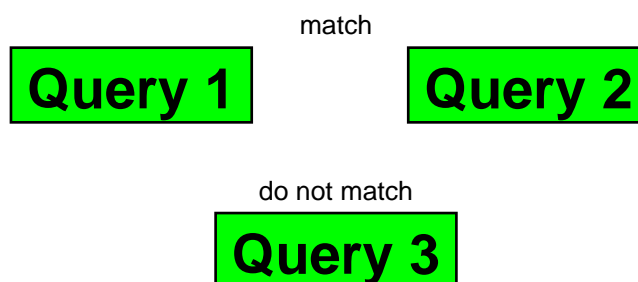
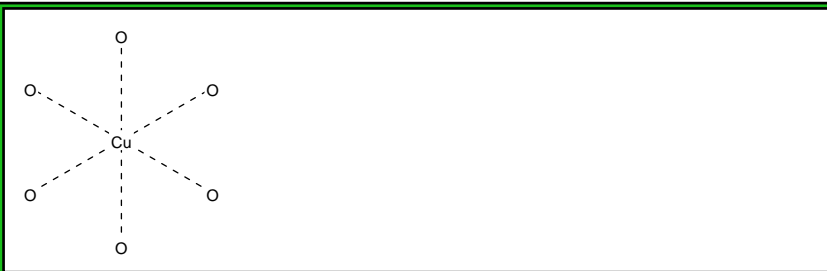
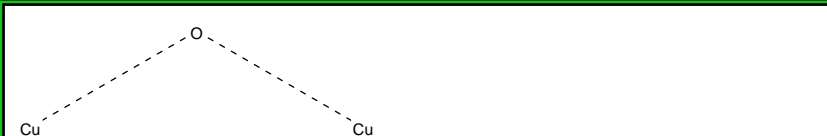


Search Overview

Search: search2
Date/Time done: Wed Jul 26 09:11:25 2017
Database(s): CSD version 5.38 updates (Nov 2016)
CSD version 5.38 (November 2016)
CSD version 5.38 (November 2016)
CSD version 5.38 updates (Feb 2017)
CSD version 5.38 updates (May 2017)
Restriction Info: No refcode restrictions applied
Filters: None
Percentage Completed: 100%
Number of Hits: 232

Summary of queries used. Search found structures that:



Query 1	
Query 2	R-factor < 3 % Powder structures exclude
Query 3	

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 1

UTAKIL

Reference: M.S.Henriques, D.I.Gorbunov, A.N.Ponomaryov, A.Saneei, M.Pourayoubi, M.Dusek, S.Zvyagin, M.Uhlarz, J.Wosnitza (2016) *Polyhedron*, **118**,154

Formula: C₃₀ H₆₀ Cu₁ N₈ O₈ P₂

Compound Name: bis(nitrato-O,O')-bis(tripiperidinophosphine oxide-O)-copper(ii)

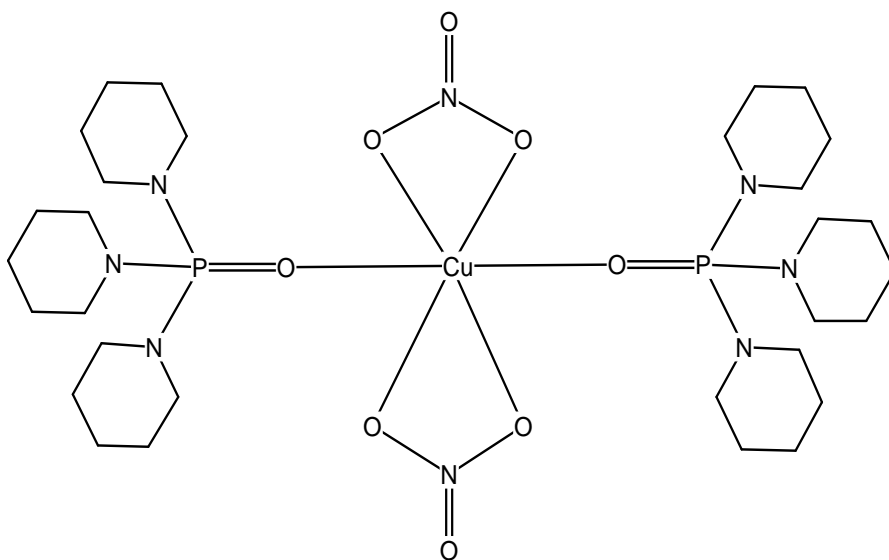
Space Group: P21/n **Cell:** **a** 8.883(0) **b** 17.136(0) **c** 12.598(0)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 103.13(0) **γ** 90.00

R-Factor (%): 2.52 **Temperature(K):** 120 **Density(g/cm³):** 1.398

Parameters

Fragment 1

DIST1 (D)	1.980
DIST2 (D)	1.980
DIST3 (D)	1.920
DIST4 (D)	1.920
DIST5 (D)	2.494
DIST6 (D)	2.494



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 2

ABACUF01

Reference: R.Baggio, D.Stoilova, G.Polla, G.Leyva, M.T.Garland
(2004) *J.Mol.Struct.* ,**697**,173

Formula: (C₆ H₁₄ Ba₂ Cu₁ O₁₆)_n

Compound Name: catena-(bis((μ₄-Formato)-(μ₃-formato)-(μ₂-formato-O,O)-bis(μ₂-aqua)-barium)-copper)

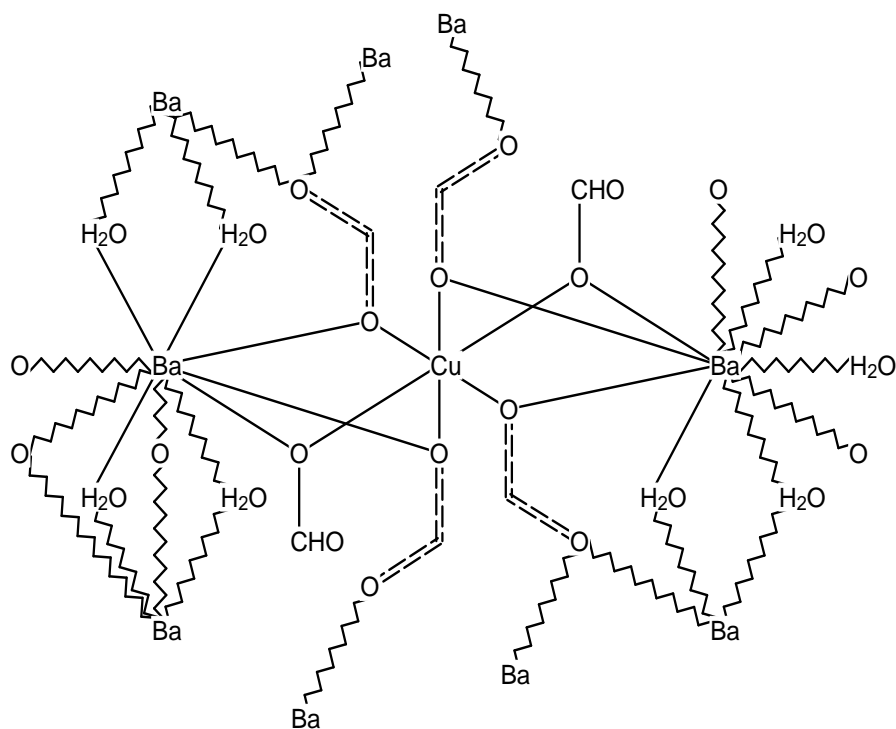
Space Group: P-1 **Cell:** **a** 8.817(0) **b** 7.128(0) **c** 6.928(0)
Space Group No.: 2 (**Å, °**) **α** 98.00(0) **β** 108.94(0) **γ** 82.55(0)

R-Factor (%): 2.23 **Temperature(K):** 293 **Density(g/cm³):** 2.782

Parameters

Fragment 1

DIST1 (D)	2.015
DIST2 (D)	1.972
DIST3 (D)	2.015
DIST4 (D)	1.972
DIST5 (D)	2.330
DIST6 (D)	2.330



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 3

ACUFUR01

Reference: M.Yamanaka, H.Uekusa, S.Ohba, Y.Saito, S.Iwata,
M.Kato, T.Tokii, Y.Muto, O.W.Steward (1991)
Acta Crystallogr., Sect.B: Struct. Sci., **47**,344

Formula: $(C_4 H_{12} Cu_2 O_{12})_n, 4n(C_1 H_4 N_2 O_1)$

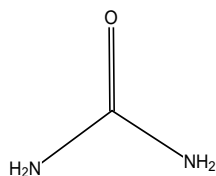
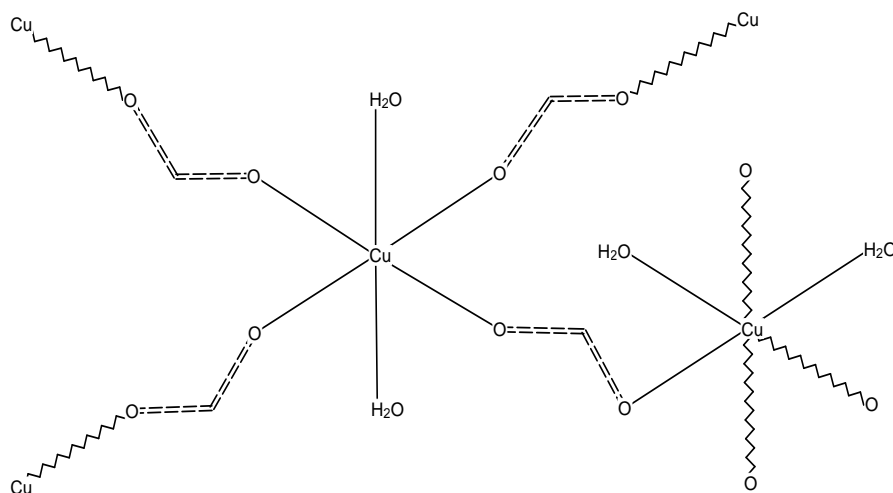
Compound Name: catena(Diaqua-bis((μ_2 -formato-O,O')-copper(ii) (urea)))

Space Group: P21/c **Cell:** **a** 8.158(0) **b** 8.368(0) **c** 8.088(5)
Space Group No.: 14 **(Å, °)** α 90.00 β 95.81(0) γ 90.00
R-Factor (%): 2.40 **Temperature(K):** 120 **Density(g/cm³):** 1.872

Parameters

Fragment 1

DIST1 (D) 1.985
DIST2 (D) 1.989
DIST3 (D) 1.985
DIST4 (D) 1.989
DIST5 (D) 2.408
DIST6 (D) 2.408



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 4

AGAMAY

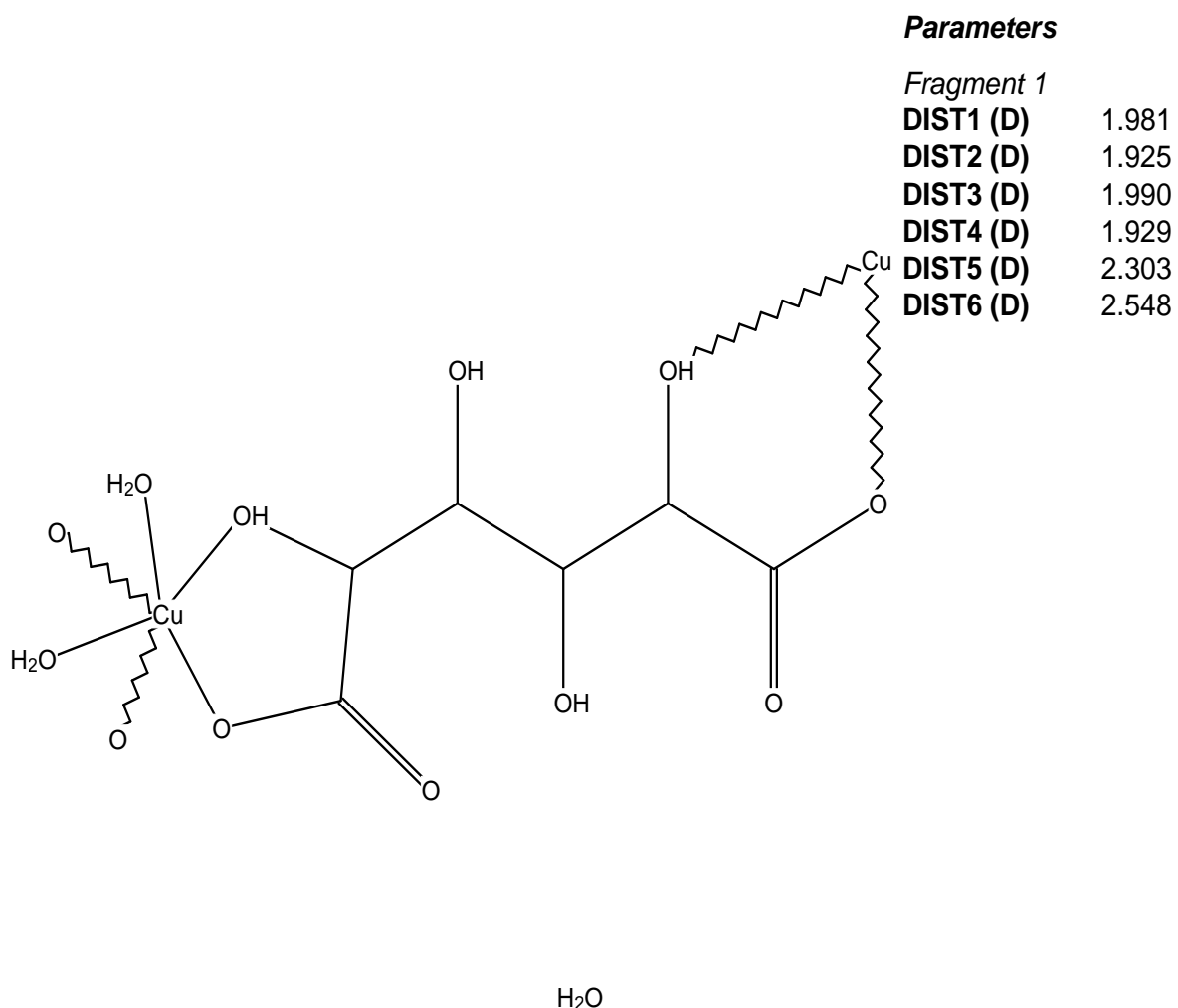
Reference: M.S.Zavakhina, D.G.Samsonenko, D.N.Dybtsev,
M.P.Yutkin, A.V.Virovets, V.P.Fedin (2013)
Izv.Akad.Nauk SSSR, Ser.Khim.(Russ.)(Russ.Chem.Bull.), 716

Formula: $(C_6 H_{12} Cu_1 O_{10})_n, 3n(H_2 O)_1$

Compound Name: catena-((μ_2 -D-Glucarato)-diaqua-copper trihydrate)

Space Group: P1 **Cell:** **a** 6.636(0) **b** 7.154(0) **c** 7.408(0)
Space Group No.: 1 **(Å, °)** α 100.12(0) β 103.45(0) γ 108.06(0)

R-Factor (%): 1.91 **Temperature(K):** 150 **Density(g/cm³):** 1.917



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 5

AMATUF

Reference: T.J.Bednarchuk, V.Kinzhybalo, O.Bednarchuk,
A.Pietraszko (2016) *J.Mol.Struct.* ,**1120**,138

Formula: $H_{12} Cu_1 O_6^{2+}, 2(C_5 H_7 N_2^{1+}), 2(O_4 S_1^{2-})$

Compound Name: hexaaqua-copper(ii) bis(4-aminopyridinium) bis(sulfate)

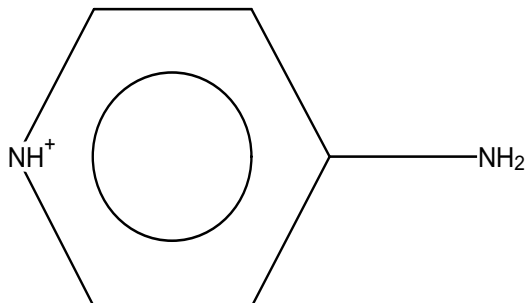
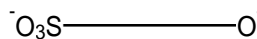
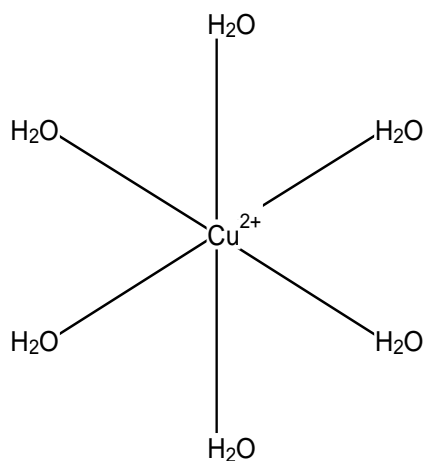
Space Group: P-1 **Cell:** **a** 6.179(3) **b** 7.059(3) **c** 12.442(5)
Space Group No.: 2 **(Å, °)** α 99.80(3) β 98.87(3) γ 99.66(3)

R-Factor (%): 2.34 **Temperature(K):** 297 **Density(g/cm³):** 1.777

Parameters

Fragment 1

DIST1 (D)	1.978
DIST2 (D)	2.036
DIST3 (D)	1.978
DIST4 (D)	2.036
DIST5 (D)	2.248
DIST6 (D)	2.248



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 6

ANIYUS

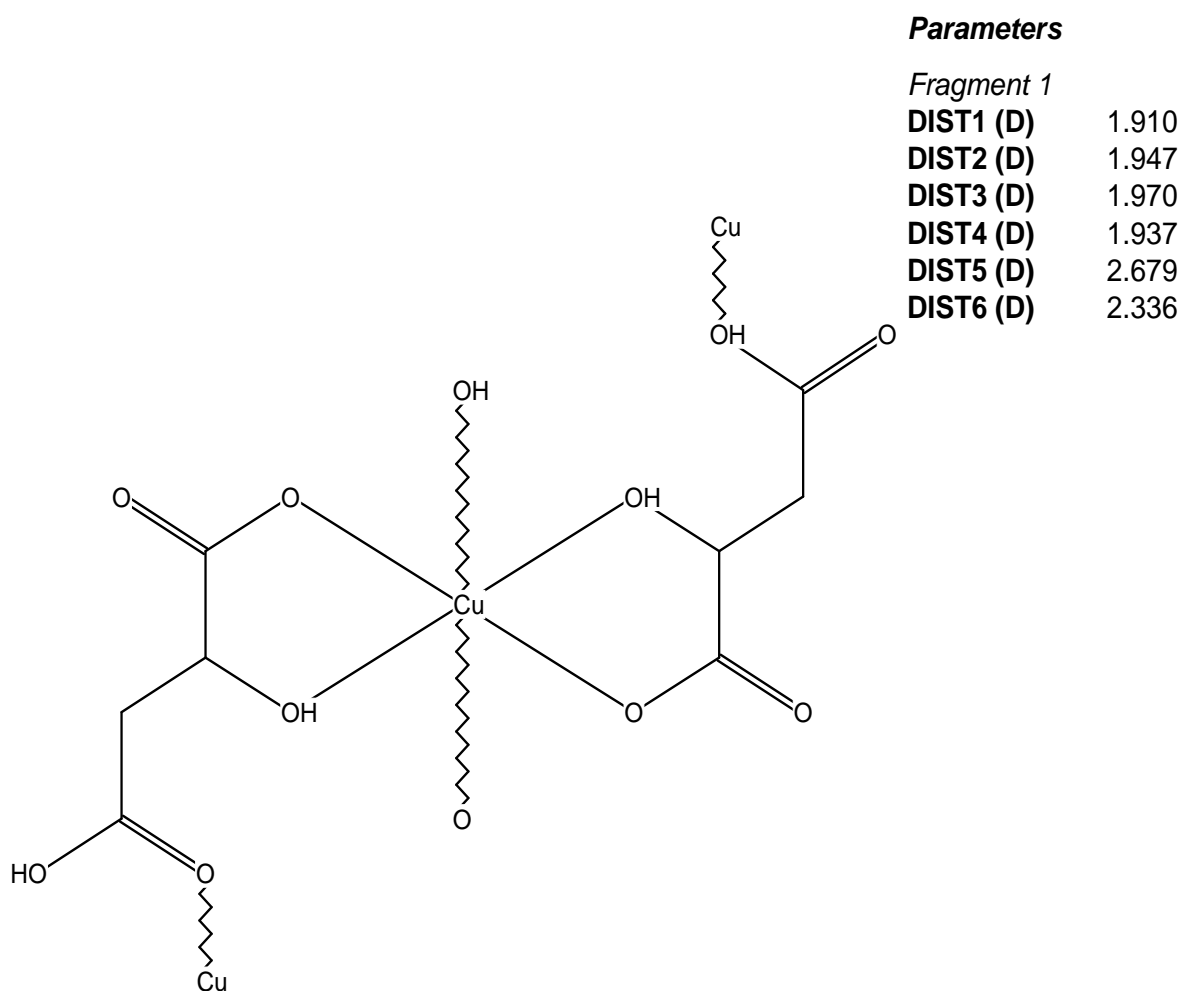
Reference: R.V.Gudavarthy, N.Burla, E.A.Kulp, S.J.Limmer, E.Sinn, J.A.Switzer (2011) *J.Mater.Chem.* ,21,6209

Formula: (C₈ H₁₀ Cu₁ O₁₀)_n,2n(H₂ O₁)

Compound Name: catena-(bis(μ₂-L-Hydrogen malato)-copper(ii) dihydrate)

Space Group: P21 **Cell:** **a** 7.584(4) **b** 10.214(5) **c** 8.169(4)
Space Group No.: 4 **(Å, °)** α 90.00 β 92.78(0) γ 90.00

R-Factor (%): 2.41 **Temperature(K):** 298 **Density(g/cm³):** 1.922



H₂O

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 7

AQOXAG

Reference: T.W.T.Muesmann, C.Zitzer, A.Mietrach, T.Kluner, J.Christoffers, M.S.Wickleder (2011) *Dalton Trans.*, **40**,3128

Formula: (C₆ H₈ Cl₄ Cu₁ O₁₀ S₂)_n

Compound Name: catena-[(μ_2 -2,3,5,6-Tetrachlorobenzene-1,4-disulfonato-O,O')-tetra-aqua-copper(ii)]

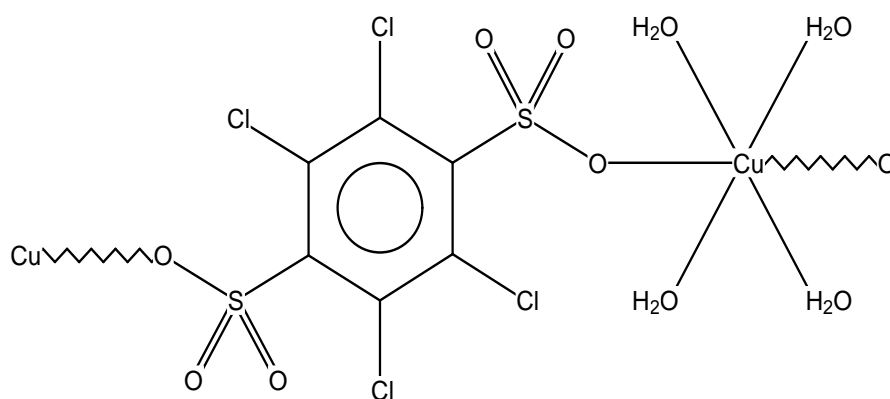
Space Group: Pnma **Cell:** **a** 7.213(0) **b** 21.478(0) **c** 9.794(0)
Space Group No.: 62 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.66 **Temperature(K):** 153 **Density(g/cm³):** 2.231

