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:

Query 1

Query 2

4M
Reference:

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)

Compound Name:
catena-((\mu_2-N,N\text{-bis(4-Pyridylmethyl)butane-1,4-diammonium})-tetra-aqua-cobalt(ii))-(cucurbituril)-polyrotaxane tetranitrate tridecahydrate

Space Group:
P21/c

Space Group No.:
14

Cell:
\begin{align*}
a & = 12.446(0) \\
\beta & = 21.324(0) \\
c & = 29.040(0)
\end{align*}

R-Factor (%)
7.98

Temperature(K)
293

Density(g/cm$^3$)
1.623

Formula: \((C_{36}H_{36}N_{24}O_{12})_n,n(C_{16}H_{32}N_{4}NiO_{4}^{4+}),4n(N_1O_3^{-}),13n(H_2O)\)

Compound Name: catena-((\(\mu_2-N,N'\)-bis(4-Pyridylmethyl)butane-1,4-diammonium)-tetr aqua-nickel(ii))-(cucurbituril)-polyrotaxane tetranitrate tridecahydrate)

Space Group: P21/c  
Cell: \(a = 12.430(3) \text{ Å}, b = 21.318(4) \text{ Å}, c = 29.012(6) \text{ Å}\)

Space Group No.: 14  
\(\alpha = 90.00^\circ, \beta = 91.80(3)^\circ, \gamma = 90.00^\circ\)

R-Factor (%): 9.45  
Temperature(K): 293  
Density(g/cm\(^3\)): 1.627

**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})^{-},40n(H_{2}O)

**Compound Name:** catena(μ₂-tris(N,N'-bis(4-Pyridylmethyl)-1,4-diaminobutane)-di-nitrato-di-silver tris(cucurbituril) hexanitrate hydrate)

**Space Group:** Cmca  
**Cell:** 
\[ a = 31.408(3) \text{ Å}, \quad b = 32.508(4) \text{ Å}, \quad c = 22.479(3) \text{ Å} \]  
**Space Group No.:** 64  
**R-Factor (%):** 11.81  
**Temperature(K):** 295  
**Density(g/cm³):** 1.516
REKHOE


Formula: \((C_{32}H_{48}Ag_2N_8^{6+})0.5n,n(C_{36}H_{36}N_{24}O_{12}),3n(C_7H_7O_3S_1^{1-}),11n(H_2O_1)\)

Compound Name: catena(\(\mu_2\)-N,N'-bis(4-Pyridylmethyl-1,4-diaminobutane)-silver cucurbituril tris(p-toluenesulfonate) undecahydrate)

Space Group: P-1

Space Group No.: 2

Cell: \(a\) 15.001(2) \(b\) 15.491(2) \(c\) 23.580(2)

Space Group No.: \(\alpha\) 91.90(1) \(\beta\) 105.54(0) \(\gamma\) 116.71(1)

R-Factor (%): 11.05

Temperature(K): 295

Density(g/cm\(^3\)): 1.495

SEWSES


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-}),87(H_{2}O)

Compound Name: (4)-tris([Cucurbituril]-([μ₂-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  
Space Group No.: 176  
Cell: a 26.707(0)  b 26.707(0)  c 23.365(0)

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

Formula: \( \text{C}_{54} \text{H}_{96} \text{N}_{18} \text{Pt}_{3}^{12+}, \text{C}_{36} \text{H}_{36} \text{N}_{24} \text{O}_{12}^{+}, \text{C}_{36} \text{H}_{36} \text{N}_{24} \text{O}_{12}^{+}, 12(\text{N}_{1} \text{O}_{3}^{1-}), 87(\text{H}_{2} \text{O}) \)

Compound Name: (4)-(tris((Cucurbituril)-(\(\mu_2\)-N,N'-bis(4-pyridylmethyl)-1,4-diammoniobutane)-(ethylenediamine)-platinum))-cyclic-oligorotaxane dodecanitrate hydrate

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

Space Group: P63/m
Space Group No.: 176
Cell: \(a = 26.707(0) \text{ Å}, b = 26.707(0) \text{ Å}, c = 23.365(0) \text{ Å}\)

