

Search Overview

Search: search6
Date/Time done: Sat Mar 07 10:08:52 2020
Database(s): CSD version 5.41 (November 2019)
Restriction Info: No refcode restrictions applied
Filters: None
Percentage Completed: 100%
Number of Hits: 16

Summary of queries used. Search found structures that:

match

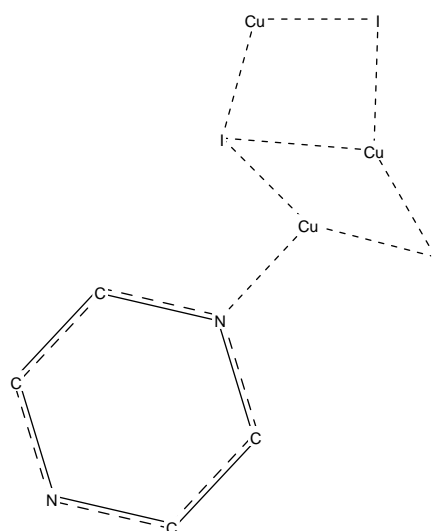
Query 2

Query 3

Query 2

Name **catena**

Query 3



Search: search6 (Sat Mar 07 10:08:52 2020): Hits 1-4

AGIYEU01

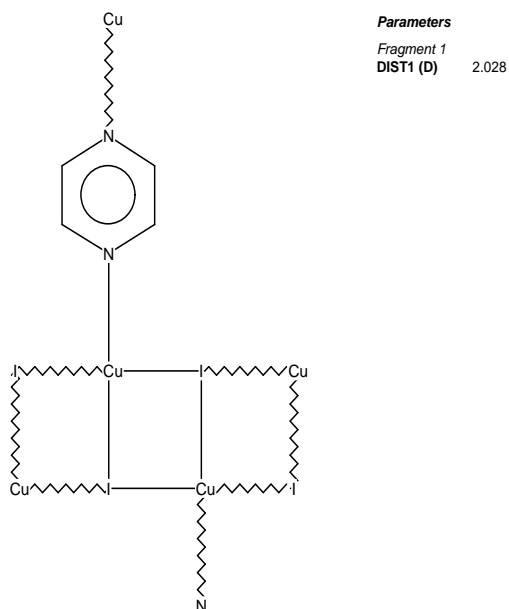
Reference: A.J.Blake, N.R.Brooks, N.R.Champness, P.A.Cooke, M.Crew, A.M.Deveson, L.R.Hanton, P.Hubberstey, D.Fenske, M.Schroder (1999) *Crystal Engineering*, **2**,181

Formula: (C₄ H₄ Cu₂ I₂ N₂)_n

Compound Name: catena-(bis(μ₃-iodo)-(μ₂-pyrazine-N,N')-di-copper(ii))

Space Group: P-1 **Cell:** a 4.134(0) b 7.058(1) c 8.041(1)
Space Group No.: 2 **(Å, °)** α 109.72(3) β 101.31(3) γ 96.54(3)

R-Factor (%): 4.82 **Temperature(K):** 203 **Density(g/cm³):** 3.604



AGIYEU02

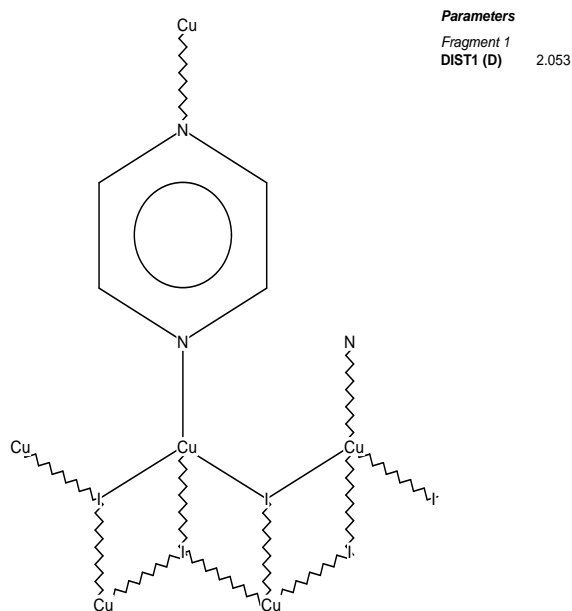
Reference: A.M.Goforth, M.D.Smith, H.-C.zur Loye (2003) *J.Chem.Cryst.*, **33**,303