Parameters

Fragment 1

DIST1 (D) 1.940
DIST2 (D) 1.958
DIST3 (D) 1.940
DIST4 (D) 1.958
DIST5 (D) 2.447
DIST6 (D) 2.447



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 8

AQOXIO

Reference: T.W.T.Muesmann, C.Zitzer, A.Mietrach, T.Kluner, J.Christoffers, M.S.Wickleder (2011) *Dalton Trans.*, **40**,3128

Formula: $H_{12} Cu_1 O_6^{2+}, C_6 F_4 O_6 S_2^{2-}$

Compound Name: Hexa-aqua-copper(ii) 2,3,5,6-tetrafluorobenzene-1,4-disulfonate

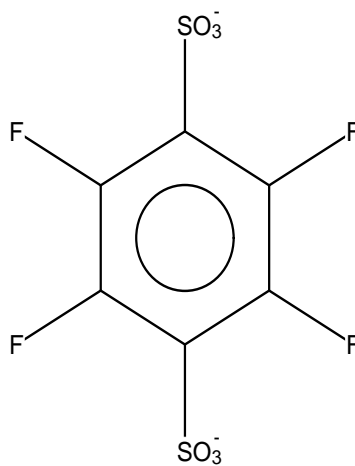
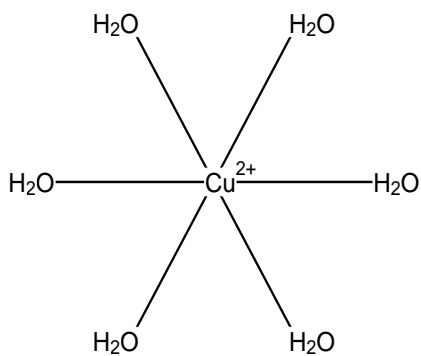
Space Group: P-1 **Cell:** **a** 5.104(0) **b** 7.447(0) **c** 10.778(0)
Space Group No.: 2 **(Å, °)** α 85.63(0) β 77.45(0) γ 76.02(0)

R-Factor (%): 2.65 **Temperature(K):** 153 **Density(g/cm³):** 2.054

Parameters

Fragment 1

DIST1 (D)	1.948
DIST2 (D)	1.979
DIST3 (D)	1.948
DIST4 (D)	1.979
DIST5 (D)	2.380
DIST6 (D)	2.380



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 9

AXAFIO

Reference: F.Pointillart, C.Train, M.Gruselle, F.Villain, H.W.Schmalle, D.Talbot, P.Gredin, S.Decurtins, M.Verdaguer (2004) *Chem.Mater.* ,**16**, 832

Formula: $(C_{30} H_{24} N_6 Ru_1^{2+})n, n(C_6 Cu_2 O_{12}^{2-})$

Compound Name: catena-[tris(2,2'-Bipyridyl)-ruthenium(ii) tris(μ_2 -oxalato)-di-copper(ii)]

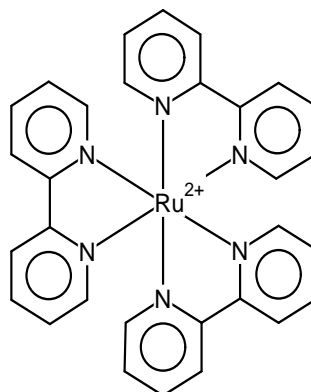
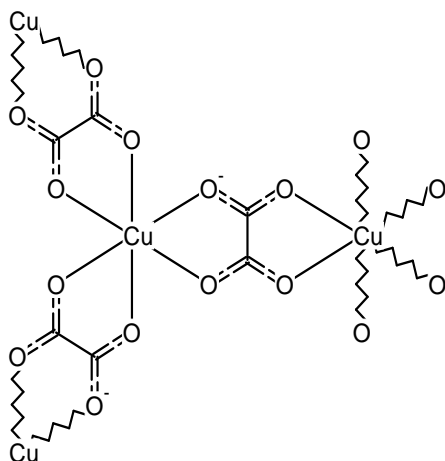
Space Group: P4132 **Cell:** **a** 15.297(0) **b** 15.297(0) **c** 15.297(0)
Space Group No.: 213 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.72 **Temperature(K):** 183 **Density(g/cm³):** 1.783

Parameters

Fragment 1

DIST1 (D)	2.109
DIST2 (D)	2.087
DIST3 (D)	2.087
DIST4 (D)	2.109
DIST5 (D)	2.109
DIST6 (D)	2.087



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 10

BESNOC01

Reference: Xin-Yan Zhang (2007)
Acta Crystallogr., Sect. E: Struct. Rep. Online ,**63**,m1254

Formula: C₈ H₁₄ Cu₁ O₁₂

Compound Name: Diaqua-bis(malato-O,O')-copper(ii)

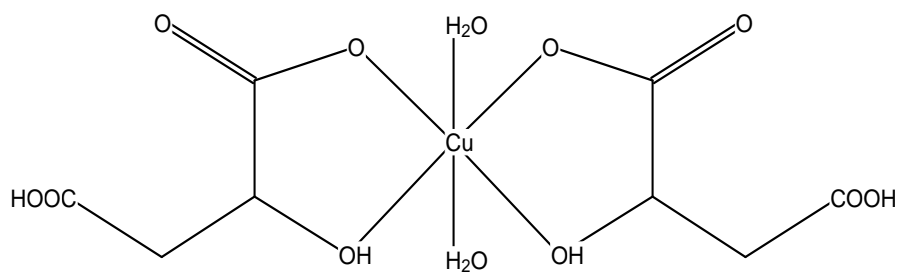
Space Group: P21/c **Cell:** **a** 8.476(0) **b** 7.438(0) **c** 10.312(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 102.68(0) γ 90.00

R-Factor (%): 2.17 **Temperature(K):** 293 **Density(g/cm³):** 1.915

Parameters

Fragment 1

DIST1 (D)	1.913
DIST2 (D)	1.951
DIST3 (D)	1.951
DIST4 (D)	1.913
DIST5 (D)	2.515
DIST6 (D)	2.515



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 11

BOVTAH02

Reference: W.Clegg, J.M.Holcroft, N.C.Martin (2015) *CrystEngComm*, 17,2857

Formula: $(C_{10}H_{14}Cu_2O_{14})_n \cdot 4(H_2O)_1$

Compound Name: catena-((μ_4 -1,2,4,5-Benzenetetracarboxylato-O,O',O'',O''')-bis(triaqua-copper) tetrahydrate)

Space Group: C2/c **Cell:** **a** 12.152(0) **b** 18.141(1) **c** 9.582(0)
Space Group No.: 15 **(Å, °)** α 90.00 β 113.50(0) γ 90.00

R-Factor (%): 2.35 **Temperature(K):** 160 **Density(g/cm³):** 1.911

Parameters

Fragment 1

DIST1 (D) 1.952

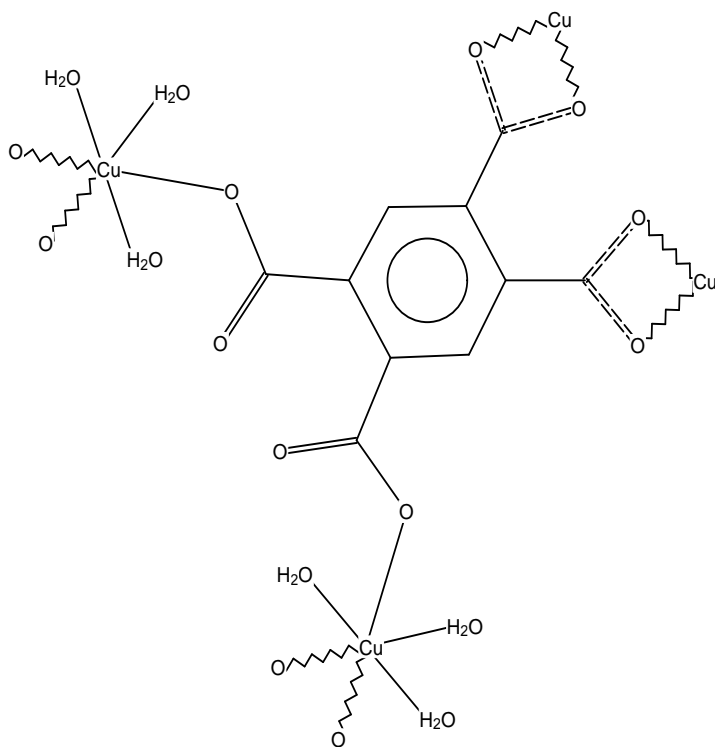
DIST2 (D) 1.955

DIST3 (D) 1.955

DIST4 (D) 2.009

H₂O **DIST5 (D)** 2.243

DIST6 (D) 2.676



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 12

BUDSCU

Reference: F.Charbonnier, R.Faure, H.Loiseleur (1977)
Acta Crystallogr., Sect.B:Struct. Crystallogr.Cryst.Chem. ,**33**,3759

Formula: (C₄ H₁₆ Cu₁ O₁₀ S₂)_n

Compound Name: catena-((μ₂-Butane-1,4-disulfonato-O,O')-tetra-aqua-copper(ii))

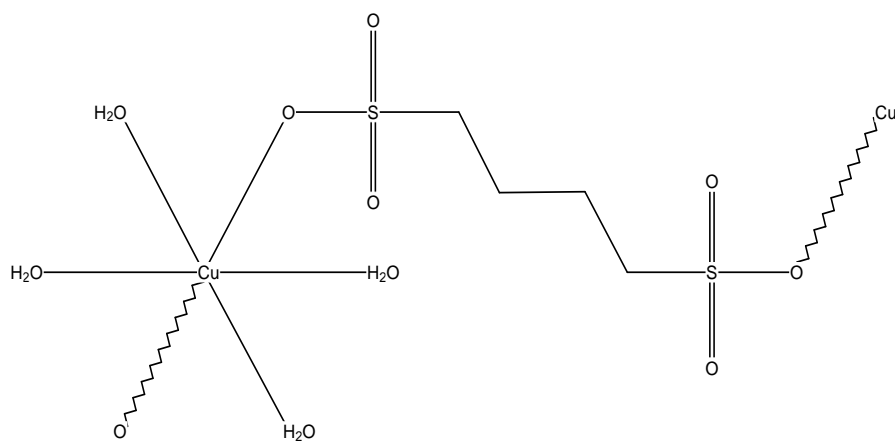
Space Group: P21/c **Cell:** **a** 6.213(0) **b** 9.081(2) **c** 11.324(3)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 108.65(1) **γ** 90.00

R-Factor (%): 2.30 **Temperature(K):** 295 **Density(g/cm³):** 1.930

Parameters

Fragment 1

DIST1 (D)	1.950
DIST2 (D)	1.947
DIST3 (D)	1.950
DIST4 (D)	1.947
DIST5 (D)	2.360
DIST6 (D)	2.360



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 13

BUGCEM

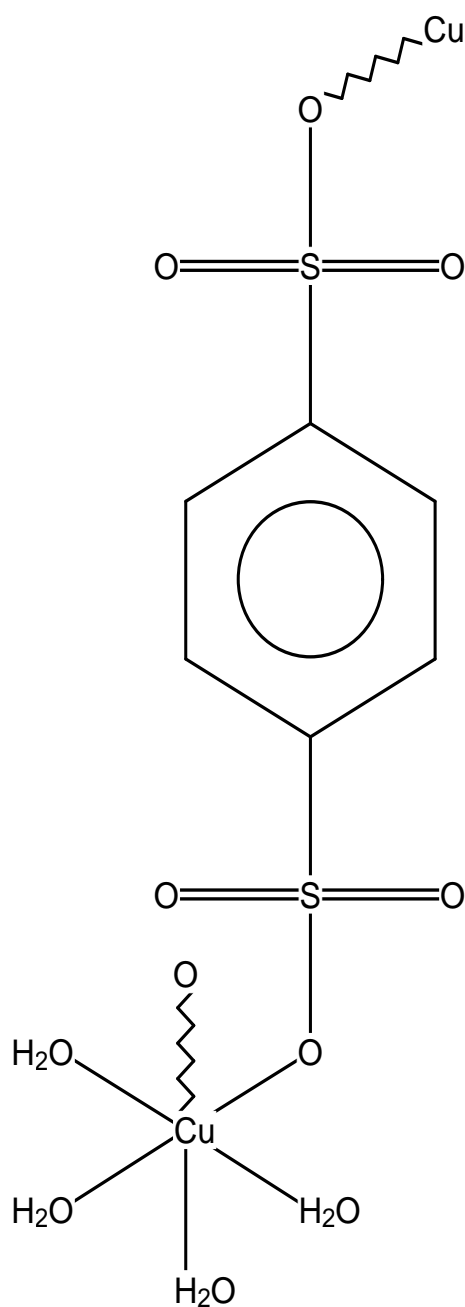
Reference: A.Mietrach, T.W.T.Muesmann, J.Christoffers,
M.S.Wickleder (2009) *Eur.J.Inorg.Chem.* ,5328

Formula: (C₆ H₁₂ Cu₁ O₁₀ S₂)_n

Compound Name: catena-((μ₂-benzene-1,4-disulfonato)-tetraaqua-copper(ii))

Space Group: P21/n **Cell:** **a** 5.975(0) **b** 10.936(0) **c** 9.922(0)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 105.17(0) **γ** 90.00

R-Factor (%): 1.98 **Temperature(K):** 153 **Density(g/cm³):** 1.973



Parameters

Fragment 1

DIST1 (D)	1.963
DIST2 (D)	1.938
DIST3 (D)	1.963
DIST4 (D)	1.938
DIST5 (D)	2.412
DIST6 (D)	2.412

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 14

BUGCIQ

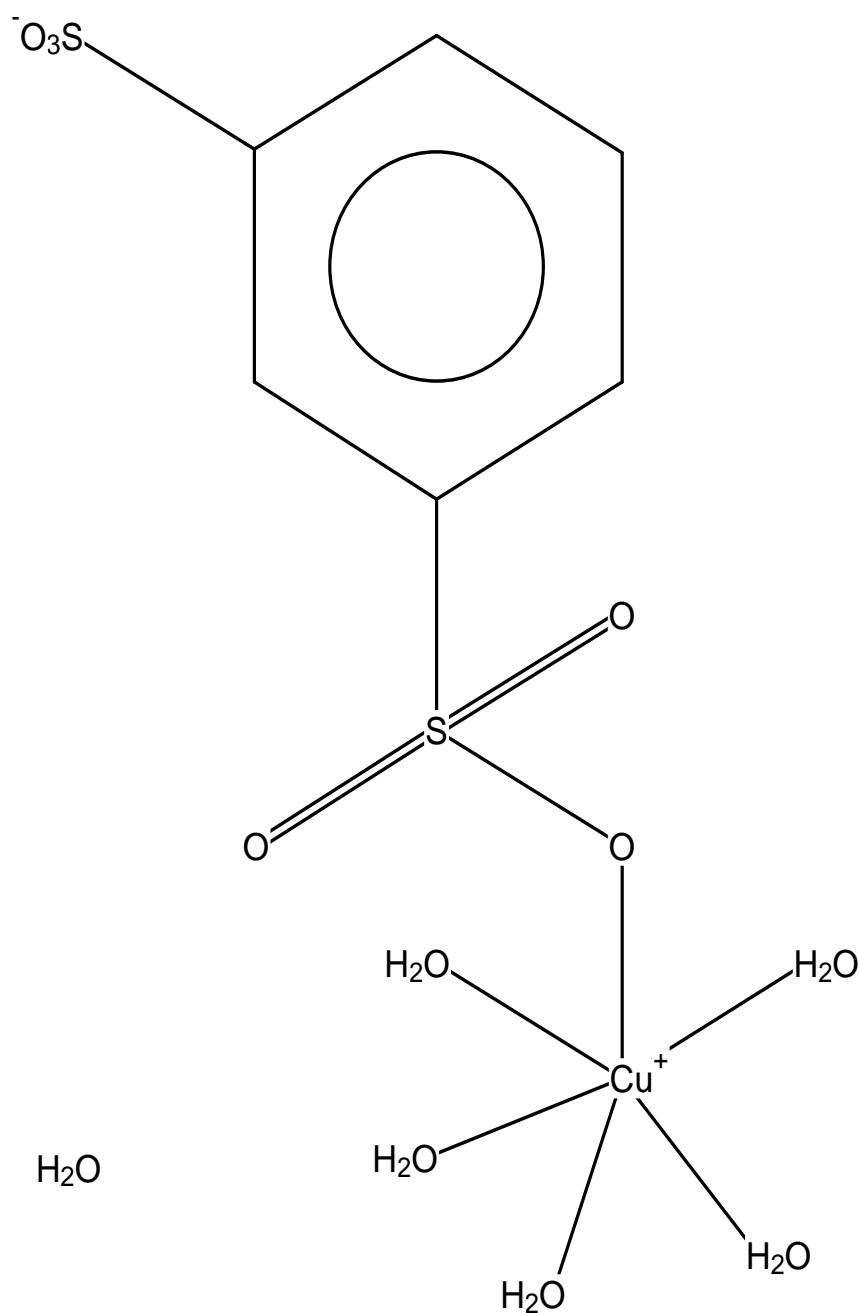
Reference: A.Mietrach, T.W.T.Muesmann, J.Christoffers,
M.S.Wickleder (2009) *Eur.J.Inorg.Chem.* ,5328

Formula: C₆ H₁₄ Cu₁ O₁₁ S₂,H₂ O₁

Compound Name: Pentaqua-(benzene-1,3-disulfonato)-copper(ii) monohydrate

Space Group: P21/n **Cell:** **a** 6.321(0) **b** 20.226(1) **c** 11.283(0)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 99.26(0) **γ** 90.00

R-Factor (%): 1.95 **Temperature(K):** 153 **Density(g/cm³):** 1.903



Parameters

Fragment 1

DIST1 (D)	1.948
DIST2 (D)	2.000
DIST3 (D)	2.004
DIST4 (D)	1.962
DIST5 (D)	2.337
DIST6 (D)	2.292

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 15

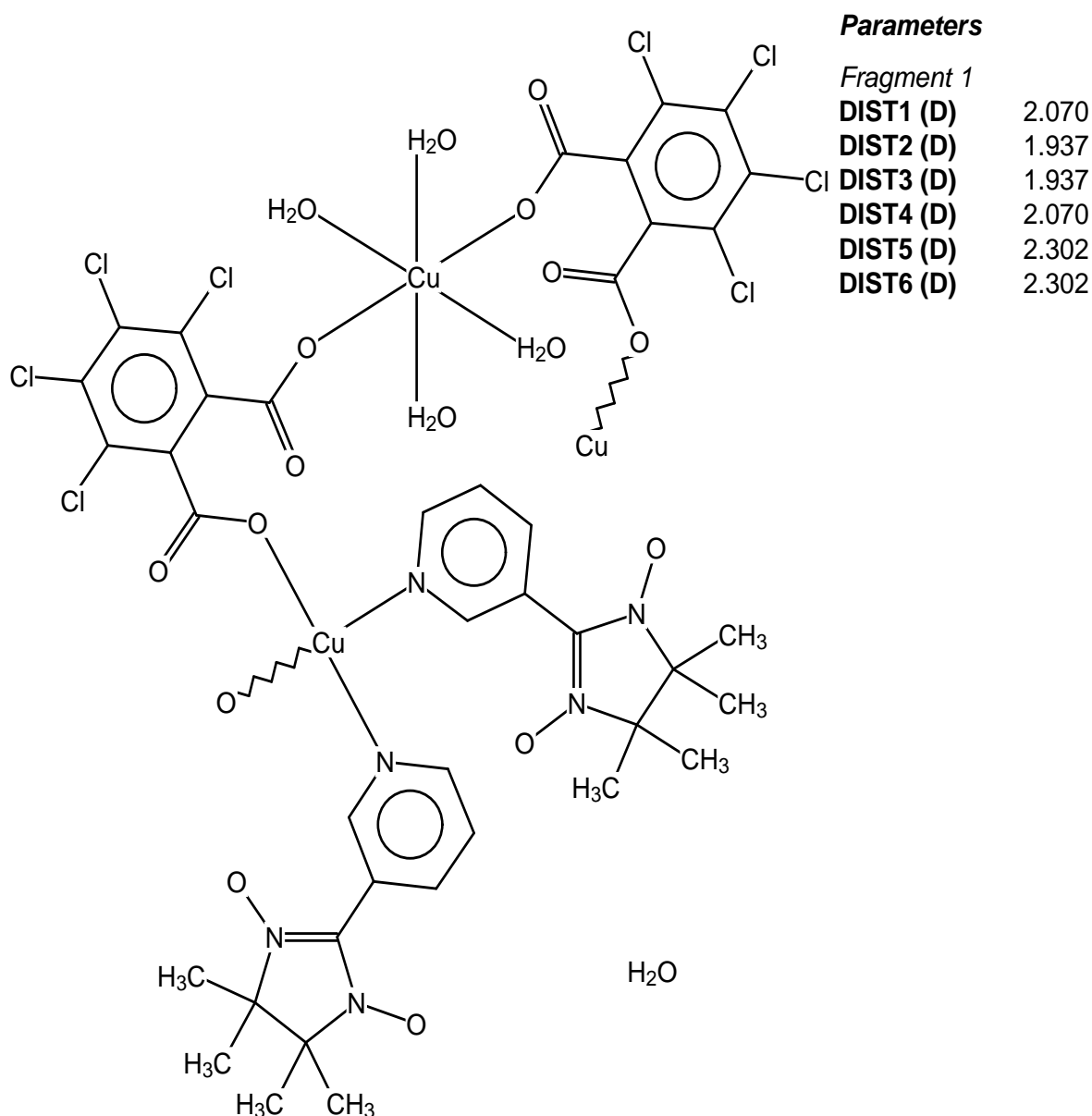
BUSWUI

Reference: Yue Ma, XiaoPing Chen, Dong Cao, ShiPing Yan, DaiZheng Liao (2009) *Sci.China,Ser.B:Chem.* ,52,1438

Formula: $(C_{40} H_{40} Cl_8 Cu_2 N_6 O_{16})_n \cdot 2n(H_2 O)_1$

Compound Name: catena-(bis(μ_2 -3,4,5,6-tetrachlorophthalato)-bis(2-(3'-pyridyl)-4,4,5,5-tetramethylimidazoline-1-oxyl-3-oxide-N)-tetra-aqua-di-copper(ii) dihydrate)

Space Group: P-1 **Cell:** **a** 7.424(2) **b** 11.256(2) **c** 16.495(4)
Space Group No.: 2 (**Å, °**) α 70.32(0) β 86.06(0) γ 80.10(0)
R-Factor (%): 2.80 **Temperature(K):** 293 **Density(g/cm³):** 1.698



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 16

CABYEJ01

Reference: Yu-fang Pan, Wen-guan Lu (2006)
Jiangxi Shifan Daxue Xuebao Ziran Kexueban(Chin.)(J.Jiangxi Normal Univ.(Nat.Sci.))
30,209