Temperature(K): 188
Density(g/cm\(^3\)): 1.584

R-Factor (%): 9.57
TUBVUH


Formula: \((\text{C}_{36}\text{H}_{36}\text{N}_{24}\text{O}_{12})_{2n},n(\text{C}_{32}\text{H}_{60}\text{Cu}_{2}\text{N}_{8}\text{O}_{6}^{8+}),8n(\text{N}_{1}\text{O}_{3}^{-}),28n(\text{H}_{2}\text{O})\)

Compound Name: catena-((3)-bis(Cucurbituril)-(bis(\(\mu_2\cdot\text{N,N'-bis(4-pyridylmethyl)-1,4-
    diaminobutane}-\text{hexa-aqua-di-copper})\))-polyrotaxane octanitrate hydrate

Space Group: P-1

Space Group No.: 2

Cell:
\(a\) 14.690(2)  \(b\) 14.923(2)  \(c\) 19.665(3)

\(\alpha\) 84.96(1)  \(\beta\) 74.98(1)  \(\gamma\) 68.90

R-Factor (%): 10.04  Temperature(K): 295  Density(g/cm\(^3\)) 1.613
Search Overview

Search: search2
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:

<table>
<thead>
<tr>
<th>Query 1</th>
<th>Query 2</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1" alt="Query 1" /></td>
<td><img src="image2" alt="Query 2" /></td>
</tr>
</tbody>
</table>

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ADOFAA


Formula: \((\text{C}_{32}\text{H}_{64}\text{Co}_2\text{N}_8\text{O}_8^{8+})\_n, n(\text{C}_{36}\text{H}_{36}\text{N}_{24}\text{O}_{12}), n(\text{C}_{36}\text{H}_{36}\text{N}_{24}\text{O}_{12}), 8n(\text{N}_1\text{O}_3^{-1}), 30n(\text{H}_2\text{O})\)

Compound Name: catena-(cis-bis(\(\mu_2\)-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,°)  
\(\alpha\) 97.17(0)  
\(\beta\) 97.34(0)  
\(\gamma\) 115.94(0)

R-Factor (%): 7.42  
Temperature(K): 293  
Density(g/cm\(^3\)): 1.569

**Formula:** 
\[(C_{32}H_{64}N_8Ni_2O_8)^{8+}n,C_{36}H_{36}N_24O_{12})n(C_{36}H_{36}N_24O_{12}),8n(N_1O_3^{-})\cdot30n(H_2O)

**Compound Name:** catena-(cis-bis(\(\mu_2-N,N'\)-bis(3-Pyridylmethyl)butane-1,4-diammonium)-bis(tetra-aqua-nickel(ii))-bis(cucurbituril)-polyrotaxane octanitrate hydrate)

**Space Group:** P-1  
**Space Group No.:** 2

**Cell:**  
\[a = 14.168(0) \quad b = 14.551(0) \quad c = 21.545(0)\]

**Space Group No.:** 2  
\[\alpha = 99.05(0) \quad \beta = 94.68(0) \quad \gamma = 114.82\]

**R-Factor (%):** 13.22  
**Temperature(K):** 188  
**Density(g/cm\(^3\)):** 1.622
**Reference:**

**Formula:**
(C\(_{36}\)H\(_{36}\)N\(_{24}\)O\(_{12}\))\(_{2}\)n,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

**R-Factor (%):** 5.63

**Temperature(K):** 293

**Density(g/cm\(^3\)):** 1.642
ADOGEF


Formula: \((\text{C}_{36}\text{H}_{36}\text{N}_{24}\text{O}_{12})2n, n(\text{C}_{32}\text{H}_{50}\text{Cu}_{1}\text{N}_8\text{O}_1\text{Cu}^{2+})_6n(\text{N}_1\text{O}_3\text{Cu}^{2+})_3.5n(\text{H}_2\text{O})_1\)