Formula: (C₄ H₄ Cu₂ I₂ N₂)_n

Compound Name: catena-(bis(μ₃-iodo)-(μ₂-pyrazine)-di-copper(i))

Space Group: P-1 **Cell:** a 4.176(0) b 7.128(0) c 8.128(0)
Space Group No.: 2 **(Å, °)** α 109.61(0) β 101.77(0) γ 96.68(0)

R-Factor (%): 2.88 **Temperature(K):** 293 **Density(g/cm³):** 3.502



BASBAA

Reference: Jin-Cheng Wu, Liang Zhao, De-Xian Wang, Mei-Xiang Wang (2012) *Inorg.Chem.*, **51**,3860

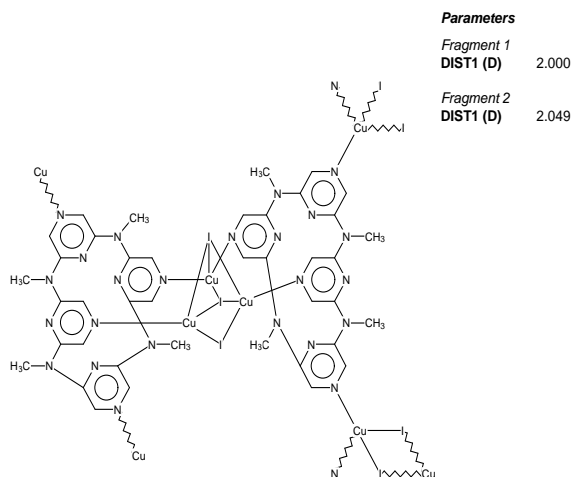
Formula: (C₄₀ H₄₀ Cu₅ I₅ N₂₄)_n

Compound Name: catena-(bis(μ₄-2,4,6,8-tetramethyl-2,4,6,8-tetraza-1,3,5,7(2,6)-tetrapyrazinacyclooctaphane)-bis(μ₃-iodo)-tris(μ₂-iodo)-penta-copper unknown solvate)

Synonym: catena-(bis(μ₄-tetramethylazacalix[4]pyrazine)-bis(μ₃-iodo)-tris(μ₂-iodo)-penta-copper unknown solvate)

Space Group: Pmnm **Cell:** a 24.142(2) b 35.780(7) c 9.209(1)
Space Group No.: 59 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 7.29 **Temperature(K):** 113 **Density(g/cm³):** 1.511



DEYNIG

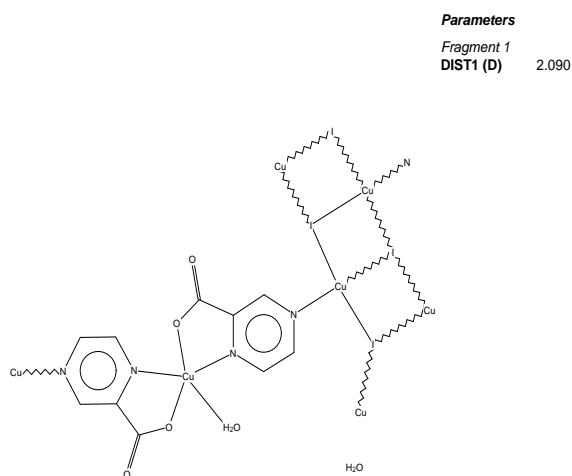
Reference: Zhen-Zhen Wen, Xi-Ling Wen, Song-Liang Cai, Sheng-Run Zheng, Jun Fan, Wei-Guang Zhang (2013) *CrystEngComm*, **15**,5359

Formula: (C₁₀ H₈ Cu₃ I₂ N₄ O₅)_n·H₂O

Compound Name: catena-[bis(μ₃-iodo)-bis(μ₂-pyrazine-2-carboxylato)-aqua-di-copper(i)-copper(ii) monohydrate]

Space Group: Pbcn **Cell:** a 7.666(1) b 31.951(7) c 15.481(3)
Space Group No.: 60 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 8.67 **Temperature(K):** 296 **Density(g/cm³):** 2.546