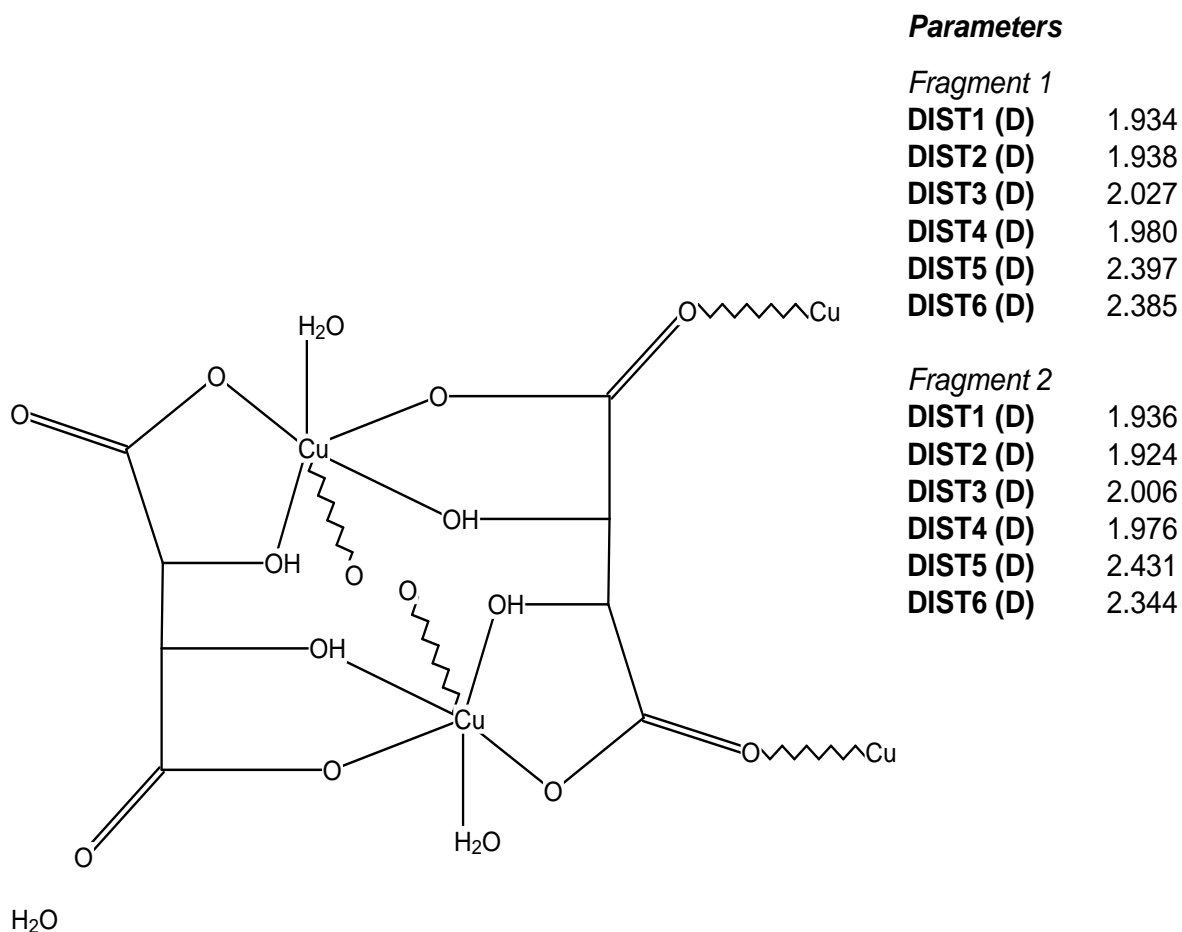
Formula: $(C_8 H_{12} Cu_2 O_{14})_n \cdot 4n(H_2 O)_1$

Compound Name: catena-((μ_4 -(S,S)-Tartrato)-(μ_2 -(S,S)-tartrato)-diaqua-di-copper(ii) tetrahydrate)

Space Group: P21 **Cell:** **a** 8.370(2) **b** 8.755(2) **c** 12.127(3)

Space Group No.: 4 **(Å, °)** α 90.00 β 104.54(2) γ 90.00

R-Factor (%): 2.32 **Temperature(K):** 296 **Density(g/cm³):** 2.051



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 17

CAMZUM

Reference: S.Bieller, H.-W.Lerner, M.Bolte (2005)
Acta Crystallogr., Sect.E:Struct.Rep.Online ,61,m928

Formula: $C_{12} H_{36} Cu_1 O_6 S_6^{2+}, 2(H_1 O_4 S_1^{1-})$

Compound Name: hexakis(Dimethylsulfoxide)copper(ii) bis(hydrogen sulfate)

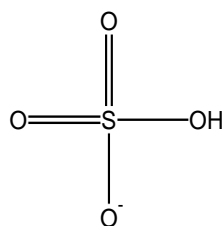
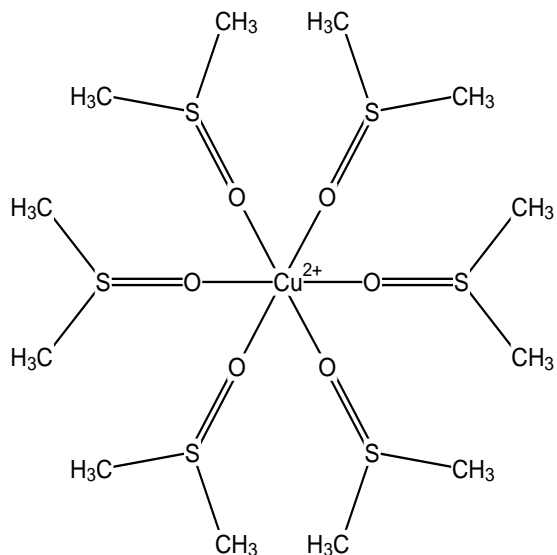
Space Group: P-1 **Cell:** **a** 8.227(0) **b** 9.466(0) **c** 9.595(0)
Space Group No.: 2 **(Å, °)** α 97.56(0) β 90.42(0) γ 90.24(0)

R-Factor (%): 2.32 **Temperature(K):** 173 **Density(g/cm³):** 1.629

Parameters

Fragment 1

DIST1 (D)	1.976
DIST2 (D)	2.022
DIST3 (D)	1.976
DIST4 (D)	2.022
DIST5 (D)	2.344
DIST6 (D)	2.344



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 18

CDACDH25

Reference: C.J.Simmons, H.Stratemeier, M.A.Hitchman, D.Reinen, V.M.Masters, M.J.Riley (2011) *Inorg.Chem.* ,50,4900

Formula: C₆ H₁₄ Cu₁ O₈

Compound Name: trans-Diaqua-bis(2-methoxyacetato-O,O')-copper(ii)

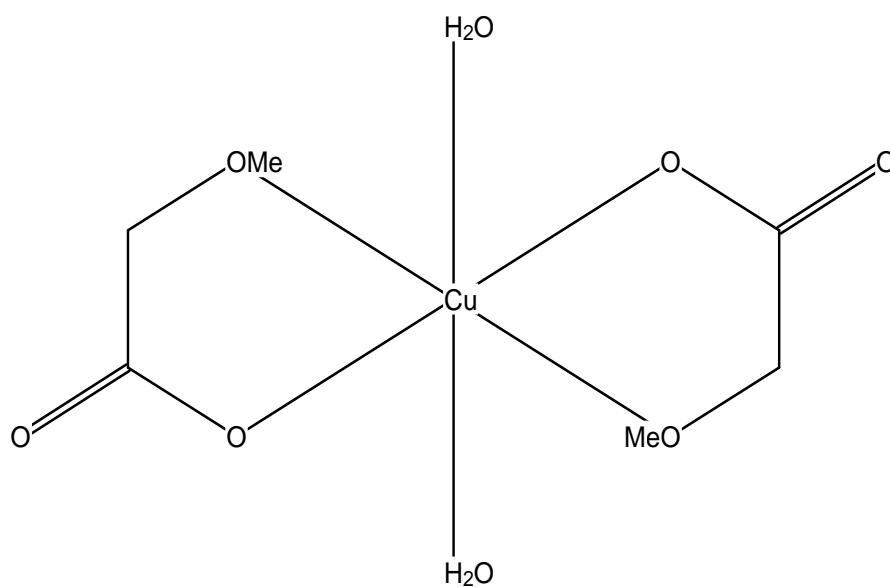
Space Group: P21/n **Cell:** **a** 6.974(0) **b** 10.181(0) **c** 7.242(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 96.88(0) γ 90.00

R-Factor (%): 2.20 **Temperature(K):** 320 **Density(g/cm³):** 1.806

Parameters

Fragment 1

DIST1 (D)	1.928
DIST2 (D)	1.928
DIST3 (D)	2.133
DIST4 (D)	2.169
DIST5 (D)	2.133
DIST6 (D)	2.169



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 19

CICYET01

Reference: M.Fainerman-Melnikova, J.K.Clegg, A.A.H.Pakchung, P.Jensen, R.Codd (2010) *CrystEngComm* ,12,4217

Formula: (C₁₄ H₂₀ Cu₂ O₂₀)_n

Compound Name: catena-[bis(μ₂-4-Pyranone-2,6-dicarboxylato)-octaaqua-di-copper]

Space Group: P-1 **Cell:** **a** 4.966(1) **b** 9.909(3) **c** 10.491(4)
Space Group No.: 2 **(Å, °)** α 94.10(0) β 94.91(0) γ 97.22(0)

R-Factor (%): 2.57 **Temperature(K):** 150 **Density(g/cm³):** 2.075

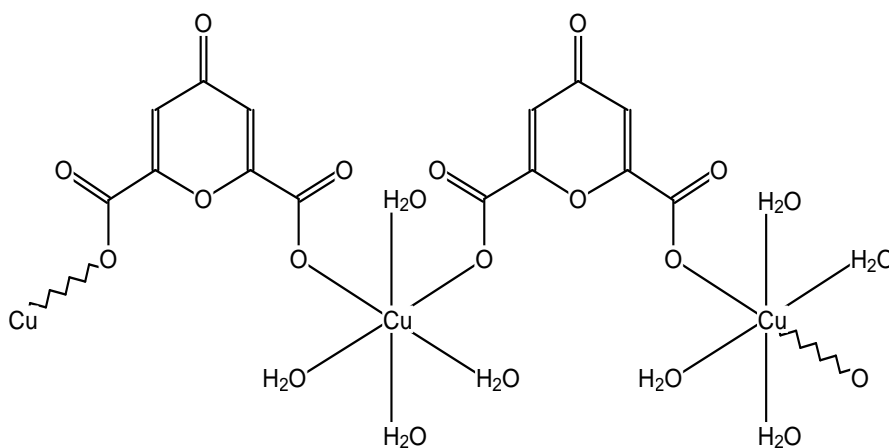
Parameters

Fragment 1

DIST1 (D) 1.973
DIST2 (D) 1.983
DIST3 (D) 1.983
DIST4 (D) 1.973
DIST5 (D) 2.455
DIST6 (D) 2.455

Fragment 2

DIST1 (D) 1.911
DIST2 (D) 1.962
DIST3 (D) 1.911
DIST4 (D) 1.962
DIST5 (D) 2.534
DIST6 (D) 2.534



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 20

CIWTOT

Reference: D.Fischer, T.M.Klapotke, M.Reymann, J.Stierstorfer
(2014) *Chem.-Eur.J.* ,**20**,6401

Formula: (C₄ H₈ Cu₁ N₁₀ O₁₀)_n

Compound Name: catena-[(μ_2 -(diazene-1,2-diyl-di-1,2,5-oxadiazole-4,3-diyl)
bis(nitroazanide))-tetraaqua-copper(ii)]

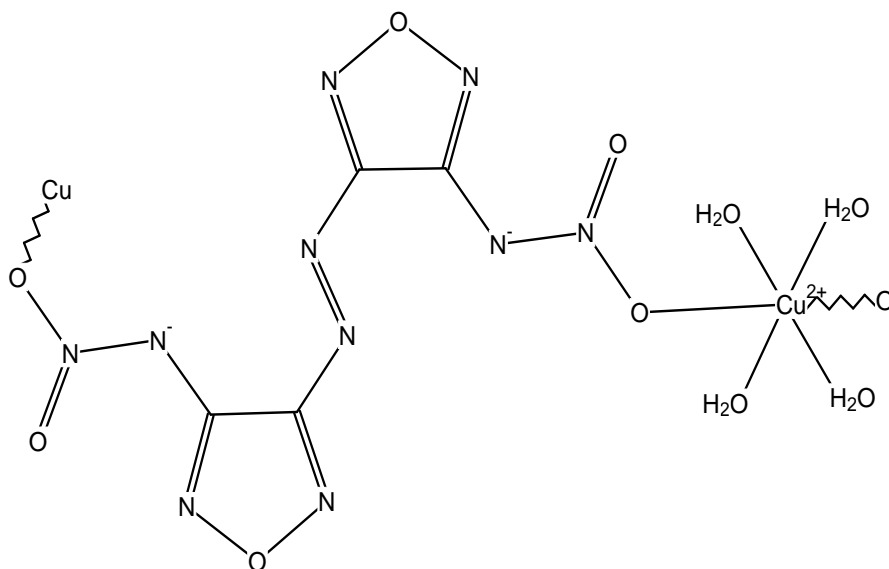
Space Group: P-1 **Cell:** **a** 4.931(0) **b** 7.937(0) **c** 8.493(0)
Space Group No.: 2 (**Å, °**) α 68.91(0) β 83.97(0) γ 86.09(0)

R-Factor (%): 2.62 **Temperature(K):** 100 **Density(g/cm³):** 2.261

Parameters

Fragment 1

DIST1 (D)	1.947
DIST2 (D)	1.991
DIST3 (D)	1.947
DIST4 (D)	1.991
DIST5 (D)	2.349
DIST6 (D)	2.349



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 21

COWTUE

Reference: Chih-Chieh Wang, Meu-Ju Ke, Cheng-Hsiao Tsai, I-Hsuan Chen, Shin-I Lin, Tzuen-Yeuan Lin, Li-Mei Wu, Gene-Hsiang Lee, Hwo-Shuenn Sheu, V.E.Fedorov (2009) *Cryst. Growth Des.* ,9,1013

Formula: (C₁₄ H₂₀ Cu₂ N₄ O₁₂)_n

Compound Name: catena-(bis(μ₂-croconato)-diaqua-bis(ethylenediamine)-di-copper(ii))

Synonym: catena-(bis(μ₂-4,5-dioxycyclopent-4-ene-1,2,3-trione)-diaqua-bis(ethylenediamine)-di-copper(ii))

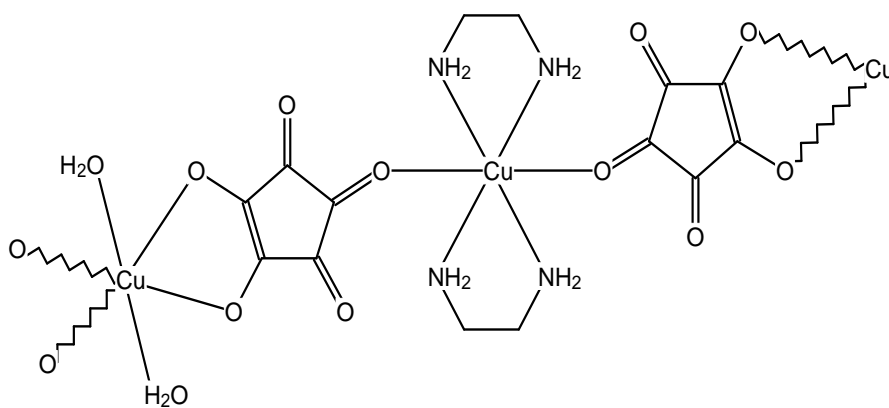
Space Group: P21/c **Cell:** **a** 10.007(0) **b** 13.944(0) **c** 7.010(0)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 98.08(0) **γ** 90.00

R-Factor (%): 2.58 **Temperature(K):** 295 **Density(g/cm³):** 1.932

Parameters

Fragment 1

DIST1 (D) 1.957
DIST2 (D) 1.991
DIST3 (D) 1.991
DIST4 (D) 1.957
DIST5 (D) 2.417
DIST6 (D) 2.417



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 22

CUACDH03

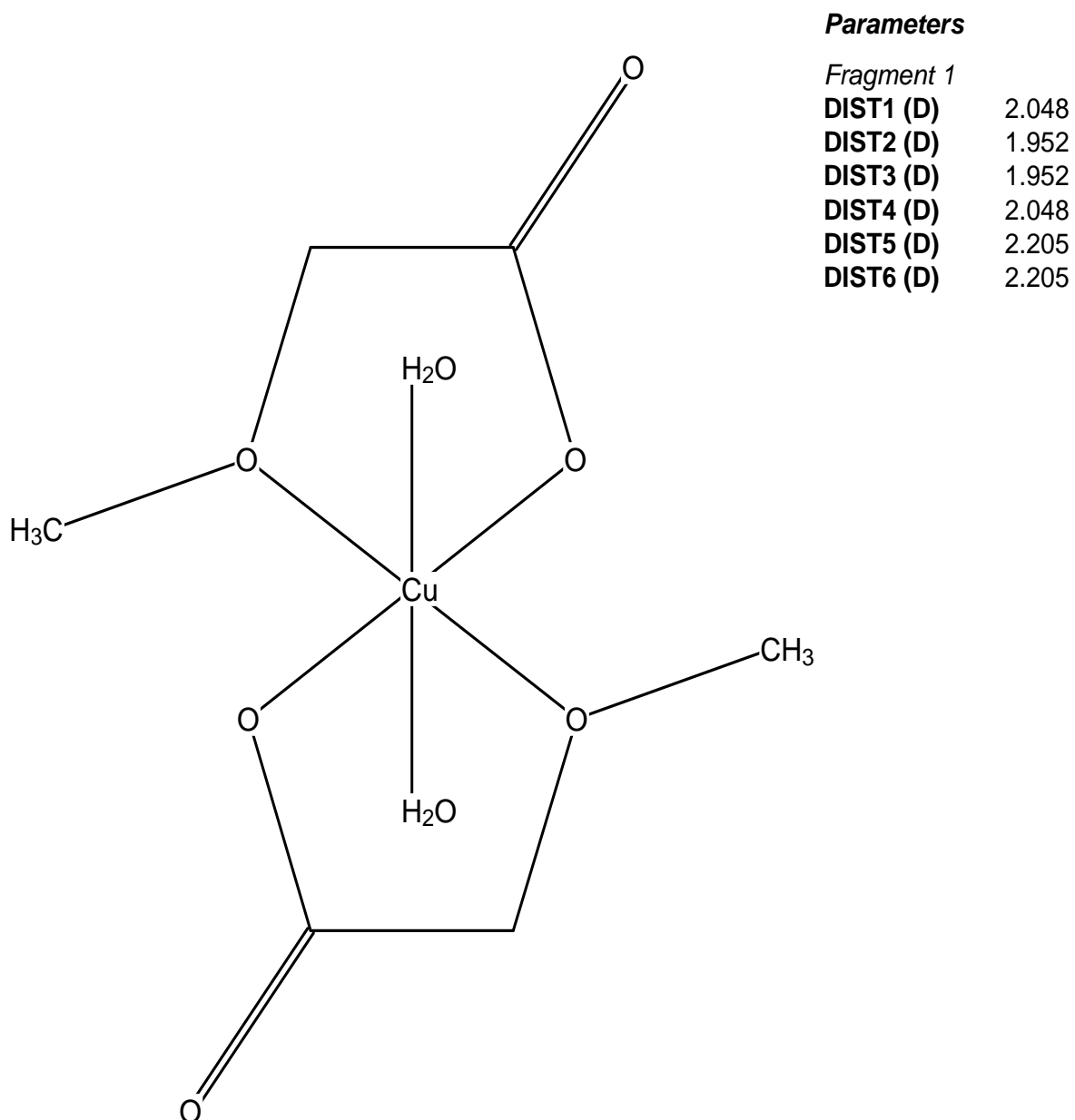
Reference: K.Prout, A.Edwards, V.Mtetwa, J.Murray, J.F.Saunders, F.J.C.Rossotti (1997) *Inorg.Chem.* ,**36**,2820

Formula: C₆ H₁₄ Cu₁ O₈

Compound Name: trans-Diaqua-bis(methoxyacetato)-copper(ii)

Space Group: P1121/n **Cell:** **a** 6.900(2) **b** 7.190(1) **c** 9.874(2)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 90.00 **γ** 95.70(1)

R-Factor (%): 2.45 **Temperature(K):** 125 **Density(g/cm³):** 1.892



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 23

CUACDH11

Reference: H.-L.Zhu, Q.-F.Zeng, D.-S.Xia, X.-L.Zhu, X.Liu,
D.-Q.Wang (2003) *Z.Kristallogr.-New Cryst.Struct.* ,**218**,315

Formula: C₆ H₁₄ Cu₁ O₈

Compound Name: Diaqua-bis(2-methoxyacetato-O,O')-copper(ii)

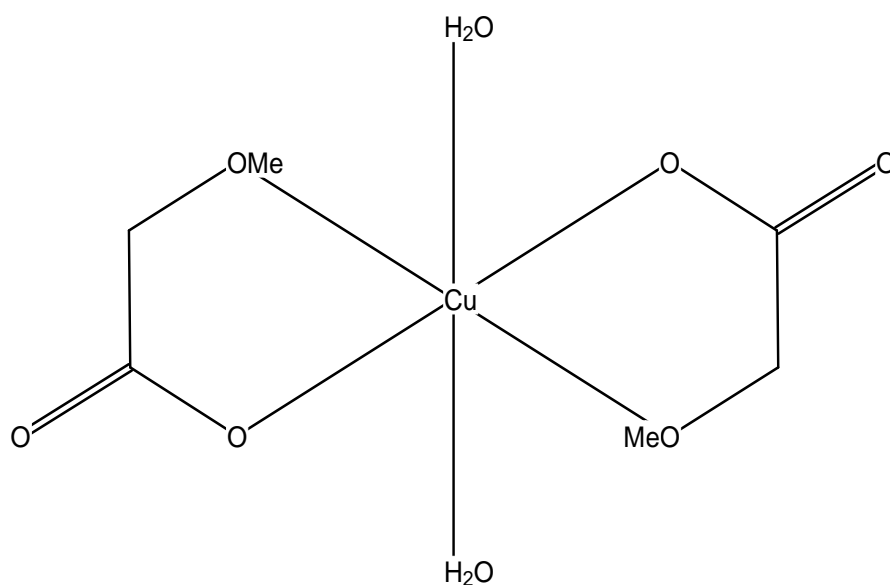
Space Group: P21/n **Cell:** **a** 6.955(1) **b** 10.123(2) **c** 7.226(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 96.57(1) γ 90.00

R-Factor (%): 2.57 **Temperature(K):** 292 **Density(g/cm³):** 1.825

Parameters

Fragment 1

DIST1 (D)	1.932
DIST2 (D)	1.932
DIST3 (D)	2.147
DIST4 (D)	2.138
DIST5 (D)	2.147
DIST6 (D)	2.138



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 24

CUACDH13

Reference: C.J.Simmons, H.Stratemeier, M.A.Hitchman, D.Reinen, V.M.Masters, M.J.Riley (2011) *Inorg.Chem.* ,50,4900

Formula: C₆ H₁₄ Cu₁ O₈

Compound Name: trans-Diaqua-bis(2-methoxyacetato-O,O')-copper(ii)