Compound Name: catena-(bis(\(\mu_2\)-N,N'-bis(3-Pyridylmethyl)butane-1,4-diammonium)-aqua-copper(ii) bis(cucurbituril) polyrotaxane hexanitrate hydrate)

Space Group: P4/n  
Space Group No.: 85  
Cell: \(a 23.751(0)\) \(b 23.751(0)\) \(c 14.116(0)\)

R-Factor (%): 10.89  
Temperature(K): 170  
Density(g/cm\(^3\)): 1.425
XIGXIU


Formula: \( \text{C}_{36}\text{H}_{36}\text{N}_{24}\text{O}_{12}\cdot \text{C}_{72}\text{H}_{128}\text{N}_{24}\text{O}_{12}\cdot \text{Pt}_{4}^{16+}\cdot \text{C}_{36}\text{H}_{36}\text{N}_{24}\text{O}_{12}\cdot \text{C}_{36}\text{H}_{36}\text{N}_{24}\text{O}_{12}\cdot \text{C}_{36}\text{H}_{36}\text{N}_{24}\text{O}_{12}\cdot \text{Pt}_{4}^{16+}\cdot \text{C}_{36}\text{H}_{36}\text{N}_{24}\text{O}_{12}\cdot \text{C}_{36}\text{H}_{36}\text{N}_{24}\text{O}_{12}\cdot \text{C}_{36}\text{H}_{36}\text{N}_{24}\text{O}_{12}\cdot \text{Pt}_{4}^{16+} \)

Compound Name: (5)-(tetrakis((Cucurbituril)-\( \mu_{2}-N,N'\)-bis(3-pyridylmethyl)-1,4-diammoniobutane)-(ethylenediamine)-platinum))-cyclic-oligorotaxane hexadecanitrate ethanol solvate hydrate

Space Group: P21

Space Group No.: 4

Cell: \( a = 15.756(0) \) \( b = 26.462(0) \) \( c = 43.249(0) \)

\( \alpha = 90.00 \) \( \beta = 94.43(0) \) \( \gamma = 90.00 \)

R-Factor (%): 8.01

Temperature(K): 188

Density(g/cm\(^3\)): 1.574
Search Overview

Search: search3
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

Formula: \((\text{C}_{22}\text{H}_{14}\text{Co}_{1}\text{N}_{6}\text{O}_{10})_n\text{n(C}_1\text{H}_1\text{Cl}_3)\)

Compound Name: catena-\([\mu_2\text{-N,N'-bis(4-Pyridylmethyl) pyromellitic diimide-N,N'}\text{-bis(nitrato-O,O')-cobalt(ii) chloroform solvate}]\)

Space Group: C2/c  
Space Group No.: 15  
Cell: \(a \ 16.720(3) \quad b \ 17.232(3) \quad c \ 12.175(2)\)  
Space Group No.: 15  
\(\alpha \ 90.00 \quad \beta \ 128.90(0) \quad \gamma \ 90.00\)  

R-Factor (%): 6.93  
Temperature(K): 293  
Density(g/cm\(^3\)): 1.705

Formula: \((\text{C}_{66}\text{H}_{42}\text{Cd}_{2}\text{N}_{16}\text{O}_{24})\text{n}\cdot2\text{n(C}_{1}\text{H}_{1}\text{Cl}_{3})\)

Compound Name: catena-(tris(μ₂-N,N'-bis(4-Pyridylmethyl)pyromellitic diimide)-tetrakis(nitrato-O,O')-di-cadmium(ii) chloroform solvate)

Space Group: P-1  
Space Group No.: 2  
Cell: \(a = 11.012(1), b = 13.190(2), c = 13.934(2)\)  
Space Group No.: 2  
\(\alpha = 95.10(0), \beta = 106.14(0), \gamma = 99.00(0)\)  
R-Factor (%): 4.00  
Temperature(K): 298  
Density(g/cm\(^3\)): 1.665

RESHUT

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

Formula: \((\text{C}_{66}\text{H}_{42}\text{Hg}_{4}\text{I}_{8}\text{N}_{12}\text{O}_{12})\text{n}\)