Search: search6 (Sat Mar 07 10:08:52 2020): Hits 5-8

DIVKUQ

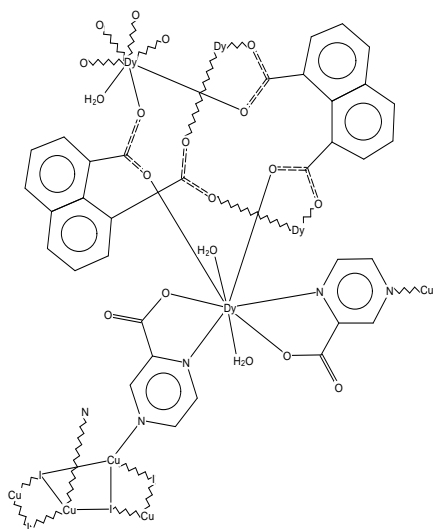
Reference: Gao-Juan Cao, Zhi-Long Wang, Cheng Rong, Qing-Lu Li (2013) *Inorg.Chem.Commun.*, **36**,163

Formula: (C₃₄ H₂₄ Cu₂ Dy₂ I₂ N₄ O₁₅)_n

Compound Name: catena-(bis(μ₄-Naphthalene-1,8-dicarboxylato)-bis(μ₃-iodo)-bis(μ₂-pyrazine-2-carboxylato)-triaqua-di-copper-di-dysprosium)

Space Group: Pbc_a **Cell:** **a** 8.160(0) **b** 29.750(1) **c** 30.838(2)
Space Group No.: 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 6.85 **Temperature(K):** 293 **Density(g/cm³):** 2.545



Parameters
Fragment 1
DIST1 (D) 2.058

ECEVEO

Reference: J.H.Chong, M.J.MacLachlan (2006) *Inorg.Chem.* **45**,1442

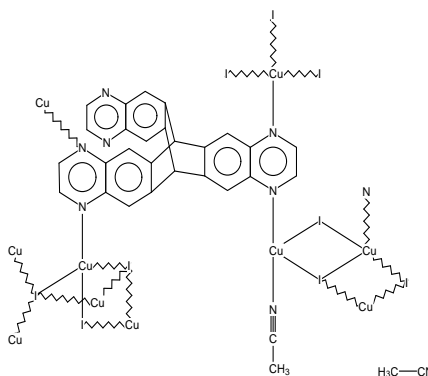
Formula: (C₂₈ H₁₇ Cu₄ I₄ N₇)_n(C₂ H₃ N)₁

Compound Name: catena-(μ₄-5,8,16,19,26,29-Hexa-azaocyclotriacta-2(11),3,5,7,9,13(22),14,16,18,20,23(32),24,26,28,30-pentadecaene)-(μ₄-iodo)-(μ₃-iodo)-bis(μ₂-iodo)-(acetonitrile)-tetra-copper(i) acetonitrile clathrate)

Synonym: catena-(μ₄-iodo)-(μ₄-tri-2,3-pyrazino(b,e,h)tritycene)-(μ₃-iodo)-bis(μ₂-iodo)-(acetonitrile)-tetra-copper(i) acetonitrile clathrate)

Space Group: P-1 **Cell:** **a** 9.837(0) **b** 11.970(0) **c** 15.862(0)
Space Group No.: 2 **(Å, °)** α 75.47(0) β 86.57(0) γ 67.83(0)

R-Factor (%): 2.60 **Temperature(K):** 173 **Density(g/cm³):** 2.490



Parameters
Fragment 1
DIST1 (D) 2.089

ECEVIS

Reference: J.H.Chong, M.J.MacLachlan (2006) *Inorg.Chem.* **45**,1442

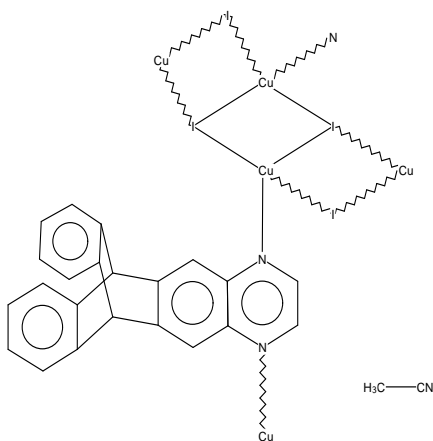
Formula: (C₂₂ H₁₄ Cu₂ I₂ N₂)_n(C₂ H₃ N)₁

Compound Name: catena-(bis(μ₃-iodo)-(μ₂-5,8-di-azahexacyclo[10.6.6.0^{2,11}.0^{4,9}.0^{13,18}.0^{19,24}]tetracos-2(11),3,5,7,9,13,15,17,19,21,23-undecaene)-di-copper(i) acetonitrile clathrate)

Synonym: catena-(μ₃-iodo)-(μ₂-2,3-pyrazino(b)tritycene)-di-copper(i) acetonitrile clathrate)

