:** a 9.772(0) b 9.838(0) c 11.991(1)  
**Space Group No.:** 13 **(Å, °)** α 90.00 β 90.77(0) γ 90.00

**R-Factor (%):** 2.71 **Temperature(K):** 173 **Density(g/cm³):** 1.833



## WEHPIJ

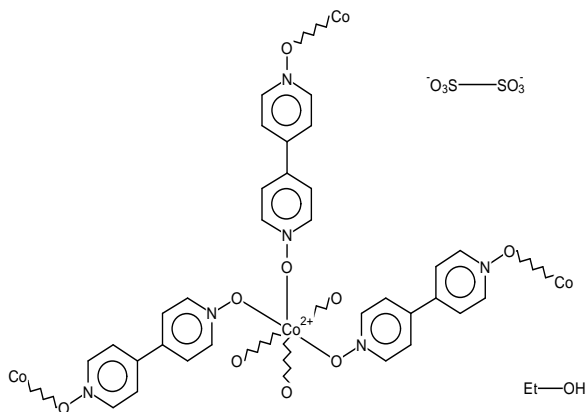
**Reference:** D.G.Mantero, A.Neels, H.Stoeckli-Evans (2006)  
*Inorg.Chem.* **45**,3287

**Formula:**  $(C_{30}H_{24}Co_1N_6O_6^{2+})_n \cdot n(O_6S_2^{2-}) \cdot 7n(C_2H_6O_1)$

**Compound Name:** catena-(tris(μ₂-4,4'-bipyridine-N,N'-dioxide-O,O')-cobalt(II) dithionate ethanol solvate)

**Space Group:** C2/c **Cell:** a 20.681(4) b 14.135(1) c 19.564(4)  
**Space Group No.:** 15 **(Å, °)** α 90.00 β 107.48(1) γ 90.00

**R-Factor (%):** 5.61 **Temperature(K):** 253 **Density(g/cm³):** 1.347



## WEHPOP

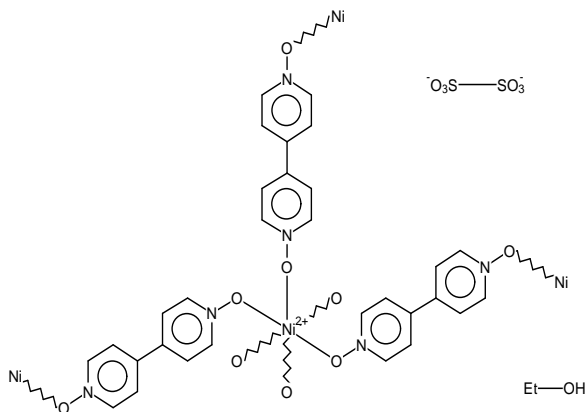
**Reference:** D.G.Mantero, A.Neels, H.Stoeckli-Evans (2006)  
*Inorg.Chem.* **45**,3287

**Formula:**  $(C_{30}H_{24}Ni_1O_6^{2+})_n \cdot n(O_6S_2^{2-}) \cdot 7n(C_2H_6O_1)$

**Compound Name:** catena-(tris(μ₂-4,4'-bipyridine-N,N'-dioxide-O,O')-nickel(II) dithionate ethanol solvate)

**Space Group:** C2/c **Cell:** a 20.828(5) b 13.499(4) c 20.020(5)  
**Space Group No.:** 15 **(Å, °)** α 90.00 β 106.18(1) γ 90.00

**R-Factor (%):** 14.96 **Temperature(K):** 253 **Density(g/cm³):** 1.359



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WEHPUV

**Reference:** D.G.Mantero, A.Neels, H.Stoeckli-Evans (2006)  
*Inorg.Chem.* **45**,3287

**Formula:** C<sub>10</sub> H<sub>18</sub> N<sub>2</sub> Ni<sub>1</sub> O<sub>7</sub> 2<sup>+</sup>·O<sub>4</sub> S<sub>1</sub> 2<sup>-</sup>·2(H<sub>2</sub> O<sub>1</sub>)

**Compound Name:** penta-aqua-(4,4'-bipyridine-N,N'-dioxide-O)-nickel(ii) sulfate dihydrate

**Space Group:** P2<sub>1</sub>/n **Cell:** **a** 7.138(0) **b** 25.244(3) **c** 10.211(1)  
**Space Group No.:** 14 **(Å, °)** **α** 90.00 **β** 92.17(0) **γ** 90.00

**R-Factor (%):** 3.14 **Temperature(K):** 253 **Density(g/cm<sup>3</sup>):** 1.695