Compound Name: catena-(bis(\(\mu_2\)-Iodo)-tris(\(\mu_2\)-N,N'-bis(4-pyridylmethyl)pyromellitic diimide-N,N')-octakis(iodo)-tetra-mercury)

Space Group: P-1

Cell:

\(\begin{array}{ccc}
\text{a} & 10.882(4) \\
\text{b} & 14.319(5) \\
\text{c} & 14.827(5)
\end{array}\)

Space Group No.: 2

\((\text{Å},°)\)

\(\begin{array}{ccc}
\text{α} & 62.90(0) \\
\text{β} & 89.98(0) \\
\text{γ} & 69.69(0)
\end{array}\)

R-Factor (%): 4.23

Temperature(K): 293

Density\((\text{g/cm}^3)\): 2.642

Formula: (C_{44}H_{28}Hg_{2}I_{4}N_{8}O_{8})n

Compound Name: catena-(bis(μ_{2}-2,6-bis(4-Pyridylmethyl)benzo(1,2-c:4,5-c')dipyrrrole-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/cm^3): 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**

4M

Formula: \((C_{26}H_{24}Cd_{1}N_{6}O_{6}^{2+})_{n},2n(Cl_{1}O_{4}^{1-})\)

Compound Name: catena-\(((\mu_{2}-N,N'-\text{bis}(3-\text{Pyridylmethyl})\text{pyromellitic di-imide}-N,N')\text{-bis(acetonitrile)}\text{-diaqua-cadmium diperchlorate})\)

Space Group: P21/c

Cell: 
\[
\begin{align*}
&a = 13.545(1) \\
b & = 8.135(1) \\
c & = 14.882(1) \\
\alpha & = 90.00 \\
\beta & = 95.57(0) \\
\gamma & = 90.00
\end{align*}
\]

Space Group No.: 14

R-Factor (%): 3.70

Temperature(K): 298

Density(g/cm³): 1.685

![Chemical structure diagram]
**FISCEQ**

**Reference:**  

**Formula:**  
\((C_{66}H_{50}N_{12}O_{16}Zn_{2}^{4+})_n4n(ClO_4^{-})_{2n}(C_2H_3N_1)\)

**Compound Name:**  
catena-(tris(\(\mu_2\)-N,N'-bis(3-Pyridylmethyl)pyromellitic di-imide-N,N')-tetra-aqua-di-zinc tetraperchlorate acetonitrile solvate)

**Space Group:**  
P-1  
**Cell:**  
\(a = 7.797(1) \text{ Å}, b = 8.706(1) \text{ Å}, c = 28.893(4) \text{ Å}\)

**Space Group No.:**  
2  
**\(\alpha\), \(\beta\), \(\gamma\):**  
\(\alpha = 81.94(0) ^\circ, \beta = 89.38(0) ^\circ, \gamma = 86.81(0) ^\circ\)

**R-Factor (%):**  
5.25  
**Temperature(K):**  
298  
**Density(g/cm^3):**  
1.608

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PALYIL


Formula: \((C_{66}H_{42}N_{16}O_{24}Zn_2)n,2n(C_1H_4O_1)\)

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

\(\alpha\) 90.00 \(\beta\) 103.43(0) \(\gamma\) 90.00

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

**Formula:** \((C_{66}H_{42}Cd_{2}N_{16}O_{24})_n, 2n(C_2H_6O_1)\)

**Compound Name:** catena-(tris\((\mu_2-N,N'\)-bis(3-Pyridylmethyl)pyromellitic diimide)-bis(nitrato-\(O\))-bis(nitrato-\(O,O'\))-di-cadmium(ii) ethanol solvate)

**Space Group:** P21/a  
**Space Group No.:** 14  
**Cell:** 
- \(a\) 15.403(1) Å  
- \(b\) 13.614(1) Å  
- \(c\) 17.400(2) Å  
- \(\alpha\) 90.00°  
- \(\beta\) 103.25(0)°  
- \(\gamma\) 90.00°  