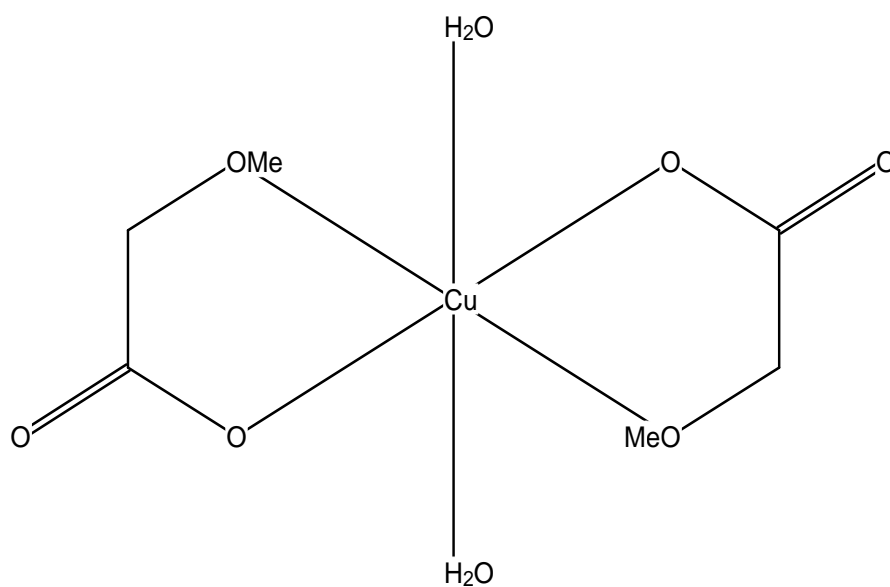
Space Group: P21/n **Cell:** **a** 6.898(0) **b** 9.858(0) **c** 7.197(0)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 95.71(0) **γ** 90.00

R-Factor (%): 1.80 **Temperature(K):** 90 **Density(g/cm³):** 1.894

Parameters

Fragment 1

DIST1 (D) 2.042
DIST2 (D) 1.955
DIST3 (D) 1.955
DIST4 (D) 2.042
DIST5 (D) 2.205
DIST6 (D) 2.205



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 25

CUACDH14

Reference: C.J.Simmons, H.Stratemeier, M.A.Hitchman, D.Reinen, V.M.Masters, M.J.Riley (2011) *Inorg.Chem.* ,50,4900

Formula: C₆ H₁₄ Cu₁ O₈

Compound Name: trans-Diaqua-bis(2-methoxyacetato-O,O')-copper(ii)

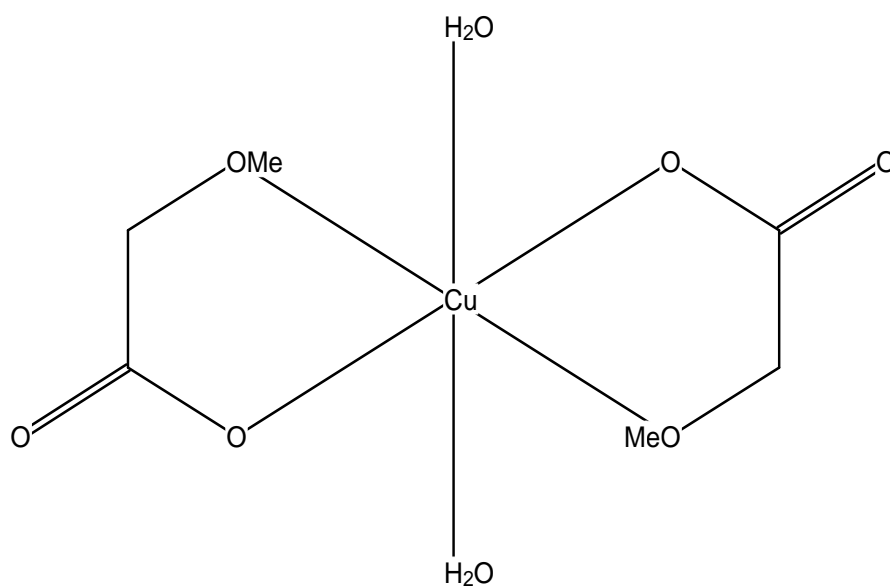
Space Group: P21/n **Cell:** **a** 6.902(0) **b** 9.881(0) **c** 7.198(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 95.73(0) γ 90.00

R-Factor (%): 1.80 **Temperature(K):** 120 **Density(g/cm³):** 1.888

Parameters

Fragment 1

DIST1 (D) 2.047
DIST2 (D) 1.954
DIST3 (D) 1.954
DIST4 (D) 2.047
DIST5 (D) 2.203
DIST6 (D) 2.203



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 26

CUACDH15

Reference: C.J.Simmons, H.Stratemeier, M.A.Hitchman, D.Reinen, V.M.Masters, M.J.Riley (2011) *Inorg.Chem.* ,50,4900

Formula: C₆ H₁₄ Cu₁ O₈

Compound Name: trans-Diaqua-bis(2-methoxyacetato-O,O')-copper(ii)

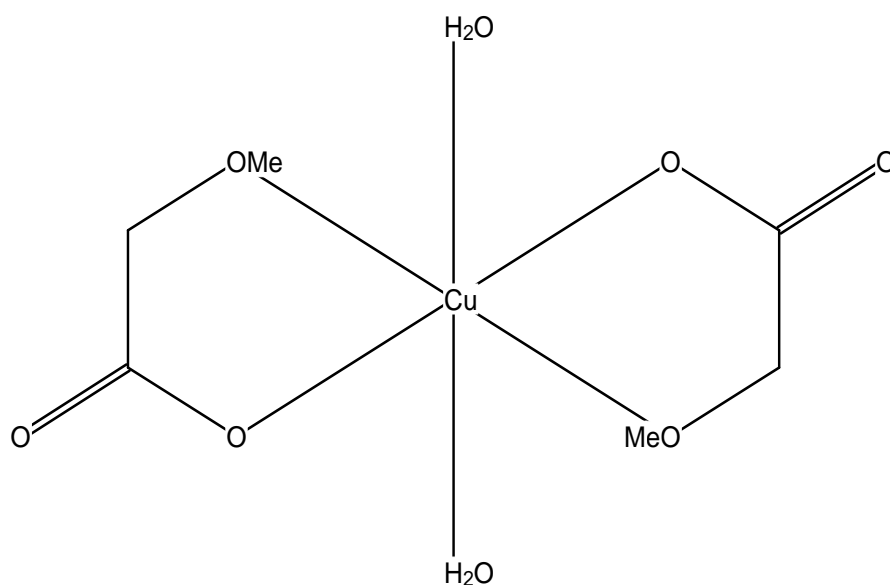
Space Group: P21/n **Cell:** **a** 6.905(0) **b** 9.899(0) **c** 7.200(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 95.75(0) γ 90.00

R-Factor (%): 1.85 **Temperature(K):** 140 **Density(g/cm³):** 1.884

Parameters

Fragment 1

DIST1 (D)	2.052
DIST2 (D)	1.952
DIST3 (D)	1.952
DIST4 (D)	2.052
DIST5 (D)	2.201
DIST6 (D)	2.201



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 27

CUACDH16

Reference: C.J.Simmons, H.Stratemeier, M.A.Hitchman, D.Reinen, V.M.Masters, M.J.Riley (2011) *Inorg.Chem.* ,50,4900

Formula: C₆ H₁₄ Cu₁ O₈

Compound Name: trans-Diaqua-bis(2-methoxyacetato-O,O')-copper(ii)

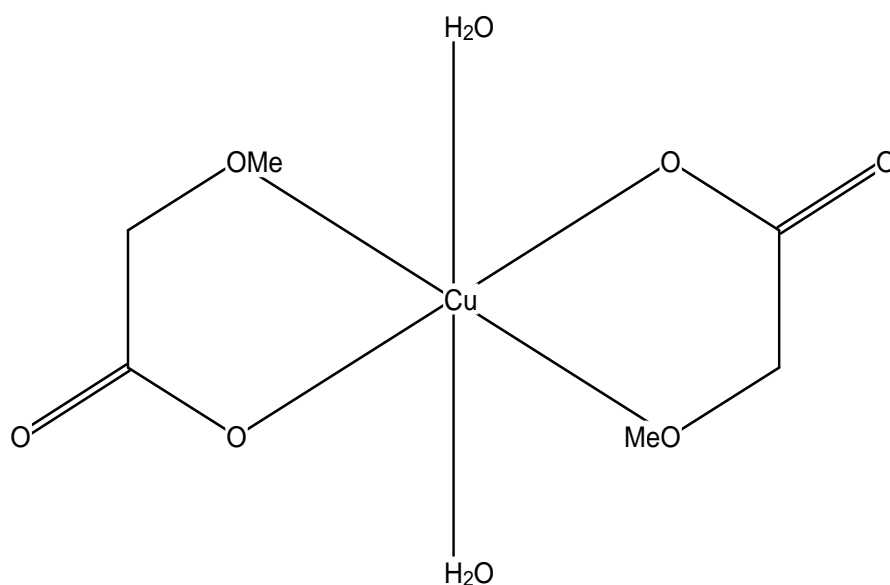
Space Group: P21/n **Cell:** **a** 6.908(0) **b** 9.920(0) **c** 7.201(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 95.78(0) γ 90.00

R-Factor (%): 1.90 **Temperature(K):** 160 **Density(g/cm³):** 1.878

Parameters

Fragment 1

DIST1 (D)	1.951
DIST2 (D)	1.951
DIST3 (D)	2.199
DIST4 (D)	2.059
DIST5 (D)	2.199
DIST6 (D)	2.059



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 28

CUACDH17

Reference: C.J.Simmons, H.Stratemeier, M.A.Hitchman, D.Reinen, V.M.Masters, M.J.Riley (2011) *Inorg.Chem.* ,50,4900

Formula: C₆ H₁₄ Cu₁ O₈

Compound Name: trans-Diaqua-bis(2-methoxyacetato-O,O')-copper(ii)

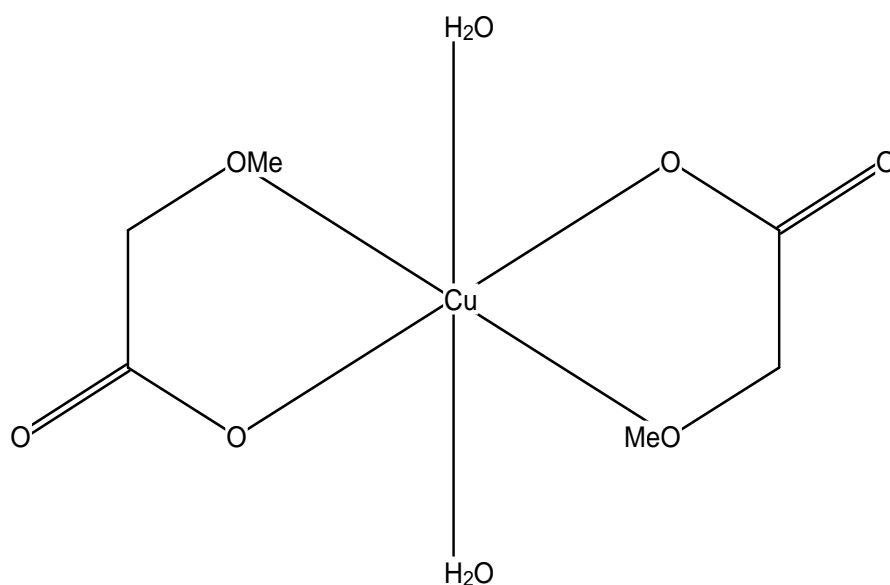
Space Group: P21/n **Cell:** **a** 6.913(0) **b** 9.945(0) **c** 7.204(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 95.84(0) γ 90.00

R-Factor (%): 1.98 **Temperature(K):** 180 **Density(g/cm³):** 1.872

Parameters

Fragment 1

DIST1 (D)	1.949
DIST2 (D)	1.949
DIST3 (D)	2.191
DIST4 (D)	2.066
DIST5 (D)	2.191
DIST6 (D)	2.066



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 29

CUACDH18

Reference: C.J.Simmons, H.Stratemeier, M.A.Hitchman, D.Reinen, V.M.Masters, M.J.Riley (2011) *Inorg.Chem.* ,50,4900

Formula: C₆ H₁₄ Cu₁ O₈

Compound Name: trans-Diaqua-bis(2-methoxyacetato-O,O')-copper(ii)

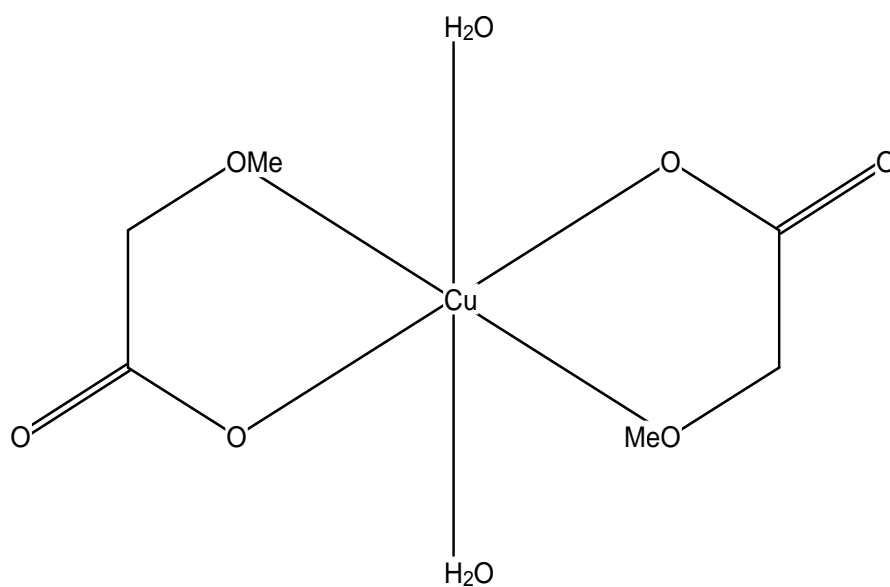
Space Group: P21/n **Cell:** **a** 6.919(0) **b** 9.973(0) **c** 7.207(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 95.94(0) γ 90.00

R-Factor (%): 2.00 **Temperature(K):** 200 **Density(g/cm³):** 1.865

Parameters

Fragment 1

DIST1 (D)	1.946
DIST2 (D)	1.946
DIST3 (D)	2.187
DIST4 (D)	2.074
DIST5 (D)	2.187
DIST6 (D)	2.074



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 30

CUACDH19

Reference: C.J.Simmons, H.Stratemeier, M.A.Hitchman, D.Reinen, V.M.Masters, M.J.Riley (2011) *Inorg.Chem.* ,50,4900

Formula: C₆ H₁₄ Cu₁ O₈

Compound Name: trans-Diaqua-bis(2-methoxyacetato-O,O')-copper(ii)

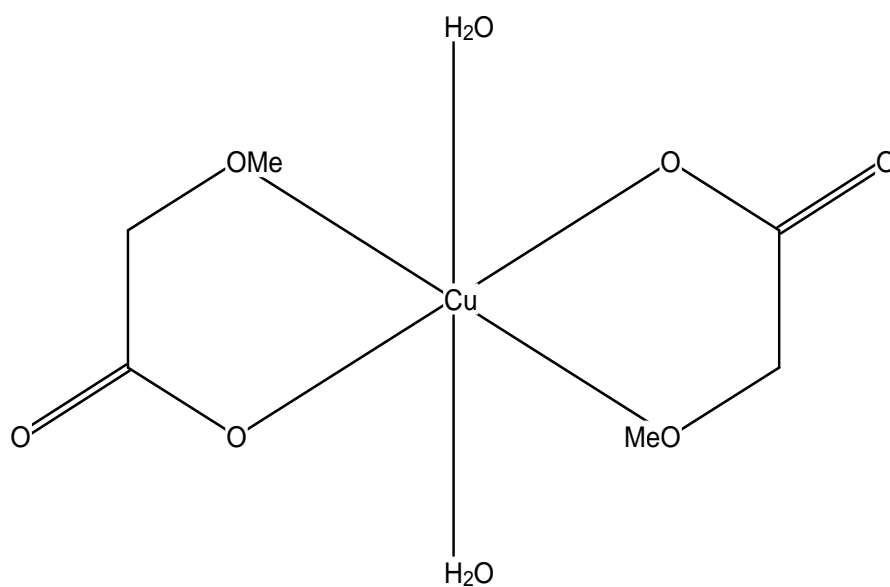
Space Group: P21/n **Cell:** **a** 6.926(0) **b** 10.005(0) **c** 7.211(0)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 96.06(0) **γ** 90.00

R-Factor (%): 2.08 **Temperature(K):** 220 **Density(g/cm³):** 1.856

Parameters

Fragment 1

DIST1 (D)	1.943
DIST2 (D)	1.943
DIST3 (D)	2.180
DIST4 (D)	2.087
DIST5 (D)	2.180
DIST6 (D)	2.087



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 31

CUACDH20

Reference: C.J.Simmons, H.Stratemeier, M.A.Hitchman, D.Reinen, V.M.Masters, M.J.Riley (2011) *Inorg.Chem.* ,**50**,4900

Formula: C₆ H₁₄ Cu₁ O₈

Compound Name: trans-Diaqua-bis(2-methoxyacetato-O,O')-copper(ii)

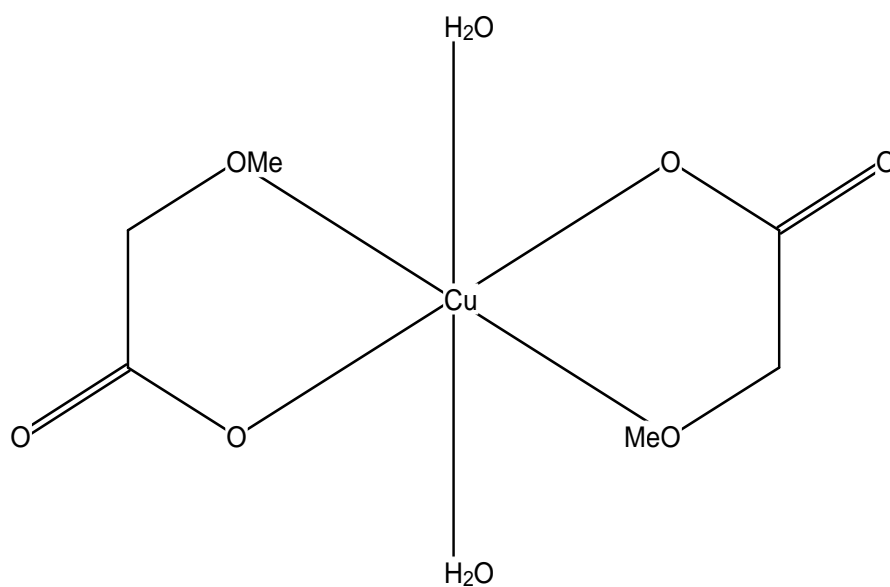
Space Group: P21/n **Cell:** **a** 6.934(0) **b** 10.038(0) **c** 7.216(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 96.19(0) γ 90.00

R-Factor (%): 2.05 **Temperature(K):** 240 **Density(g/cm³):** 1.847

Parameters

Fragment 1

DIST1 (D) 1.939
DIST2 (D) 1.939
DIST3 (D) 2.172
DIST4 (D) 2.102
DIST5 (D) 2.172
DIST6 (D) 2.102



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 32

CUACDH21

Reference: C.J.Simmons, H.Stratemeier, M.A.Hitchman, D.Reinen, V.M.Masters, M.J.Riley (2011) *Inorg.Chem.* ,50,4900

Formula: C₆ H₁₄ Cu₁ O₈

Compound Name: trans-Diaqua-bis(2-methoxyacetato-O,O')-copper(ii)

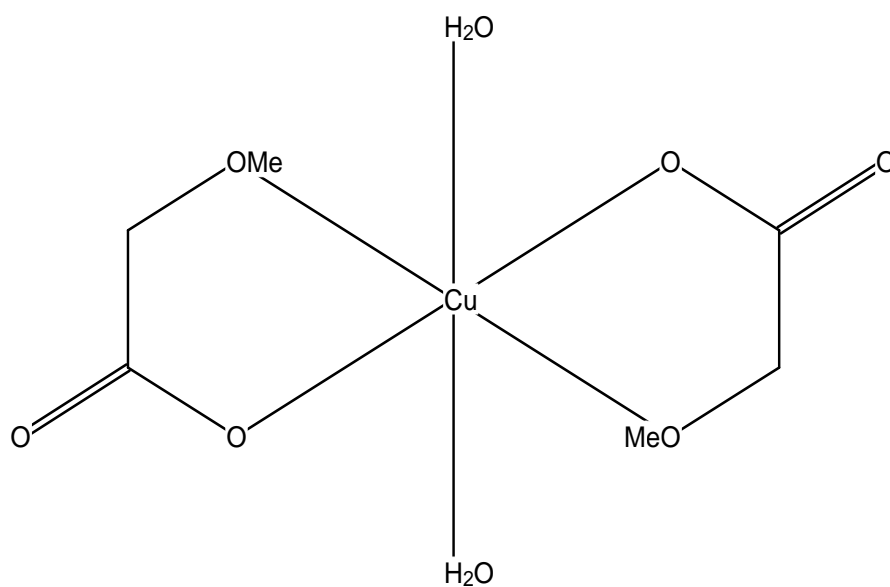
Space Group: P21/n **Cell:** **a** 6.942(0) **b** 10.072(0) **c** 7.221(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 96.34(0) γ 90.00

R-Factor (%): 2.20 **Temperature(K):** 260 **Density(g/cm³):** 1.838

Parameters

Fragment 1

DIST1 (D)	1.937
DIST2 (D)	1.937
DIST3 (D)	2.163
DIST4 (D)	2.114
DIST5 (D)	2.163
DIST6 (D)	2.114



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 33

CUACDH22

Reference: C.J.Simmons, H.Stratemeier, M.A.Hitchman, D.Reinen, V.M.Masters, M.J.Riley (2011) *Inorg.Chem.* ,50,4900

Formula: C₆ H₁₄ Cu₁ O₈

Compound Name: trans-Diaqua-bis(2-methoxyacetato-O,O')-copper(ii)

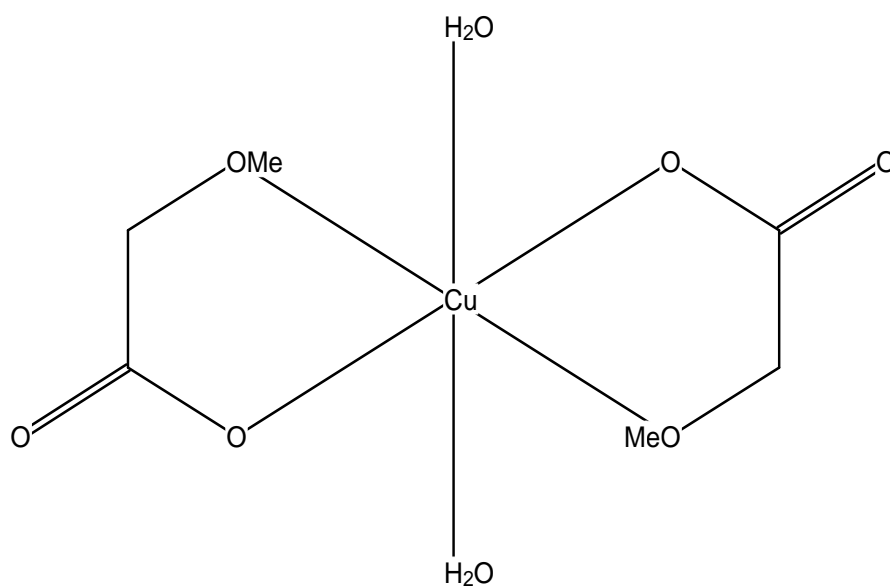
Space Group: P21/n **Cell:** **a** 6.953(0) **b** 10.110(0) **c** 7.227(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 96.52(0) γ 90.00

R-Factor (%): 2.19 **Temperature(K):** 280 **Density(g/cm³):** 1.828

Parameters

Fragment 1

DIST1 (D)	1.933
DIST2 (D)	1.933
DIST3 (D)	2.150
DIST4 (D)	2.134
DIST5 (D)	2.150
DIST6 (D)	2.134



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 34

CUACDH23

Reference: C.J.Simmons, H.Stratemeier, M.A.Hitchman, D.Reinen, V.M.Masters, M.J.Riley (2011) *Inorg.Chem.* ,50,4900