Space Group: P2₁/c **Cell:** **a** 9.157(1) **b** 31.760(4) **c** 8.246(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 99.38(0) γ 90.00

R-Factor (%): 5.26 **Temperature(K):** 173 **Density(g/cm³):** 2.045



Parameters
Fragment 1
DIST1 (D) 2.057

EMELOX

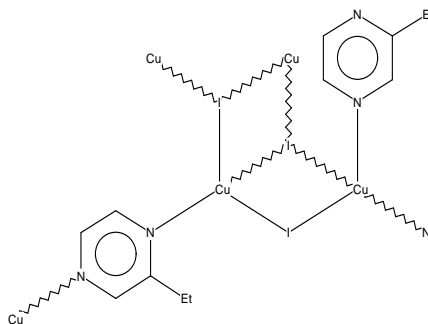
Reference: C.Nather, I.Jess, N.Lehner, D.Hinz-Hubner (2003) *Solid State Sciences*, **5**,1343

Formula: (C₁₂ H₁₆ Cu₂ I₂ N₄)_n

Compound Name: catena-(μ₃-iodo)-(μ₂-2-ethylpyrazine-N,N')-(μ₂-iodo)-(2-ethylpyrazine-N⁴)-di-copper)

Space Group: P2₁/n **Cell:** **a** 10.434(0) **b** 14.803(0) **c** 11.109(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 96.71(0) γ 90.00

R-Factor (%): 3.71 **Temperature(K):** 293 **Density(g/cm³):** 2.328



Parameters
Fragment 1
DIST1 (D) 2.080

Search: search6 (Sat Mar 07 10:08:52 2020): Hits 9-12

LIDXUS

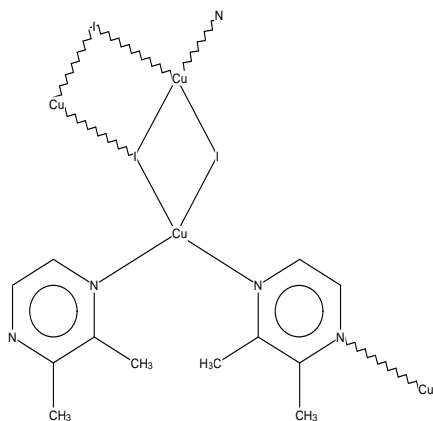
Reference: I.Jess, P.Taborsky, J.Pospisil, C.Nather (2007) *Dalton Trans.*, 2263

Formula: (C₁₂ H₁₆ Cu₂ I₂ N₄)_n

Compound Name: catena-(μ₃-iodo)-(μ₂-iodo)-(μ₂-2,3-dimethylpyrazine)-(2,3-dimethylpyrazine)-di-copper(I)

Space Group: P2₁/n **Cell:** a 9.851(0) b 12.848(0) c 13.584(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 103.15(0) γ 90.00

R-Factor (%): 3.63 **Temperature(K):** 220 **Density(g/cm³):** 2.369



Parameters

Fragment 1
DIST1 (D) 2.062

Fragment 2
DIST1 (D) 2.050

MUHQOV

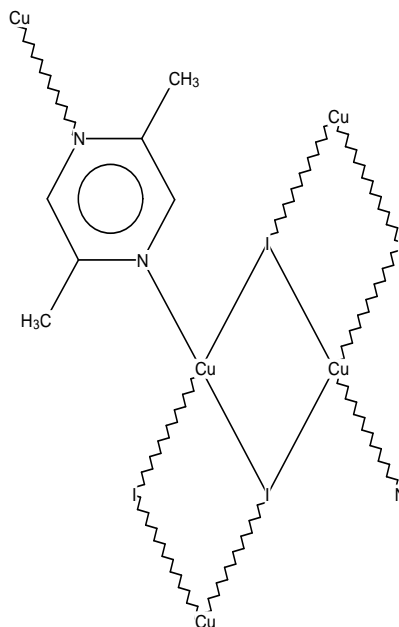
Reference: C.Nather, J.Greve, I.Jess (2002) *Solid State Sciences*, 4, 813

Formula: (C₆ H₈ Cu₂ I₂ N₂)_n

Compound Name: catena-(bis(μ₃-iodo)-(μ₂-2,5-dimethylpyrazine)-di-copper(I))

Space Group: P-1 **Cell:** a 4.294(0) b 8.181(1) c 8.215(1)
Space Group No.: 2 **(Å, °)** α 110.87(1) β 102.17(1) γ 94.54(1)