**R-Factor (%):** 3.93  
**Temperature(K):** 293  
**Density(g/cm\(^3\)):** 1.646
PEVYUL

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

Formula: $(C_{22}H_{14}Hg_1I_2N_4O_4)n.0.4n(C_1H_4O_1)$

Compound Name: catena-$(\mu_2-N,N'-\text{bis(3-Pyridylmethyldiphthalic di-imide)})$-di-iodo-mercury(ii) methanol solvate

Space Group: P2/n
Space Group No.: 13

Cell: $a = 10.812(2) \, \text{Å}$, $b = 6.226(1) \, \text{Å}$, $c = 19.627(4) \, \text{Å}$

R-Factor (%): 4.28

Temperature (K): 293

Density (g/cm$^3$): 2.198
Summary of queries used. Search found structures that:

match

Query 1

Query 2

4M

Formula: \((C_{30}H_{32}Fe\,N_6\,O_4\,S_2)n,0.5n(C_3H_6\,O_1)\)

Compound Name: catena-(bis(\(\mu_2\)-meso-2,3-bis(4-Pyridyl)butane-2,3-diol)-dithiocyanato-iron(ii) hemikis(acetone) clathrate)

Space Group: P4/ncc  
Space Group No.: 130  
Cell: \(a = 14.574(3)\,\text{Å}, \quad b = 14.574(3)\,\text{Å}, \quad c = 17.964(4)\,\text{Å}\)  
\(\alpha = 90.00^\circ, \quad \beta = 90.00^\circ, \quad \gamma = 90.00^\circ\)  
R-Factor (%): 7.11  
Temperature(K): 220  
Density(g/cm\(^3\)): 1.201

Formula: \((\text{C}_{30}\text{H}_{32}\text{FeN}_6\text{O}_4\text{S}_2)n,0.5n(\text{C}_3\text{H}_6\text{O})\)

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  
Space Group No.: 130  
Cell: \(a\ 14.224(1)\ b\ 14.224(1)\ c\ 17.580(4)\)  
α 90.00  β 90.00  γ 90.00

R-Factor (%): 8.31  
Temperature(K): 173  
Density(g/cm³): 1.288
CIDGEC


Formula: \((\text{C}_{30}\text{H}_{32}\text{Fe}_1\text{N}_6\text{O}_4\text{S}_2)\text{n}\)

Compound Name: catena-(bis(\(\mu_2\)-meso-2,3-bis(4-Pyridyl)butane-2,3-diol)-dithiocyanato-iron(ii))

Space Group: P4/ncc
Space Group No.: 130
Cell: \(a = 14.726(1)\) \(\text{Å}\), \(b = 14.726(1)\) \(\text{Å}\), \(c = 17.899(3)\) \(\text{Å}\)

Space Group No.: 130

\(\alpha = 90.00\) \(^\circ\), \(\beta = 90.00\) \(^\circ\), \(\gamma = 90.00\) \(^\circ\)

R-Factor (%): 7.00
Temperature(K): 375
Density(g/cm\(^3\)): 1.130

GEQCOV


Formula: \((C_{14}H_{16}HgI_2N_2O_2)_{n}2n(C_2H_6O_1S_1)\)

Compound Name: catena-\((\mu_2\text{-meso-2,3-bis(4-Pyridyl)-2,3-butanediol})\text{-di-iodo-mercury dimethylsulfoxide solvate})\)

Space Group: Pnma  
Space Group No.: 62  
Cell: \(a\) 10.821(2) \(b\) 25.196(5) \(c\) 10.039(2)  
\(\alpha\) 90.00 \(\beta\) 90.00 \(\gamma\) 90.00

R-Factor (%): 6.11  
Temperature(K): 291  
Density(g/cm\(^3\)): 2.075

**OHOSEK**


**Formula:** \((C_{30}H_{32}Fe_1N_6O_4S_2)n,2n(C_2H_3N_1)\)

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

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


Formula: (C$_{30}$H$_{32}$Fe$_1$N$_6$O$_4$S$_2$)$_n$,(n(C$_3$H$_8$O$_1$))

Compound Name: catena-(bis(µ$_2$-2,3-bis(4-pyridyl)butane-2,3-diol)-bis(isothiocyanato)-iron n-propanol solvate)