Formula: C₆ H₁₄ Cu₁ O₈

Compound Name: trans-Diaqua-bis(2-methoxyacetato-O,O')-copper(ii)

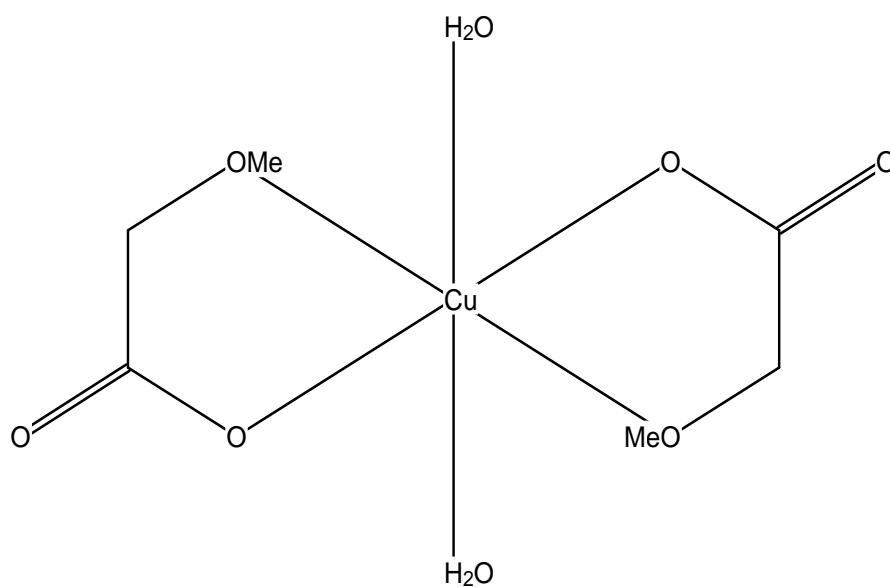
Space Group: P21/n **Cell:** **a** 6.960(0) **b** 10.141(0) **c** 7.232(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 96.67(0) γ 90.00

R-Factor (%): 2.17 **Temperature(K):** 298 **Density(g/cm³):** 1.819

Parameters

Fragment 1

DIST1 (D)	1.931
DIST2 (D)	1.931
DIST3 (D)	2.143
DIST4 (D)	2.146
DIST5 (D)	2.143
DIST6 (D)	2.146



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 35

CUACDH24

Reference: C.J.Simmons, H.Stratemeier, M.A.Hitchman, D.Reinen, V.M.Masters, M.J.Riley (2011) *Inorg.Chem.* ,50,4900

Formula: C₆ H₁₄ Cu₁ O₈

Compound Name: trans-Diaqua-bis(2-methoxyacetato-O,O')-copper(ii)

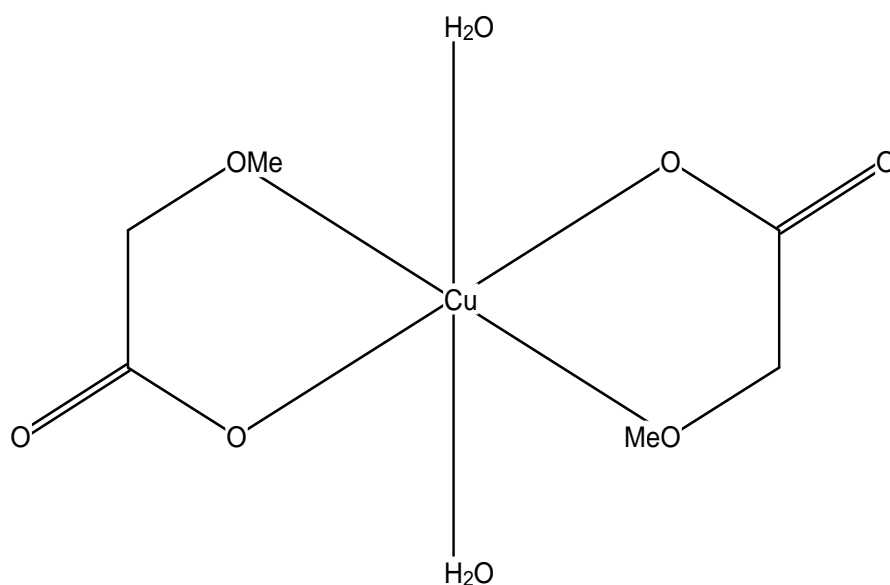
Space Group: P21/n **Cell:** **a** 6.968(0) **b** 10.163(0) **c** 7.238(0)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 96.78(0) **γ** 90.00

R-Factor (%): 2.30 **Temperature(K):** 310 **Density(g/cm³):** 1.812

Parameters

Fragment 1

DIST1 (D)	1.930
DIST2 (D)	1.930
DIST3 (D)	2.138
DIST4 (D)	2.159
DIST5 (D)	2.138
DIST6 (D)	2.159



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 36

CUACDH26

Reference: C.J.Simmons, H.Stratemeier, M.A.Hitchman, D.Reinen, V.M.Masters, M.J.Riley (2011) *Inorg.Chem.* ,50,4900

Formula: C₆ H₁₄ Cu₁ O₈

Compound Name: trans-Diaqua-bis(2-methoxyacetato-O,O')-copper(ii)

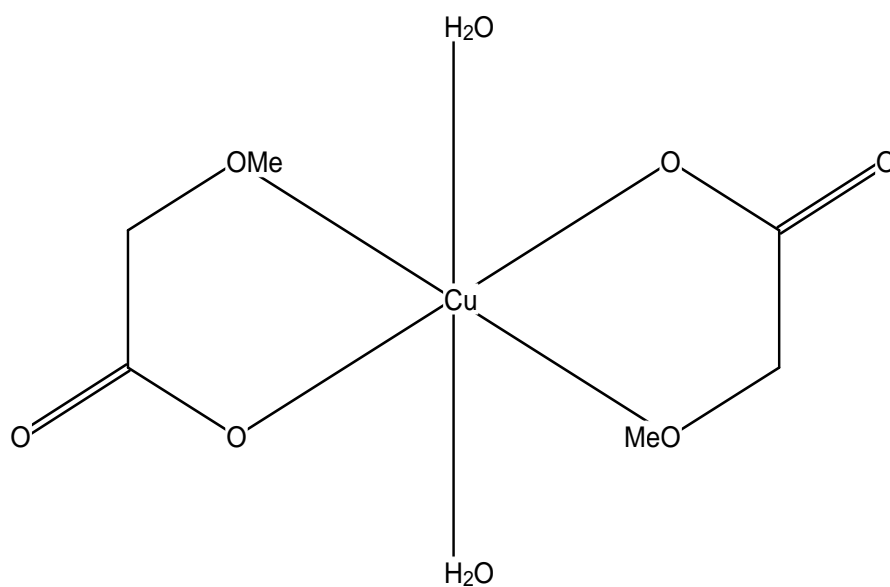
Space Group: P21/n **Cell:** **a** 6.980(0) **b** 10.201(0) **c** 7.247(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 96.98(0) γ 90.00

R-Factor (%): 2.37 **Temperature(K):** 330 **Density(g/cm³):** 1.801

Parameters

Fragment 1

DIST1 (D)	1.927
DIST2 (D)	1.927
DIST3 (D)	2.126
DIST4 (D)	2.175
DIST5 (D)	2.126
DIST6 (D)	2.175



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 37

CUACDH27

Reference: C.J.Simmons, H.Stratemeier, M.A.Hitchman, D.Reinen, V.M.Masters, M.J.Riley (2011) *Inorg.Chem.* ,50,4900

Formula: C₆ H₁₄ Cu₁ O₈

Compound Name: trans-Diaqua-bis(2-methoxyacetato-O,O')-copper(ii)

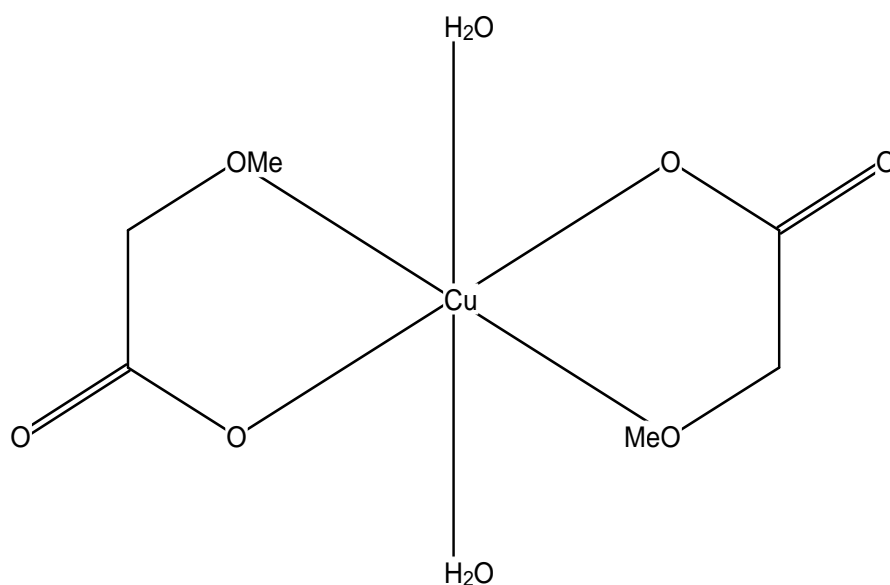
Space Group: P21/n **Cell:** **a** 6.986(0) **b** 10.218(0) **c** 7.252(0)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 97.07(0) **γ** 90.00

R-Factor (%): 2.30 **Temperature(K):** 340 **Density(g/cm³):** 1.795

Parameters

Fragment 1

DIST1 (D)	1.927
DIST2 (D)	1.927
DIST3 (D)	2.122
DIST4 (D)	2.185
DIST5 (D)	2.122
DIST6 (D)	2.185



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 38

CUACDH28

Reference: C.J.Simmons, H.Stratemeier, M.A.Hitchman, D.Reinen, V.M.Masters, M.J.Riley (2011) *Inorg.Chem.* ,50,4900

Formula: C₆ H₁₄ Cu₁ O₈

Compound Name: trans-Diaqua-bis(2-methoxyacetato-O,O')-copper(ii)

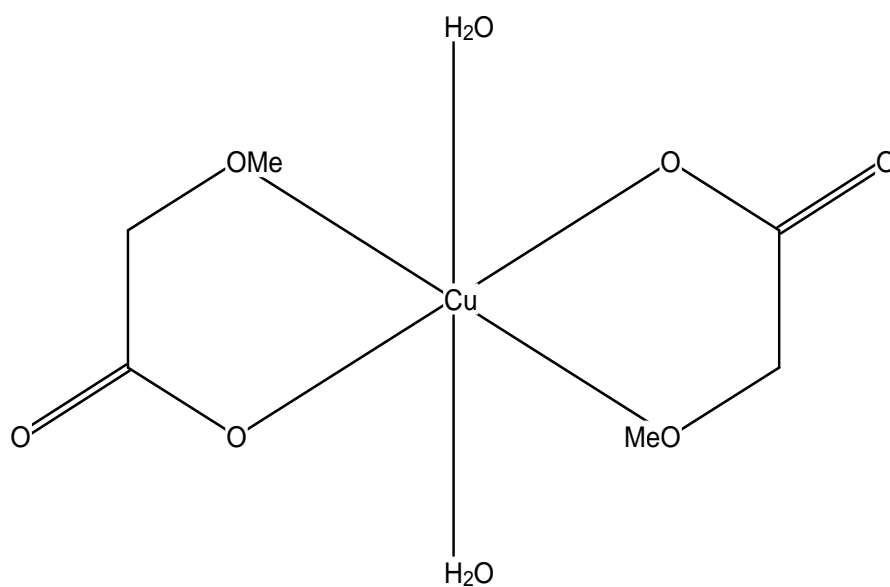
Space Group: P21/n **Cell:** **a** 6.992(0) **b** 10.233(0) **c** 7.256(0)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 97.17(0) **γ** 90.00

R-Factor (%): 2.40 **Temperature(K):** 350 **Density(g/cm³):** 1.791

Parameters

Fragment 1

DIST1 (D)	1.927
DIST2 (D)	1.927
DIST3 (D)	2.115
DIST4 (D)	2.196
DIST5 (D)	2.115
DIST6 (D)	2.196



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 39

CUCROC01

Reference: A.Cornia, A.C.Fabretti, A.Giusti, F.Ferraro, D.Gatteschi
(1993) *Inorg.Chim.Acta* ,**212**,87

Formula: (C₁₀ H₁₂ Cu₂ O₁₆)_n

Compound Name: catena-(Tri-aqua-(μ₂-croconato-O,O,O')-copper(ii))

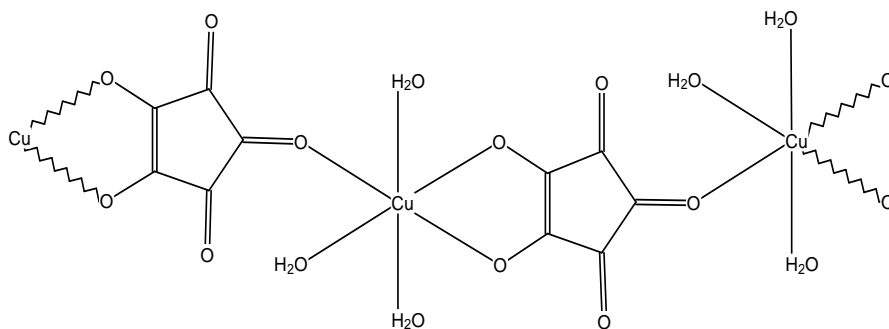
Space Group: Pbc_a **Cell:** **a** 11.770(2) **b** 8.085(2) **c** 15.571(2)
Space Group No.: 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.60 **Temperature(K):** 295 **Density(g/cm³):** 2.310

Parameters

Fragment 1

DIST1 (D)	2.010
DIST2 (D)	1.957
DIST3 (D)	1.979
DIST4 (D)	2.037
DIST5 (D)	2.309
DIST6 (D)	2.334



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 40

CUDTAR05

Reference: Yen-Hsiang Liu, Szu-Hsuan Lee, Jung-Chun Chiang, Po-Chen Chen, P.-H.Chien, Chen-I Yang (2013) *Dalton Trans.* ,**42**, 16857

Formula: $(C_8 H_{12} Cu_2 O_{14})_n \cdot 4(H_2 O)_1$

Compound Name: catena-((μ_4 -(R,R)-Tartrato)-(μ_2 -(R,R)-tartrato)-diaqua-di-copper(ii) tetrahydrate)

Space Group: P21 **Cell:** **a** 8.350(1) **b** 8.747(1) **c** 12.039(1)
Space Group No.: 4 **(\AA , $^\circ$)** α 90.00 β 104.28(0) γ 90.00
R-Factor (%): 2.33 **Temperature(K):** 200 **Density(g/cm³):** 2.071

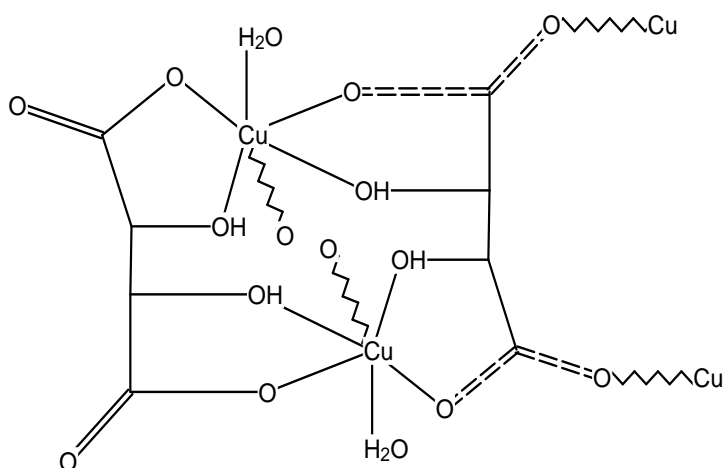
Parameters

Fragment 1

DIST1 (D) 1.941
DIST2 (D) 1.920
DIST3 (D) 2.007
DIST4 (D) 1.971
DIST5 (D) 2.423
DIST6 (D) 2.329

Fragment 2

DIST1 (D) 1.932
DIST2 (D) 1.939
DIST3 (D) 2.019
DIST4 (D) 1.969
DIST5 (D) 2.402
DIST6 (D) 2.369



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 41

CUFOHY02

Reference: M.I.Kay (1975) *Ferroelectrics* ,9,171

Formula: $(C_2 H_6 Cu_1 O_6)_n, 2n(H_2 O_1)$

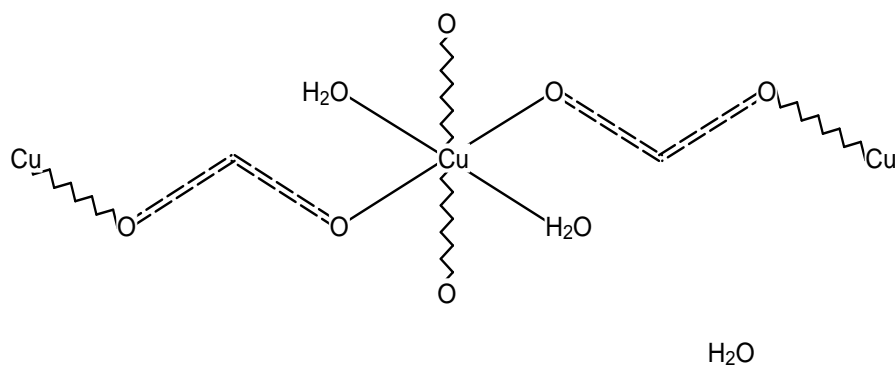
Compound Name: catena-(Diaqua-bis(μ_2 -formate-O,O')-copper(ii) dihydrate)

Space Group:	P21/a	Cell:	a 8.150	b 8.180	c 6.350
Space Group No.:	14	(Å, °)	α 90.00	β 101.08	γ 90.00
R-Factor (%):	2.30	Temperature(K):	295	Density(g/cm³):	1.804

Parameters

Fragment 1

DIST1 (D)	1.999
DIST2 (D)	1.965
DIST3 (D)	1.965
DIST4 (D)	1.999
DIST5 (D)	2.401
DIST6 (D)	2.401



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 42

CUFOHY06

Reference: N.Burger, H.Fuess (1979) *Ferroelectrics* ,22,847

Formula: $(C_2 D_6 Cu_1 O_6)_n, 2n(D_2 O_1)$

Compound Name: catena-(bis(Dideutero-aqua)-bis(μ_2 -deutero-formato-O,O')-copper) bis(deuterium oxide) solvate

Space Group: P21/a **Cell:** **a** 8.184(4) **b** 8.137(4) **c** 6.323(4)

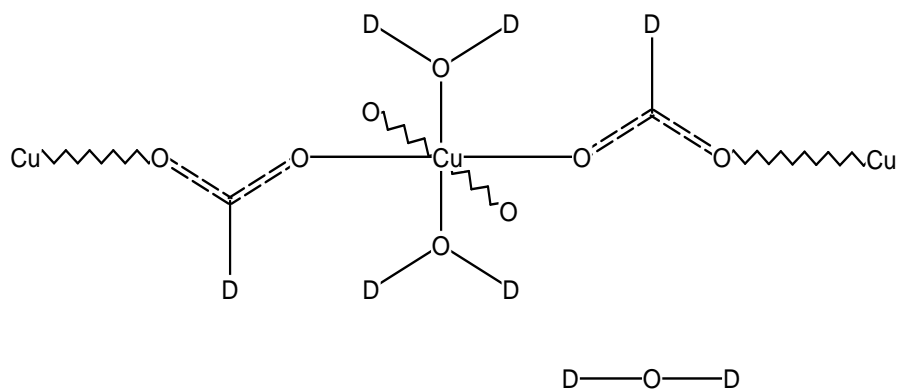
Space Group No.: 14 **(Å, °)** α 90.00 β 100.79(4) γ 90.00

R-Factor (%): 2.20 **Temperature(K):** 296 **Density(g/cm³):** 1.891

Parameters

Fragment 1

DIST1 (D)	1.995
DIST2 (D)	1.964
DIST3 (D)	1.964
DIST4 (D)	1.995
DIST5 (D)	2.386
DIST6 (D)	2.386



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 43

CUGLYC11

Reference: Qing-Song Ye, Ming-Jin Xie, Wei-Ping Liu, Xi-Zhu Chen, Qiao-Wen Chang, Yao Yu (2010) *Z.Kristallogr.-New Cryst.Struct.* ,**225**, 481

Formula: (C₄ H₆ Cu₁ O₆)_n

Compound Name: catena-(bis(μ₂-Glycolato)-copper(ii))

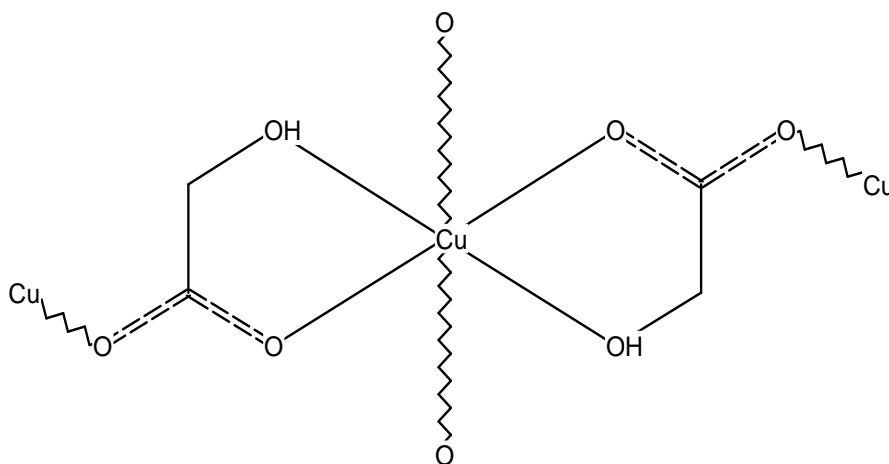
Space Group: P21/n **Cell:** **a** 5.110(0) **b** 8.677(1) **c** 7.746(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 106.84(0) γ 90.00

R-Factor (%): 2.58 **Temperature(K):** 293 **Density(g/cm³):** 2.159

Parameters

Fragment 1

DIST1 (D)	1.932
DIST2 (D)	1.919
DIST3 (D)	1.919
DIST4 (D)	1.932
DIST5 (D)	2.546
DIST6 (D)	2.546



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 44

CUGLYC13

Reference: S.Yoneyama, T.Kodama, K.Kikuchi, Y.Kawabata, K.Kikuchi, T.Ono, Y.Hosokoshi, W.Fujita (2013) *CrystEngComm* ,15, 10193

Formula: (C₄ H₆ Cu₁ O₆)_n

Compound Name: catena-(bis(μ₂-Glycolato)-copper(ii))