R-Factor (%): 2.31 **Temperature(K):** 293 **Density(g/cm³):** 3.126



Parameters

Fragment 1
DIST1 (D) 2.058

MUHQOV01

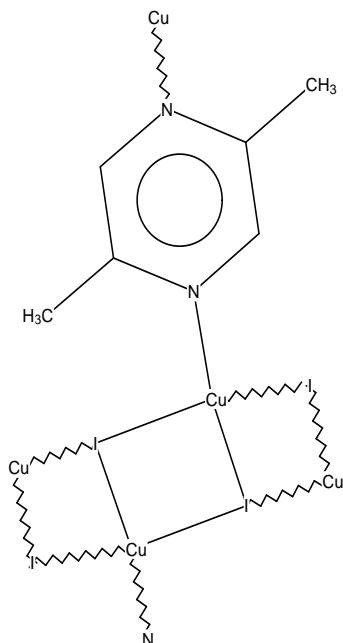
Reference: N.Kitada, T.Ishida (2014) *CrystEngComm*, 16,8035

Formula: (C₆ H₈ Cu₂ I₂ N₂)_n

Compound Name: catena-(bis(μ₃-iodo)-(μ₂-2,5-dimethylpyrazine)-copper(I))

Space Group: P-1 **Cell:** a 4.297(1) b 8.220(3) c 8.247(3)
Space Group No.: 2 **(Å, °)** α 110.85(3) β 102.04(3) γ 94.82(3)

R-Factor (%): 5.90 **Temperature(K):** 293 **Density(g/cm³):** 3.097



Parameters

Fragment 1
DIST1 (D) 2.066

RABBUS

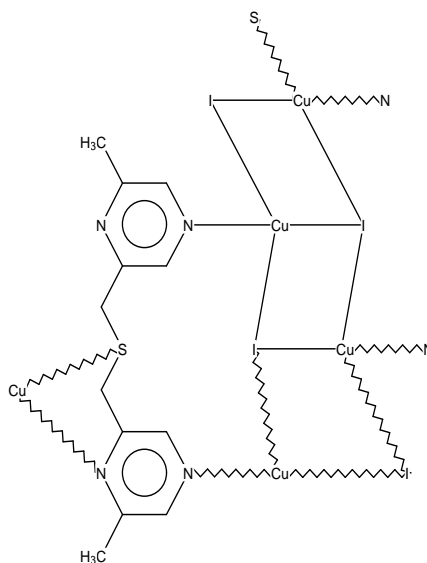
Reference: J.J.M.Amoore, L.R.Hanton, M.D.Spicer (2003) *Dalton Trans.*, 1056

Formula: (C₁₂ H₁₄ Cu₃ I₃ N₄ S₁)_n

Compound Name: catena-(bis(μ₃-iodo)-(μ₃-bis(6-methylpyrazin-2-ylmethyl) thioether-N, N', N'', S)-(μ₂-iodo)-tri-copper(I))

Space Group: P-1 **Cell:** a 8.384(0) b 9.241(0) c 13.799(0)
Space Group No.: 2 **(Å, °)** α 87.94(0) β 86.21(0) γ 67.20(0)

R-Factor (%): 2.95 **Temperature(K):** 123 **Density(g/cm³):** 2.762



Parameters

Fragment 1
DIST1 (D) 2.070

Fragment 2
DIST1 (D) 2.053

Search: search6 (Sat Mar 07 10:08:52 2020): Hits 13-16

RUPTED

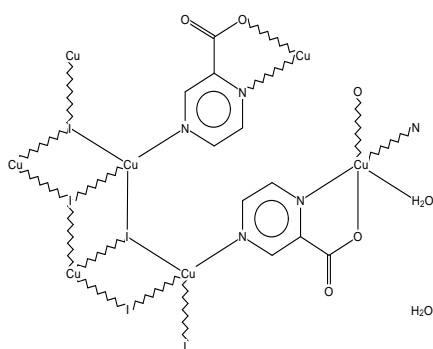
Reference: Yu-Jia Ding, Chun-Pei Zhang, Yong-Qing Wang, Xiao-Ming Lin, Ximiao Zhu, Da-Liang Zhang, Xian-Jian Duan, Yue-Peng Cai (2015) *CrystEngComm*, **17**,6693

Formula: (C₁₀ H₈ Cu₃ I₂ N₄ O₅)_n.0.5n(H₂ O₁)