Space Group: P4/ncc
Space Group No.: 130

Cell: $a$ 14.726(1) $b$ 14.726(1) $c$ 17.899(3)

$\alpha$ 90.00 $\beta$ 90.00 $\gamma$ 90.00

R-Factor (%): 8.06

Temperature(K): 220

Density(g/cm$^3$): 1.233

Formula: \((C_{30}H_{32}Fe_1N_6O_4S_2)n,3n(C_2H_6O_1)\)

Compound Name: catena-(bis(\(\mu_2\)-2,3-bis(4-pyridyl)butane-2,3-diol)-bis(isothiocyanato)-iron ethanol solvate)

Space Group: P4/ncc  
Space Group No.: 130

Cell: \(\alpha 14.639(5)\), \(\beta 14.639(5)\), \(\gamma 17.851(12)\)

Cell (Å,°): \(\alpha 90.00\), \(\beta 90.00\), \(\gamma 90.00\)

R-Factor (%): 8.80  
Temperature(K): 200  
Density(g/cm\(^3\)): 1.387

**Formula:** \((C_{30}H_{32}FeN_6O_4S_2)n,3n(C_2H_6O_1)\)

**Compound Name:** catena-(bis(\(\mu_2\)-2,3-bis(4-pyridyl)butane-2,3-diol)-bis(isothiocyanato)-iron ethanol solvate)

**Space Group:** Pccn

**Cell:**

- \(a\) = 14.493(0) Å
- \(b\) = 14.512(0) Å
- \(c\) = 17.887(0) Å

**Space Group No.:** 56

**\(R\)-Factor (%):** 10.88

**Temperature(K):** 100

**Density\((g/cm^3)\):** 1.410

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Electronic Supplementary Material (ESI) for Chemical Society Reviews

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**Formula:** \((\text{C}_{30}\text{H}_{32}\text{Fe}_1\text{N}_6\text{O}_4\text{S}_2)\text{n}\times 3\text{n(C}_1\text{H}_4\text{O}_1)\)

**Compound Name:** catena-(bis(\(\mu_2\)-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)  
\(\alpha\) 90.00  
\(\beta\) 90.00  
\(\gamma\) 90.00  

**Space Group No.:** 130  
**R-Factor (%):** 7.90  
**Temperature(K):** 200  
**Density(g/cm\(^3\)):** 1.298
OHOSUA01


Formula: \((C_{30}H_{32}Fe_{1}N_{6}O_{4}S_{2})n,3n(C_{1}H_{4}O_{1})\)

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

Space Group: Pccn  
Space Group No.: 56  
\(\alpha\) 90.00  
\(\beta\) 90.00  
\(\gamma\) 90.00  

R-Factor (%): 6.31  
Temperature(K): 100  
Density(g/cm³): 1.360
SOTRID


Formula: \((C_{20}H_{28}Cu_1N_4O_4S_4)n,2n(C_2H_6O_1S_1)\)

Compound Name: catena-\((\mu_2\text{-meso-2,3-bis(4-Pyridyl)-2,3-butanediol-N,N')-bis(dimethylsulfoxide-O)-bis(isothiocyanato)-copper(ii) dimethylsulfoxide solvate}\)

Space Group: P-1  
Space Group No.: 2  
Cell: \(a 7.548(1)\)  \(b 10.822(3)\)  \(c 10.930(3)\)

\(\alpha 96.75(0)\)  \(\beta 91.45(0)\)  \(\gamma 105.34(0)\)

R-Factor (%): 4.13  
Temperature(K): 291  
Density(g/cm\(^3\)): 1.433

\[
\begin{align*}
\text{Cu} & \quad \text{N} \\
\text{N} & \quad \text{O} \\
\text{O} & \quad \text{N} \\
\text{S} & \quad \text{O} \\
\text{S} & \quad \text{N}
\end{align*}
\]
Wlhyao


Formula: \( (C_{14}H_{16}Cu_{1}I_{1}N_{2}O_{2})_n \cdot n(C_2H_6O_1S_1) \)