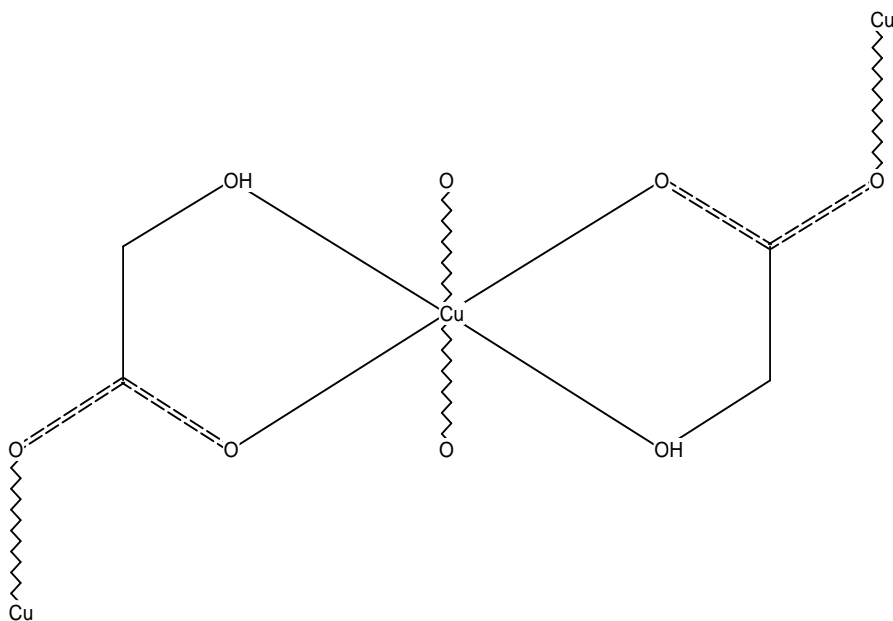
Space Group: P21/n **Cell:** **a** 5.091(0) **b** 8.694(1) **c** 7.730(1)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 107.14(0) **γ** 90.00

R-Factor (%): 2.55 **Temperature(K):** 249 **Density(g/cm³):** 2.170

Parameters

Fragment 1

DIST1 (D) 1.935
DIST2 (D) 1.922
DIST3 (D) 1.922
DIST4 (D) 1.935
DIST5 (D) 2.529
DIST6 (D) 2.529



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 45

CUHMAM01

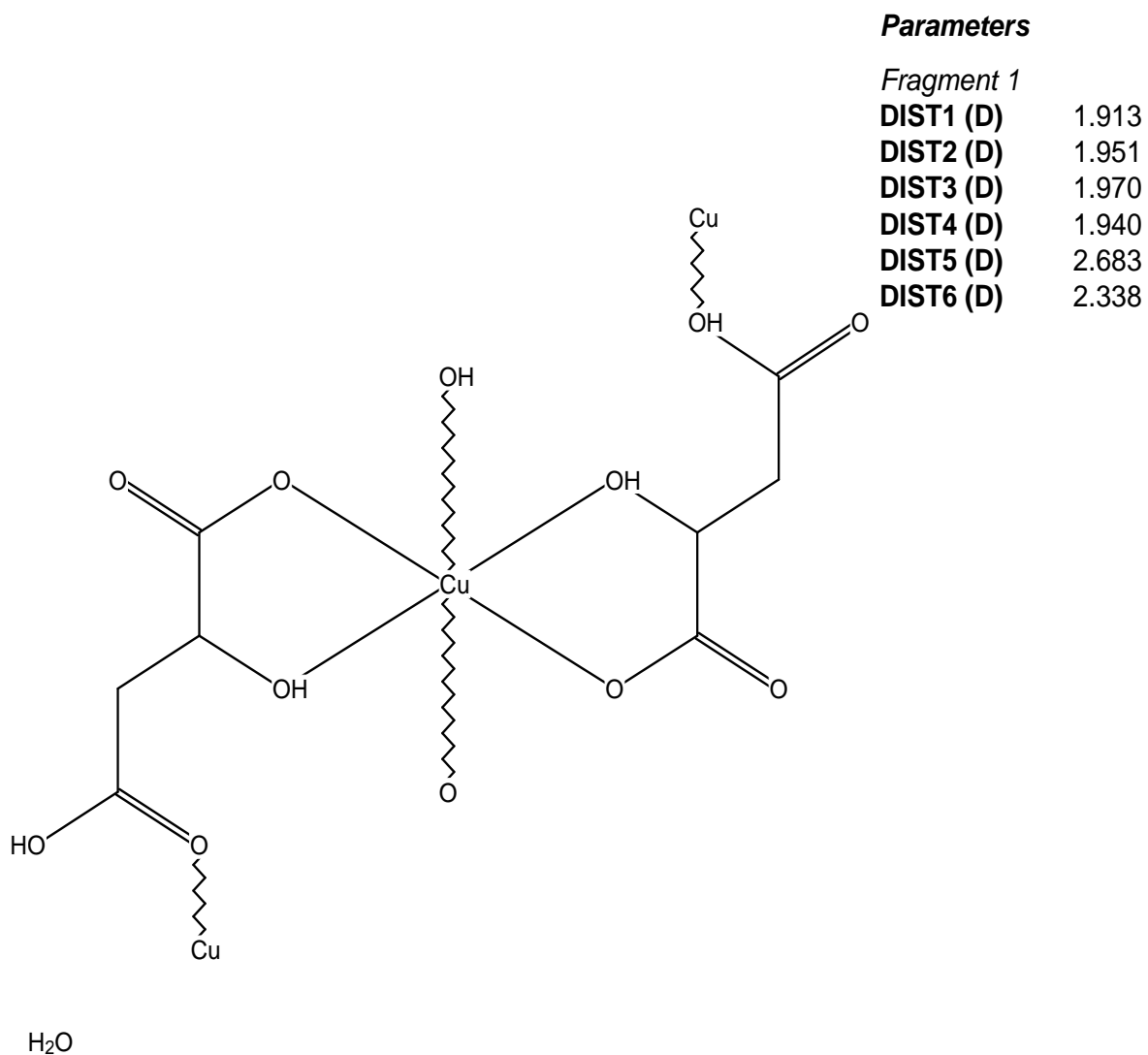
Reference: R.V.Gudavarthy, N.Burla, E.A.Kulp, S.J.Limmer, E.Sinn, J.A.Switzer (2011) *J.Mater.Chem.* ,**21**,6209

Formula: (C₈ H₁₀ Cu₁ O₁₀)_n,2n(H₂ O₁)

Compound Name: catena-(bis(μ₂-D-Hydrogen malato)-copper(ii) dihydrate)

Space Group: P21 **Cell:** **a** 7.591(6) **b** 10.230(8) **c** 8.184(6)
Space Group No.: 4 **(Å, °)** α 90.00 β 92.80(1) γ 90.00

R-Factor (%): 2.40 **Temperature(K):** 298 **Density(g/cm³):** 1.913



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 46

CUHOPT03

Reference: H.Bartl, H.Kuppers (1980)
Z.Kristallogr.,Kristallgeom.,Kristallphys.,Kristallchem. ,**152**,161

Formula: C₁₆ H₁₄ Cu₁ O₁₀

Compound Name: bis(Hydrogen phthalato-O,O')-diaqua-copper(ii)

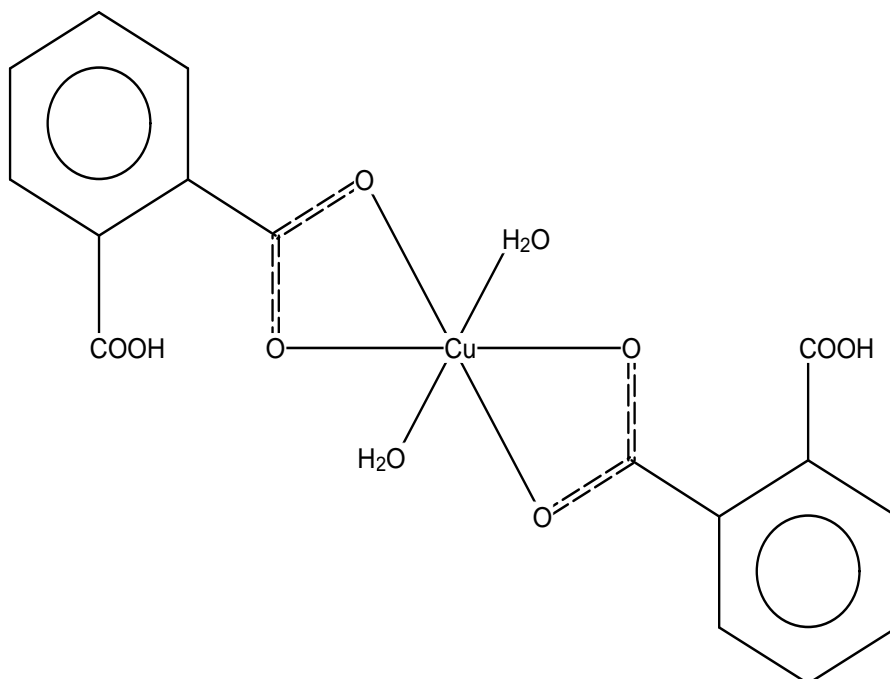
Space Group: P21/c **Cell:** **a** 8.360(2) **b** 14.395(4) **c** 7.086(2)
Space Group No.: 14 **(Å, °)** α 90.00 β 112.18(5) γ 90.00

R-Factor (%): 2.90 **Temperature(K):** 295 **Density(g/cm³):** 1.808

Parameters

Fragment 1

DIST1 (D)	1.931
DIST2 (D)	1.925
DIST3 (D)	1.925
DIST4 (D)	1.931
DIST5 (D)	2.637
DIST6 (D)	2.637



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 47

CUXZEB

Reference: T.D.Keene, I.Zimmermann, A.Neels, O.Sereda, J.Hauser, Shi-Xia Liu, S.Decurtins (2010) *Cryst.Growth Des.* ,**10**,1854

Formula: $2(\text{C}_7\text{H}_{10}\text{N}_1^{1+}), \text{C}_6\text{H}_8\text{Cu}_1\text{O}_{10}^{2-}$

Compound Name: bis(Benzylammonium) diaqua-bis(malonato)-copper(ii)

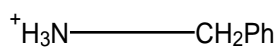
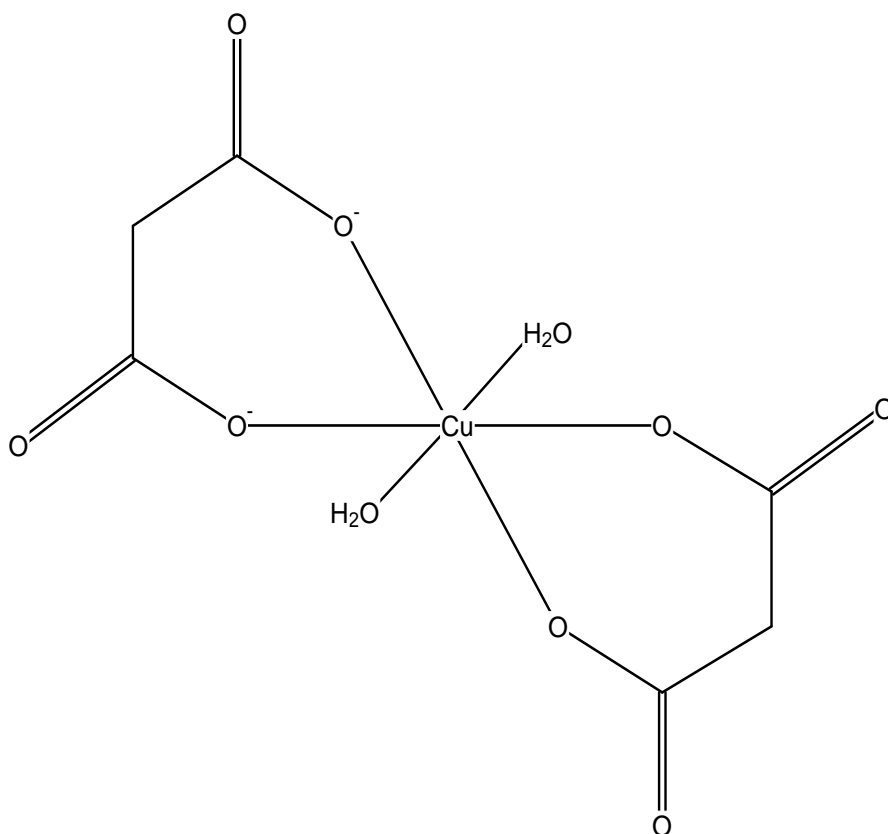
Space Group: P212121 **Cell:** **a** 8.458(0) **b** 11.712(0) **c** 22.049(1)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.75 **Temperature(K):** 173 **Density(g/cm³):** 1.581

Parameters

Fragment 1

DIST1 (D)	1.941
DIST2 (D)	1.938
DIST3 (D)	1.941
DIST4 (D)	1.936
DIST5 (D)	2.406
DIST6 (D)	2.691



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 48

CUXZOL

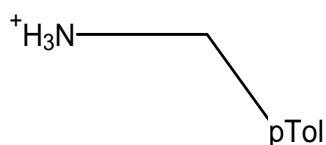
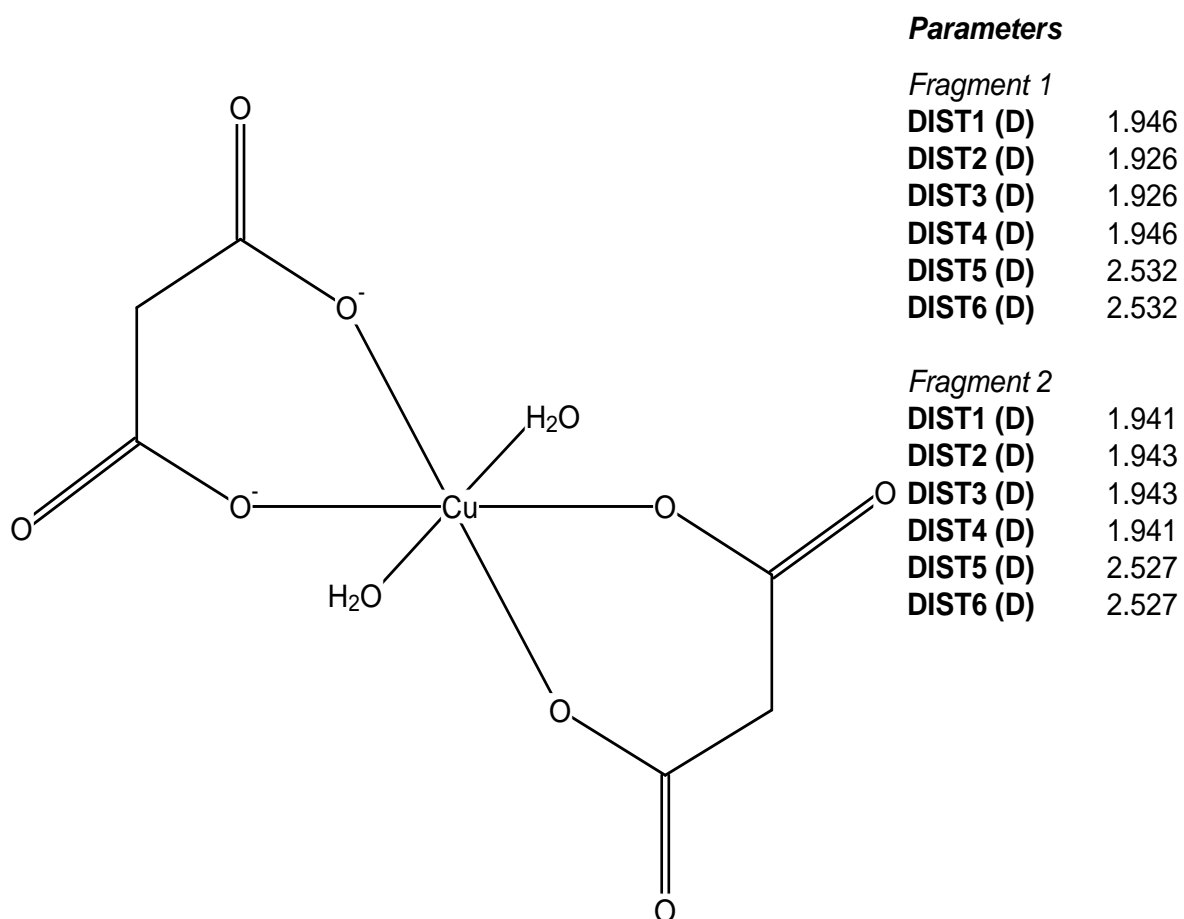
Reference: T.D.Keene, I.Zimmermann, A.Neels, O.Sereda, J.Hauser, Shi-Xia Liu, S.Decurtins (2010) *Cryst.Growth Des.* ,**10**,1854

Formula: $2(\text{C}_8 \text{H}_{12} \text{N}_1^{1+}), \text{C}_6 \text{H}_8 \text{Cu}_1 \text{O}_{10}^{2-}$

Compound Name: bis(4-Methylbenzylammonium) diaqua-bis(malonato)-copper(ii)

Space Group: P-1 **Cell:** **a** 8.448(0) **b** 11.675(1) **c** 13.117(1)
Space Group No.: 2 **(Å, °)** α 88.50(1) β 72.58(0) γ 88.84(1)

R-Factor (%): 2.83 **Temperature(K):** 173 **Density(g/cm³):** 1.475



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 49

CUXZUR

Reference: T.D.Keene, I.Zimmermann, A.Neels, O.Sereda, J.Hauser, Shi-Xia Liu, S.Decurtins (2010) *Cryst.Growth Des.* ,**10**,1854

Formula: $2(\text{C}_8 \text{H}_{10} \text{N}_1 \text{O}_2^{1+}), \text{C}_6 \text{H}_8 \text{Cu}_1 \text{O}_{10}^{2-}$

Compound Name: bis(4-Carboxybenzylammonium) diaqua-bis(malonato)-copper(ii)

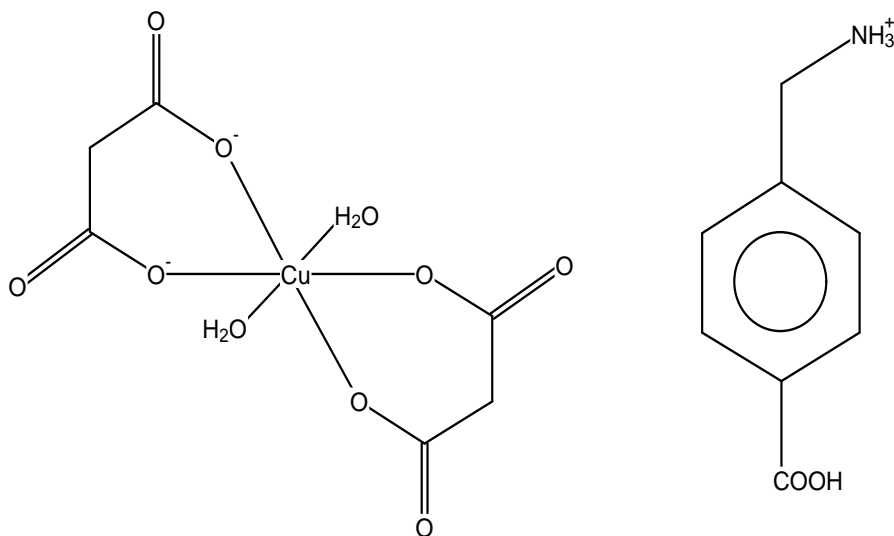
Space Group: P21/c **Cell:** **a** 13.864(0) **b** 8.245(0) **c** 11.765(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 102.54(0) γ 90.00

R-Factor (%): 2.85 **Temperature(K):** 173 **Density(g/cm³):** 1.538

Parameters

Fragment 1

DIST1 (D)	1.943
DIST2 (D)	1.947
DIST3 (D)	1.943
DIST4 (D)	1.947
DIST5 (D)	2.486
DIST6 (D)	2.486



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 50

CUYBII

Reference: T.D.Keene, I.Zimmermann, A.Neels, O.Sereda, J.Hauser, Shi-Xia Liu, S.Decurtins (2010) *Cryst.Growth Des.* ,**10**,1854

Formula: $2(\text{C}_8 \text{H}_{12} \text{N}_1^{1+}), \text{C}_6 \text{H}_8 \text{Cu}_1 \text{O}_{10}^{2-}$

Compound Name: bis(Phenylethylammonium) diaqua-bis(malonato)-copper(ii)

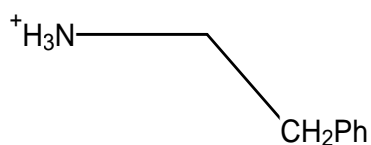
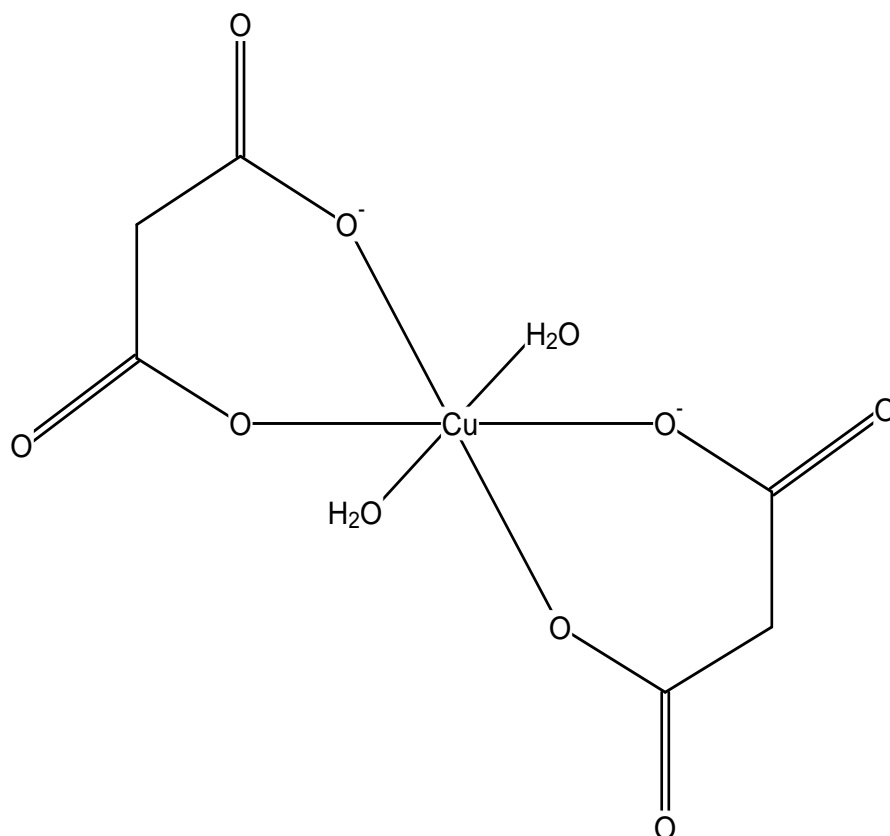
Space Group: P21 **Cell:** **a** 11.426(1) **b** 8.356(0) **c** 12.868(1)
Space Group No.: 4 **(Å, °)** α 90.00 β 95.21(1) γ 90.00

R-Factor (%): 2.74 **Temperature(K):** 173 **Density(g/cm³):** 1.488

Parameters

Fragment 1

DIST1 (D)	1.938
DIST2 (D)	1.961
DIST3 (D)	1.952
DIST4 (D)	1.967
DIST5 (D)	2.421
DIST6 (D)	2.380



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 51

DAQNUE

Reference: Qinglin He, Enbo Wang (1999) *Inorg.Chem.Commun.* ,2, 399

Formula: $2(\text{C}_5\text{H}_6\text{N}_1^{1+}), 2(\text{H}_3\text{O}_1^{1+}), \text{As}_6\text{Cu}_1\text{Mo}_6\text{O}_{30}^{4-}$

Compound Name: bis(Pyridinium) dioxonium hexakis(μ_4 -oxo)-dodecakis(μ_2 -oxo)-dodecaoxo-arsenic(iii)-copper(ii)-molybdenum(vi)