Compound Name: catena-[bis(μ₃-iodo)-bis(μ₂-pyrazine-2-carboxylato)-aqua-tri-copper hemihydrate]

Space Group: Pbcn **Cell:** a 7.668(0) b 31.909(3) c 15.427(1)
Space Group No.: 60 **Cell:** (Å, °) α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.22 **Temperature(K):** 296 **Density(g/cm³):** 2.526



Parameters
 Fragment 1
DIST1 (D) 2.088
 Fragment 2
DIST1 (D) 2.080

VEVGUY

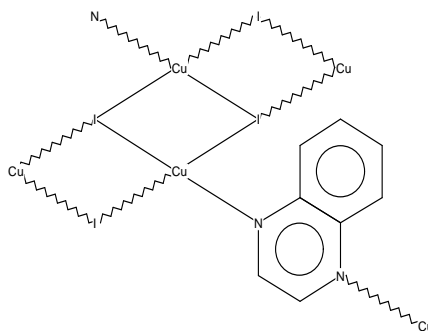
Reference: P.M.Graham, R.D.Pike, M.Sabat, R.D.Bailey, W.T.Pennington (2000) *Inorg.Chem.*, **39**,5121

Formula: (C₈ H₆ Cu₂ I₂ N₂)_n

Compound Name: catena-(bis(μ₃-iodo)-(μ₂-quinoxaline-N,N')-di-copper(i))

Space Group: P21/c **Cell:** a 4.372(0) b 17.718(2) c 14.748(0)
Space Group No.: 14 **Cell:** (Å, °) α 90.00 β 110.16(0) γ 90.00

R-Factor (%): 6.18 **Temperature(K):** 295 **Density(g/cm³):** 3.165



Parameters
 Fragment 1
DIST1 (D) 2.046

WURYUF

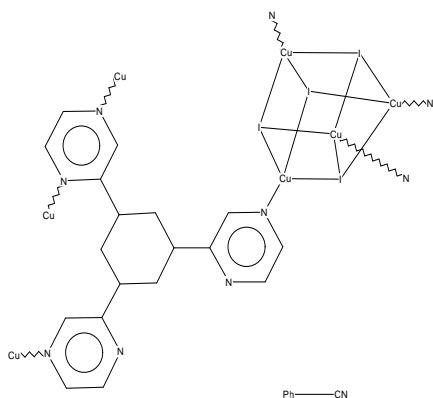
Reference: T.Hayashi, A.Kobayashi, H.Ohara, M.Yoshida, T.Matsumoto, Ho-Chol Chang, M.Kato (2015) *Inorg.Chem.*, **54**,8905

Formula: (C₁₈ H₁₈ Cu₄ I₄ N₆)_n.n(C₇ H₅ N₁)

Compound Name: catena-((μ₄-2,2',2''-Cyclohexane-1,3,5-triyltripyrazine)-tetrakis(μ₃-iodo)-tetra-copper benzonitrile solvate)

Space Group: P21/c **Cell:** a 14.765(5) b 17.932(6) c 16.285(5)
Space Group No.: 14 **Cell:** (Å, °) α 90.00 β 105.68(0) γ 90.00

R-Factor (%): 6.26 **Temperature(K):** 100 **Density(g/cm³):** 1.893



Parameters
 Fragment 1
DIST1 (D) 2.037

ZEBNUP

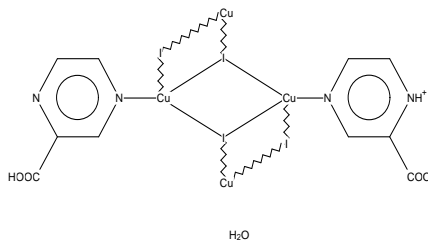
Reference: M.A.S.Goher, T.C.W.Mak (1995) *Polyhedron*, **14**,2587

Formula: (C₁₀ H₈ Cu₂ I₂ N₄ O₄)_n.3n(H₂ O₁)

Compound Name: catena(bis((μ₃-iodo)-(pyridine-2-carboxylate)-copper(ii)) trihydrate)

Space Group: P-1 **Cell:** a 6.813(1) b 8.273(1) c 16.719(2)
Space Group No.: 2 **Cell:** (Å, °) α 93.44(1) β 97.05(1) γ 96.19(1)

R-Factor (%): 3.47 **Temperature(K):** 295 **Density(g/cm³):** 2.447



Parameters
 Fragment 1
DIST1 (D) 2.063
 Fragment 2
DIST1 (D) 2.053