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: \( a = 19.122(1) \text{ Å}, \quad b = 18.499(1) \text{ Å}, \quad c = 7.254(0) \text{ Å} \)

Space Group No.: 12

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

![Chemical Structure](image)

Formula: \((\text{C}_{14}\text{H}_{16}\text{Cu}_{1}\text{I}_{1}\text{N}_{2}\text{O}_{2})_{n}n(\text{C}_{2}\text{H}_{6}\text{O}_{1}\text{S}_{1}).n(\text{C}_{1}\text{H}_{4}\text{O}_{1}).0.25n(\text{H}_{2}\text{O}_{1})\)

Compound Name: catena-\((\mu_{2}-2,3\text{-bis}(4\text{-Pyridyl})-2,3\text{-butanediol-}N,N')\cdot(\mu_{2}\text{-iodo})\cdot\text{copper(i) dimethylsulfoxide methanol solvate hydrate}\)

Space Group: C2/m  
Space Group No.: 12  
Cell: \(a\) 19.122(2)  \(b\) 18.499(2) \(c\) 7.254(0)  
Space Group No.: 12  
\(\alpha\) 90.00  \(\beta\) 91.42(0)  \(\gamma\) 90.00  

R-Factor (%): 4.01  
Temperature(K): 291  
Density(g/cm\(^3\)): 1.423
Summary of queries used. Search found structures that:

- **Query 1**
- **Query 2**

![Query 1](image1.png)

![Query 2](image2.png)

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(\(\mu_2\)-Chloro)-tris(\(\mu_2\)-(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  
\(\alpha\) 67.55(0)  \(\beta\) 86.75(0)  \(\gamma\) 83.63(0)

R-Factor (%): 8.27  
Temperature(K): 173  
Density(g/cm\(^3\)): 1.155

DARSIZ


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)

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  
Space Group No.: 96

Cell: a 17.962(0)  b 17.962(0)  c 31.649(1)

R-Factor (%): 12.40  
Temperature(K): 173  
Density(g/cm^3): 1.031

Formula: 

\[(C_{60}H_{40}Cd_1Cl_4N_4O_6^{2+})_n2n(Cl_1O_4^{-1})\_n(C_3H_7N_1O_1)\_4n(C_1H_4O_1)\_n(H_2O)\]

Compound Name: catena-(bis(\(\mu_2-(R)-6,6'\)-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: 

\[
\begin{array}{ccc}
\alpha & 90.00 & \beta & 90.00 & \gamma & 90.00 \\
(\text{Å},\,°) & a & 17.962(0) & b & 17.962(0) & c & 31.649(1)
\end{array}
\]

R-Factor (%): 12.40

Temperature(K): 173

Density(g/cm\(^3\)): 1.031

Formulas: (C\textsubscript{120}H\textsubscript{72}Cd\textsubscript{3}Cl\textsubscript{8}N\textsubscript{14}O\textsubscript{26})\textsubscript{n}, 7n(C\textsubscript{1}H\textsubscript{4}O\textsubscript{1}), 5n(H\textsubscript{2}O\textsubscript{1})

Compound Name: catena-(tetrakis(\textsubscript{\mu}\textsubscript{2}-(R)-6,6'-Dichloro-2,2'-dihydroxy-4,4'-bis(4-pyridyl)-1,1'-binaphthyl-N,N')-bis(\textsubscript{\mu}\textsubscript{2}-nitrato-O,O')-tetakis(nitrato-O,O')-tri-cadmium(ii) methanol solvate pentahydrate)

Space Group: P4122
Space Group No.: 91

Cell: 
\begin{align*}
\text{a} & : 20.305(1) \\
\text{b} & : 20.305(1) \\
\text{c} & : 49.641(4)
\end{align*}

\begin{align*}
\text{\alpha} & : 90.00 \\
\text{\beta} & : 90.00 \\
\text{\gamma} & : 90.00
\end{align*}

R-Factor (%): 6.39
Temperature(K): 173
Density(g/cm\textsuperscript{3}): 0.993