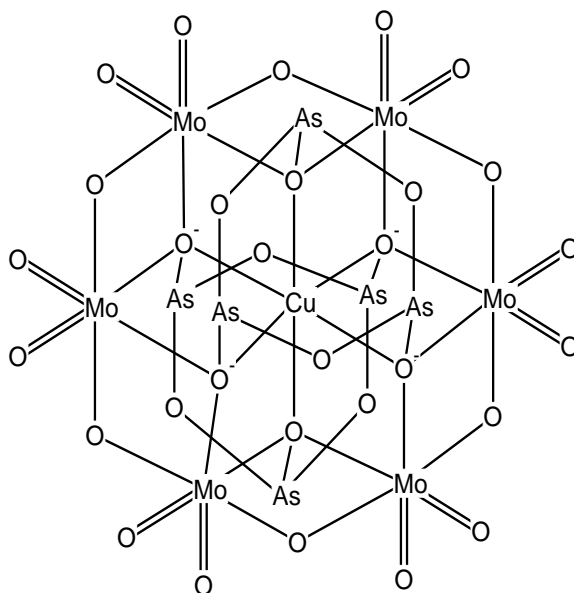
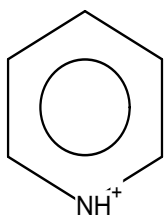
Space Group: P21/n **Cell:** **a** 9.303(2) **b** 20.731(4) **c** 12.617(3)
Space Group No.: 14 (**Å, °**) α 90.00 β 104.17(3) γ 90.00

R-Factor (%): 2.69 **Temperature(K):** 295 **Density(g/cm³):** 2.487

Parameters

Fragment 1

DIST1 (D)	2.069
DIST2 (D)	2.069
DIST3 (D)	2.048
DIST4 (D)	2.048
DIST5 (D)	2.051
DIST6 (D)	2.051



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 52

DICWER

Reference: B.L.Rodrigues, M.D.D.Costa, N.G.Fernandes (1999)
Acta Crystallogr., Sect. C: Cryst. Struct. Commun. ,55,1997

Formula: (C₁₆ H₁₄ Cu₁ O₁₀)_n

Compound Name: catena-[β-(bis(μ₂-Hydrogenphthalato-O,O')-diaqua-copper(ii))]

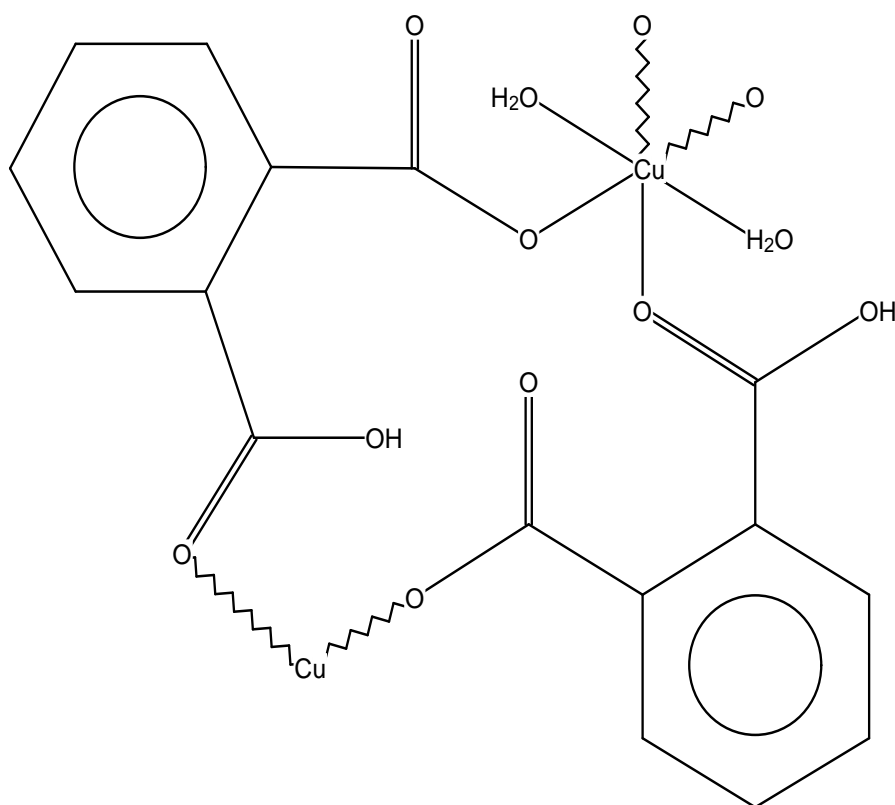
Space Group: P21/c **Cell:** **a** 13.177(2) **b** 5.111(1) **c** 12.972(2)
Space Group No.: 14 **(Å, °)** α 90.00 β 116.63(1) γ 90.00

R-Factor (%): 2.90 **Temperature(K):** 295 **Density(g/cm³):** 1.828

Parameters

Fragment 1

DIST1 (D)	1.974
DIST2 (D)	1.974
DIST3 (D)	1.944
DIST4 (D)	1.944
DIST5 (D)	2.461
DIST6 (D)	2.461



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 53

DILCIL

Reference: Yin-Qiu Liu, Xi-Rui Zeng (2007)
Acta Crystallogr., Sect. E: Struct. Rep. Online, **63**, m2414

Formula: $\text{H}_{12} \text{Cu}_1 \text{O}_6^{2+}, 2(\text{C}_6 \text{H}_5 \text{O}_4 \text{S}_1^{-})$

Compound Name: Hexaaqua-copper(ii) bis(4-hydroxybenzenesulfonate)

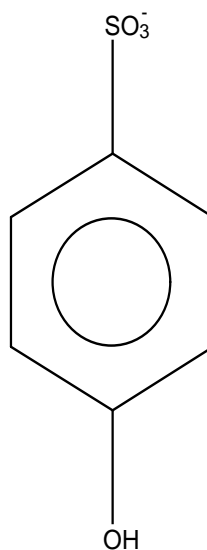
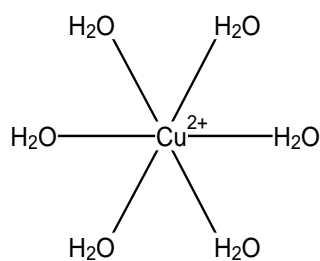
Space Group: P21/n **Cell:** **a** 6.930(1) **b** 6.187(1) **c** 23.531(4)
Space Group No.: 14 **(Å, °)** α 90.00 β 91.53(0) γ 90.00

R-Factor (%): 2.73 **Temperature(K):** 293 **Density(g/cm³):** 1.706

Parameters

Fragment 1

DIST1 (D)	1.942
DIST2 (D)	1.965
DIST3 (D)	1.942
DIST4 (D)	1.965
DIST5 (D)	2.384
DIST6 (D)	2.384



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 54

DIXGIB

Reference: Zhong-Xiang Du, Jun-Xia Li, Jian-Hua Qin (2008)
Z.Kristallogr.-New Cryst.Struct. ,**223**,105

Formula: $(C_{20} H_{24} Cu_1 Na_2 O_{24})_n \cdot 2n(H_2 O_1)$

Compound Name: catena-(hexakis(μ_2 -aqua)-bis(μ_2 -dihydrogen-1,2,4,5-benzenetetracarboxylate-O,O')-diaqua-di-sodium(i)-copper(ii) dihydrate)

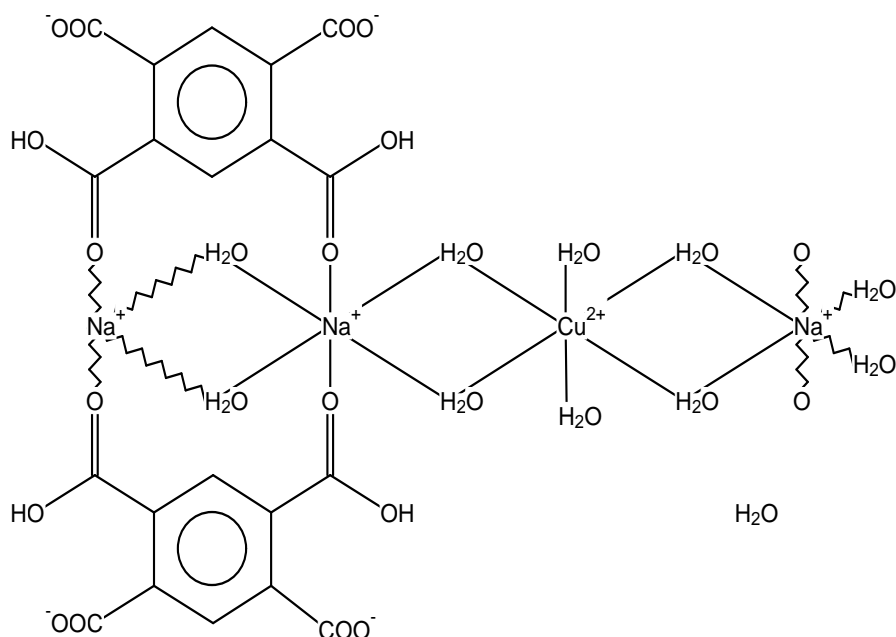
Space Group: C2/m **Cell:** **a** 7.356(0) **b** 20.271(2) **c** 10.464(1)
Space Group No.: 12 (**Å, °**) α 90.00 β 104.49(0) γ 90.00

R-Factor (%): 2.38 **Temperature(K):** 291 **Density(g/cm³):** 1.746

Parameters

Fragment 1

DIST1 (D)	1.974
DIST2 (D)	2.030
DIST3 (D)	2.030
DIST4 (D)	1.974
DIST5 (D)	2.301
DIST6 (D)	2.301



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 55

DIZYER

Reference: G.Steinhauser, K.Karaghiosoff, T.M.Klapotke (2008)
Z.Anorg.Allg.Chem. ,**634**,892

Formula: $2(\text{C}_1 \text{H}_6 \text{N}_1^{1+}), \text{Cu}_1 \text{N}_4 \text{O}_{12}^{2-}$

Compound Name: bis(Methylammonium) bis(nitrato-O,O')-bis(nitrato-O)-copper(ii)

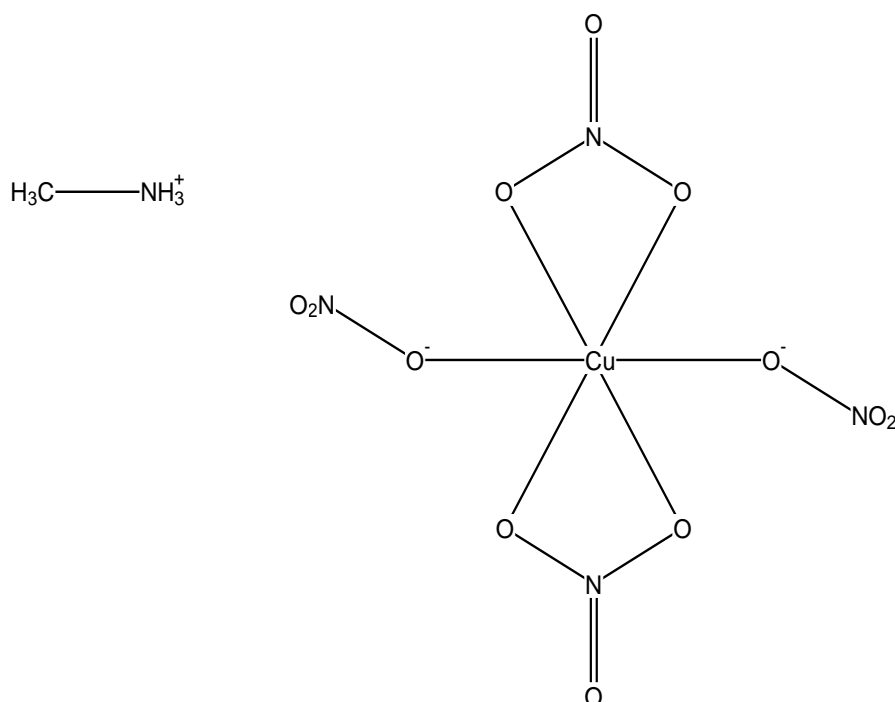
Space Group: P21/c **Cell:** **a** 8.453(0) **b** 8.692(0) **c** 9.394(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 104.82(0) γ 90.00

R-Factor (%): 2.39 **Temperature(K):** 200 **Density(g/cm³):** 1.870

Parameters

Fragment 1

DIST1 (D) 1.957
DIST2 (D) 1.967
DIST3 (D) 1.967
DIST4 (D) 1.957
DIST5 (D) 2.527
DIST6 (D) 2.527



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 56

DODDOP

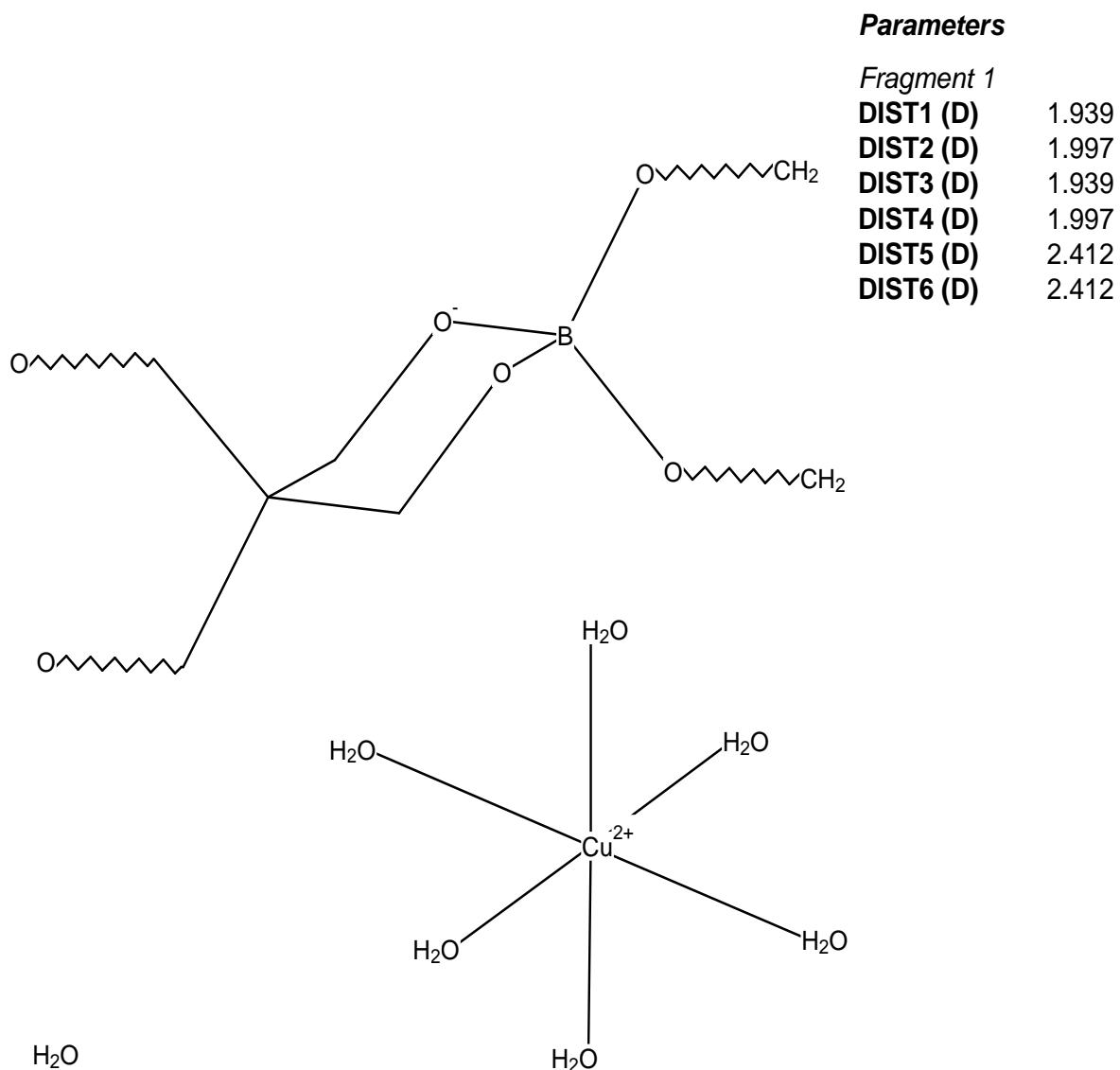
Reference: I.I.Zviedre, V.K.Bel'skii, E.M.Shvarts (1985)
Latv.PSR Zinat.Akad.Vestis,Khim.Ser. ,672

Formula: $(\text{H}_{12}\text{Cu}_1\text{O}_6^{2-})_n, 2n(\text{C}_5\text{H}_8\text{B}_1\text{O}_4^{1-}), 4n(\text{H}_2\text{O}_1)$

Compound Name: poly(Penta-erythritol-borate) hexa-aqua-copper(ii) tetrahydrate

Space Group: P-1 **Cell:** **a** 5.636(1) **b** 11.155(2) **c** 8.847(2)
Space Group No.: 2 (**Å, °**) α 109.06(1) β 104.24(1) γ 92.60(10)

R-Factor (%): 2.90 **Temperature(K):** 295 **Density(g/cm³):** 1.742



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 57

DOGYUU01

Reference: Y.Li, D.Sun, H.Zang, L.Han, G.Su (2010)
Acta Crystallogr., Sect. E: Struct. Rep. Online ,66,m1576

Formula: (C₁₀ H₁₈ Cu₃ N₄ O₁₆ P₄)_n

Compound Name: catena-(bis(μ₄-1-hydroxy-2-(imidazol-3-ium-1-yl)ethane-1,1-diyldiphosphonato)-diaqua-tri-copper(ii))

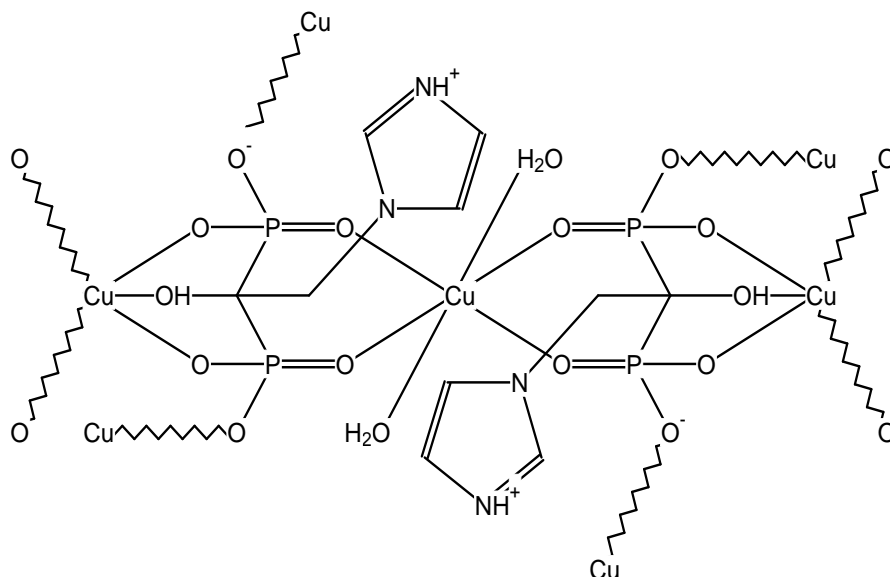
Space Group: P-1 **Cell:** **a** 7.417(0) **b** 8.150(1) **c** 9.523(1)
Space Group No.: 2 **(Å, °)** α 104.75(0) β 107.66(0) γ 101.48(0)

R-Factor (%): 2.74 **Temperature(K):** 293 **Density(g/cm³):** 2.510

Parameters

Fragment 1

DIST1 (D)	1.950
DIST2 (D)	1.959
DIST3 (D)	1.950
DIST4 (D)	1.959
DIST5 (D)	2.575
DIST6 (D)	2.575



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 58

DOKPOI01

Reference: N.Lah, P.Segedin, I.Leban (2002) *Acta Chim.Slov.* ,49,251

Formula: (C₄ H₆ Cu₁ O₈)_n

Compound Name: catena-(bis(μ₂-Formato-O,O')-bis(formic acid-O)-copper(ii))

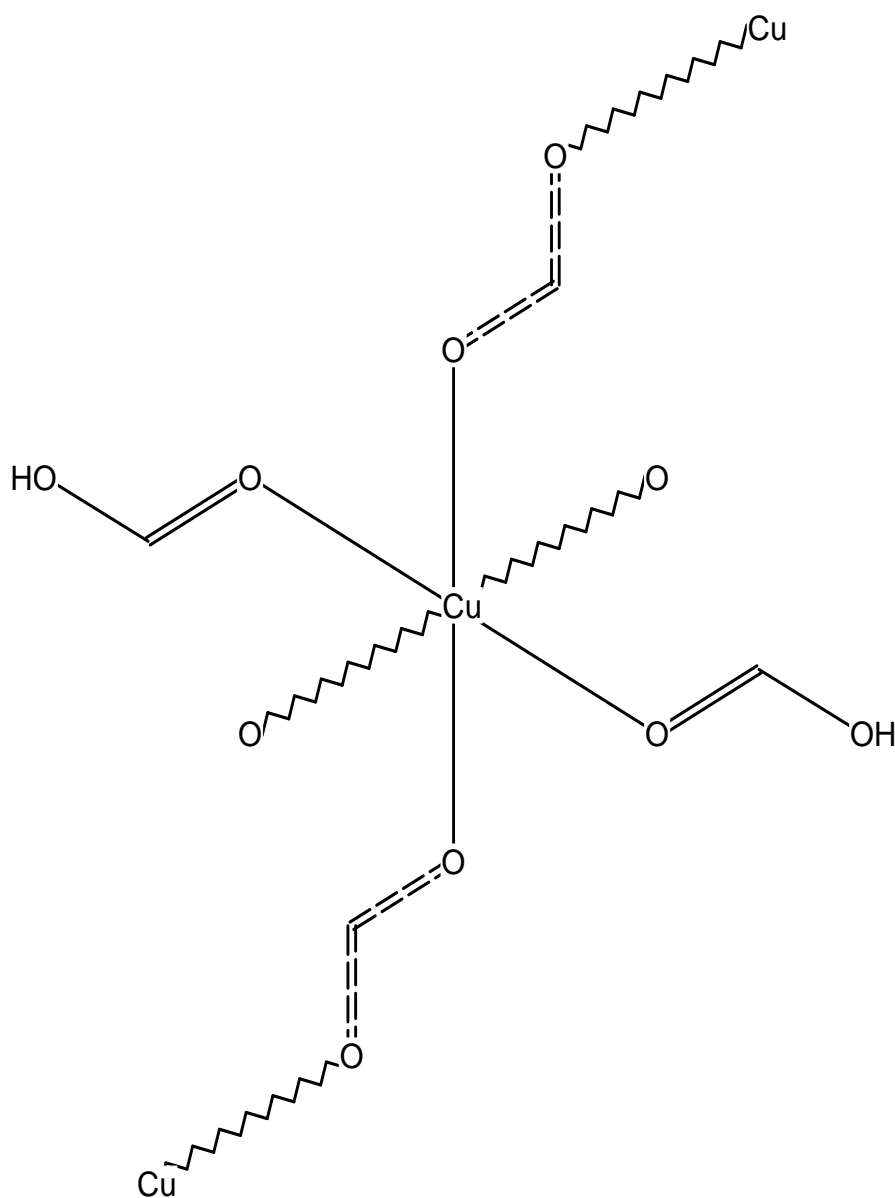
Space Group: Pbcu **Cell:** **a** 7.877(0) **b** 8.478(0) **c** 12.142(0)
Space Group No.: 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.24 **Temperature(K):** 150 **Density(g/cm³):** 2.012

Parameters

Fragment 1

DIST1 (D)	1.975
DIST2 (D)	1.945
DIST3 (D)	1.945
DIST4 (D)	1.975
DIST5 (D)	2.435
DIST6 (D)	2.435



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 59

EJEWAT

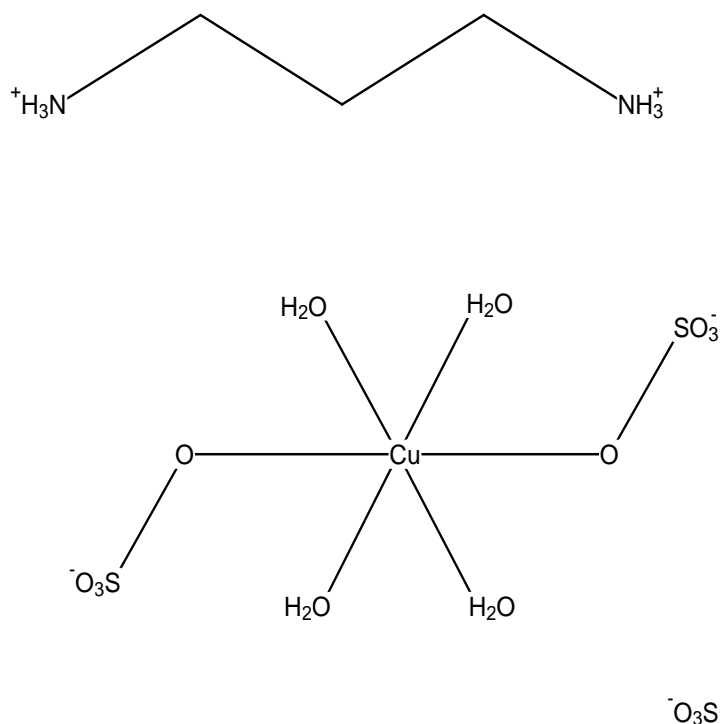
Reference: Chun-Hong Chen, Rong Mu, Li Zhang, Guan-Cheng Xu (2016) *CrystEngComm*, **18**,2719

Formula: $H_8 Cu_1 O_{12} S_2^{2-} \cdot 2(C_3 H_{12} N_2^{2+}) \cdot 2(H_1 O_4 S_1^{1-})$

Compound Name: bis(propane-1,3-diaminium) bis(hydrogen sulfate) tetra-aqua-bis(sulfato)-copper

Space Group: P-1 **Cell:** **a** 10.649(4) **b** 10.677(4) **c** 10.799(4)
Space Group No.: 2 **(Å, °)** α 94.77(0) β 100.76(0) γ 95.75(0)

R-Factor (%): 2.61 **Temperature(K):** 100 **Density(g/cm³):** 1.876



Parameters

Fragment 1

DIST1 (D) 1.997
DIST2 (D) 1.949
DIST3 (D) 1.997
DIST4 (D) 1.949
DIST5 (D) 2.442
DIST6 (D) 2.442

Fragment 2

DIST1 (D) 1.996
DIST2 (D) 1.948
DIST3 (D) 1.996
DIST4 (D) 1.948
DIST5 (D) 2.472
DIST6 (D) 2.472

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 60

ELEHOU

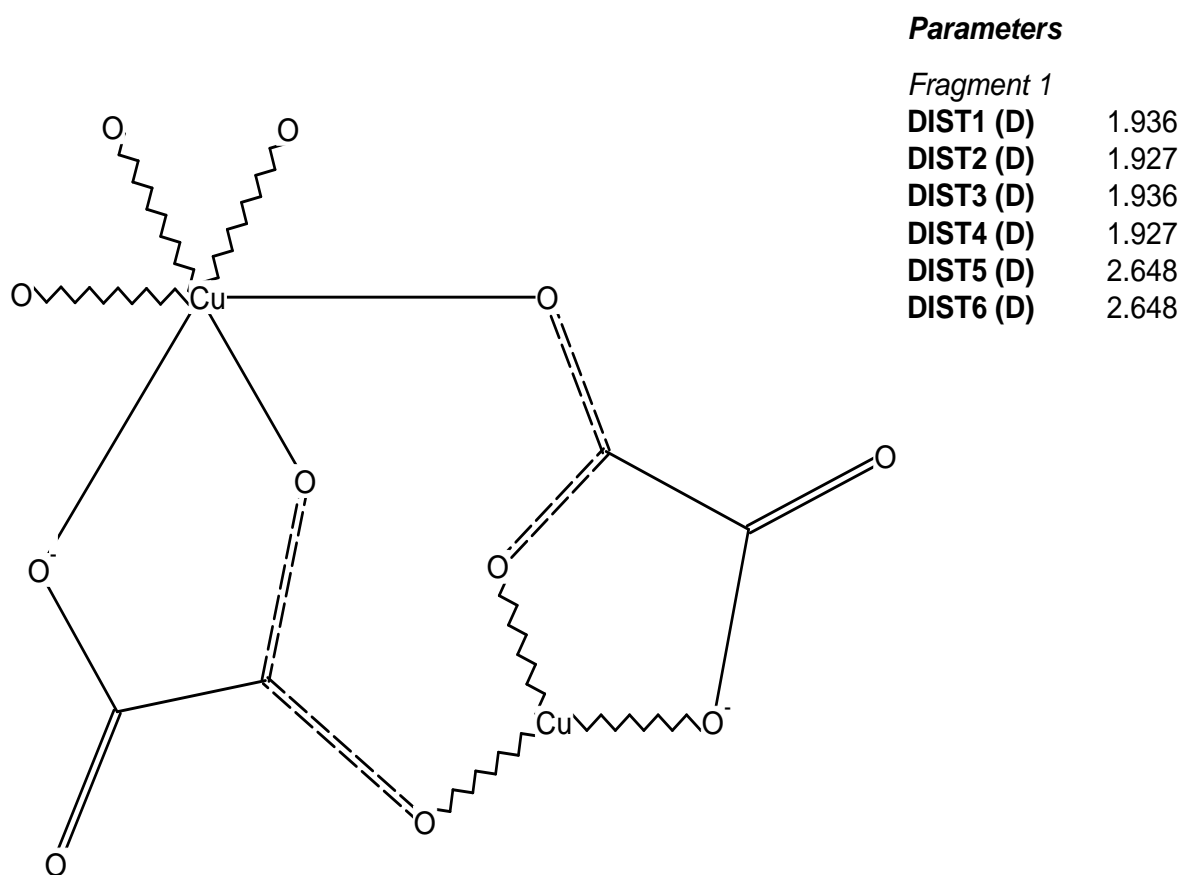
Reference: K.Matelkova, L.Kuckova, A.Maslejova, Jan Moncol, V.Jorik, J.Kozisek (2016) *Chem.Papers* ,70,82

Formula: $(C_4 Cu_1 O_8^{2-})_n \cdot 2n(K_1^{1+})$

Compound Name: catena-(Di-potassium bis(μ_2 -oxalato)-copper)

Space Group: P21/c **Cell:** **a** 4.880(0) **b** 6.652(0) **c** 13.502(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 104.50(0) γ 90.00

R-Factor (%): 1.83 **Temperature(K):** 150 **Density(g/cm³):** 2.487



K⁺

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 61

ELOHES

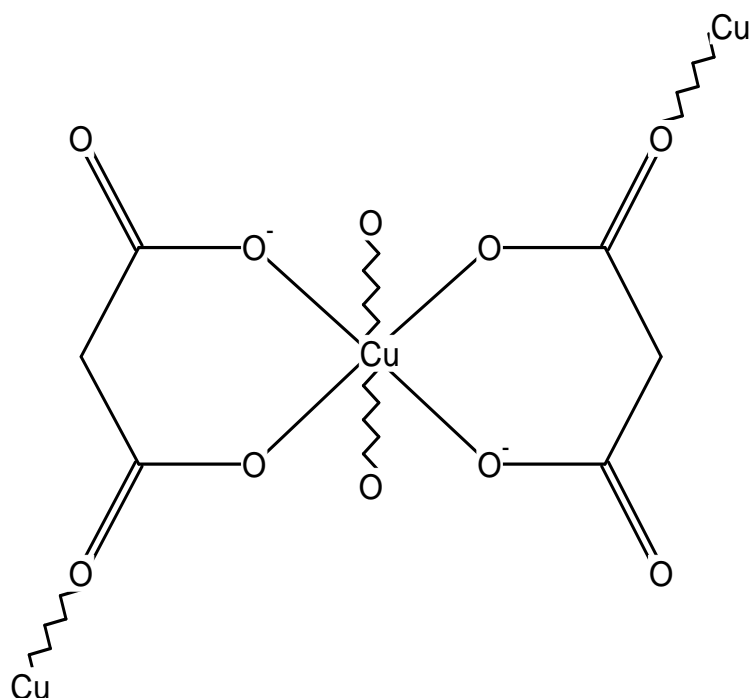
Reference: F.S.Delgado, J.Sanchiz, C.Ruiz-Perez, F.Lloret, M.Julve (2003) *Inorg.Chem.* ,**42**,5938

Formula: $(C_{12}H_{12}N_2^{2+})_n, n(C_6H_4Cu_1O_8^{2-})_n, 4n(H_2O)_1$

Compound Name: catena-(1,2-bis(4-pyridinium)ethene bis(μ_2 -malonato)-copper(ii) tetrahydrate)

Space Group: P-1 **Cell:** **a** 4.883(1) **b** 9.585(1) **c** 11.813(2)
Space Group No.: 2 **(Å, °)** α 77.29(3) β 82.18(3) γ 84.92(3)

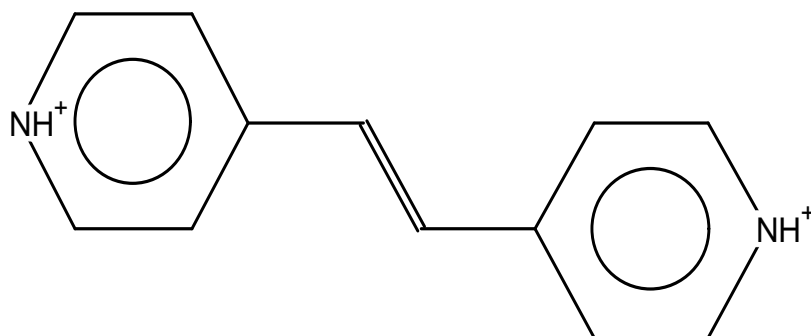
R-Factor (%): 2.81 **Temperature(K):** 293 **Density(g/cm³):** 1.631



Parameters

Fragment 1

DIST1 (D)	1.937
DIST2 (D)	1.931
DIST3 (D)	1.931
DIST4 (D)	1.937
DIST5 (D)	2.611
DIST6 (D)	2.611



H₂O

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 62

ELUBEU

Reference: T.G.Horner, P.Klufers (2016) *Eur.J.Inorg.Chem.* ,1798

Formula: $C_8 H_4 Cu_1 O_{12}^{6-}, 12(H_2 O_1), 4(Na_1^{1+}), 2(K_1^{1+})$

Compound Name: di-potassium tetra-sodium bis(L-tartrato)-copper(ii) dodecahydrate

Synonym: di-potassium tetra-sodium bis(2,3-dioxidobutanedioato)-copper(ii) dodecahydrate

Space Group: P1 **Cell:** **a** 8.973(0) **b** 8.983(0) **c** 9.393(0)

Space Group No.: 1 **(Å, °)** **α** 69.77(0) **β** 65.96(0) **γ** 76.43(0)

R-Factor (%): 2.21 **Temperature(K):** 100 **Density(g/cm³):** 1.911

Parameters

Fragment 1

DIST1 (D) 1.927

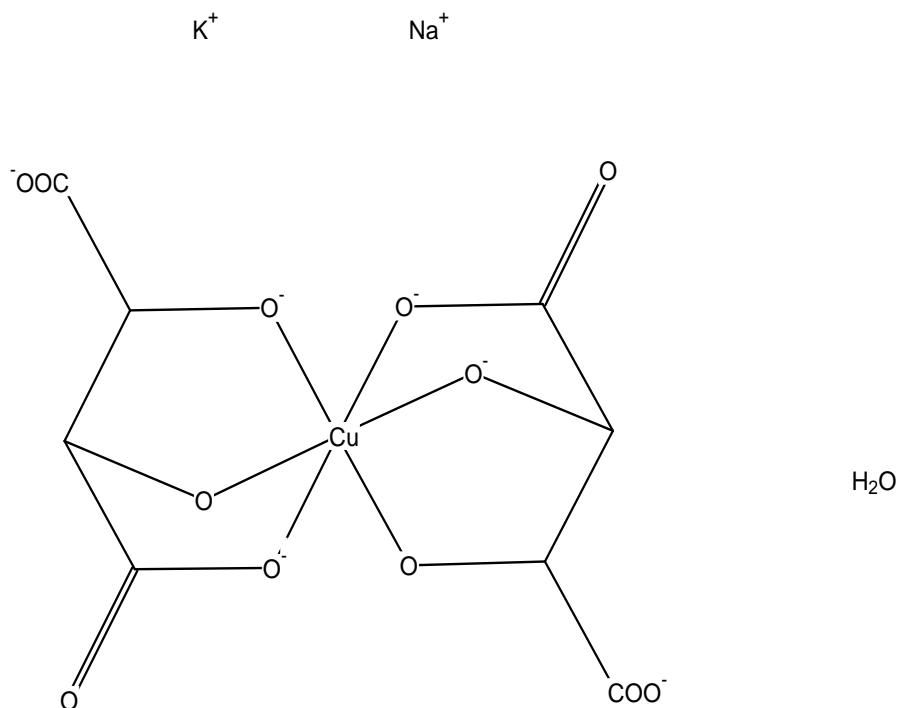
DIST2 (D) 1.996

DIST3 (D) 1.923

DIST4 (D) 1.971

DIST5 (D) 2.553

DIST6 (D) 2.680



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 63

ENIXUU01

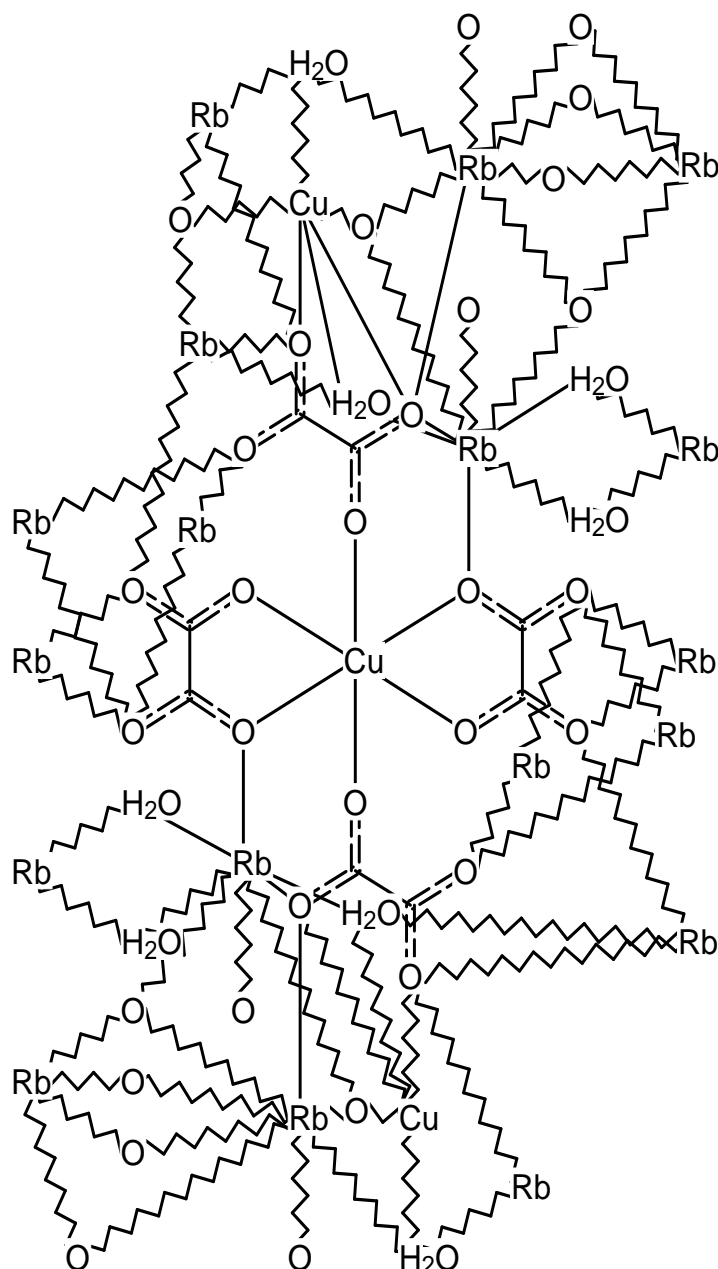
Reference: U.Kolitsch (2004)
Acta Crystallogr., Sect. C: Cryst. Struct. Commun. ,60,m129

Formula: $(C_8 H_8 Cu_2 O_{20} Rb_4)_n$

Compound Name: catena-(bis(μ_8 -Oxalato)-bis(μ_6 -oxalato)-bis(μ_3 -aqua)-bis(μ_2 -aqua)-dicopper(ii)-tetra-rubidium(i))

Space Group: P-1 **Cell:** **a** 7.000(1) **b** 8.949(2) **c** 8.982(2)
Space Group No.: 2 (**Å, °**) α 108.05(3) β 97.69(3) γ 97.99(3)

R-Factor (%): 2.41 **Temperature(K):** 293 **Density(g/cm³):** 2.850



Parameters

Fragment 1

DIST1 (D)	1.936
DIST2 (D)	1.936
DIST3 (D)	1.949
DIST4 (D)	1.949
DIST5 (D)	2.508
DIST6 (D)	2.508

Fragment 2

DIST1 (D)	1.943
DIST2 (D)	1.944
DIST3 (D)	1.944
DIST4 (D)	1.943
DIST5 (D)	2.651
DIST6 (D)	2.651

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 64

ERIGUI

Reference: Yue Cui, Qian Gao, Huan-Huan Wang, Lin Wang, Ya-Bo Xie (2011) *Acta Crystallogr., Sect. E: Struct. Rep. Online* ,**67**,m782

Formula: C₂₀ H₁₄ Cu₁ O₁₀

Compound Name: Diaquabis(2-oxo-2H-chromene-3-carboxylato)copper(ii)

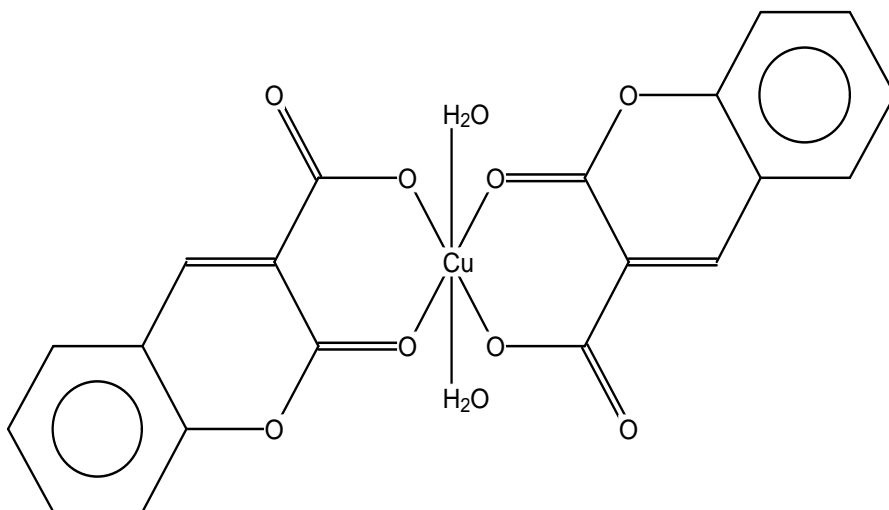
Space Group: P-1 **Cell:** **a** 6.588(1) **b** 6.830(1) **c** 10.460(2)
Space Group No.: 2 **(Å, °)** α 85.98(3) β 89.79(3) γ 65.38(3)

R-Factor (%): 2.63 **Temperature(K):** 293 **Density(g/cm³):** 1.860

Parameters

Fragment 1

DIST1 (D)	2.001
DIST2 (D)	1.942
DIST3 (D)	1.942
DIST4 (D)	2.001
DIST5 (D)	2.323
DIST6 (D)	2.323



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 65

FASYIJ

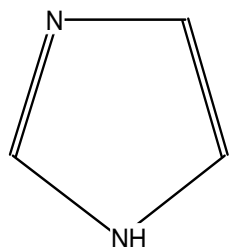
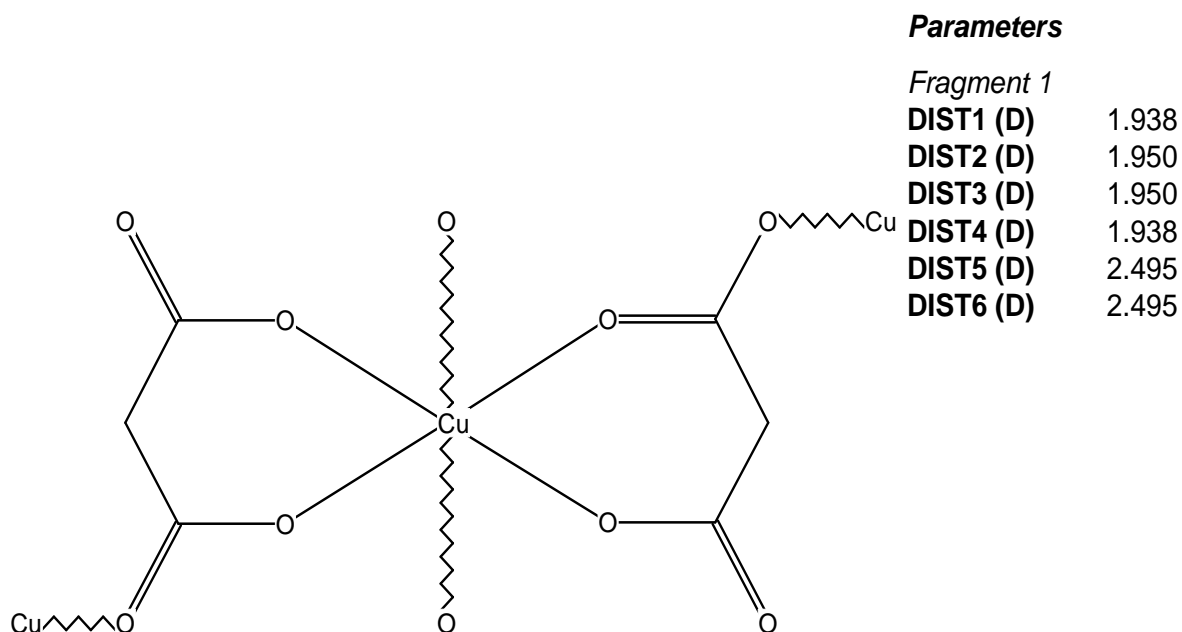
Reference: Hui Zhang, Yi-Min Feng (2012)
Z.Kristallogr.-New Cryst.Struct., **227**,237

Formula: $(C_6 H_4 Cu_1 O_8)_n, 2n(C_3 H_4 N_2), 2n(H_2 O_1)$

Compound Name: catena(bis(μ_2 -malonato)-copper(ii) imidazole dihydrate)

Space Group: P21/c **Cell:** **a** 12.290(3) **b** 7.778(1) **c** 9.100(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 101.16(3) γ 90.00

R-Factor (%): 2.77 **Temperature(K):** 293 **Density(g/cm³):** 1.712



H₂O

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 66

FEJXIC01

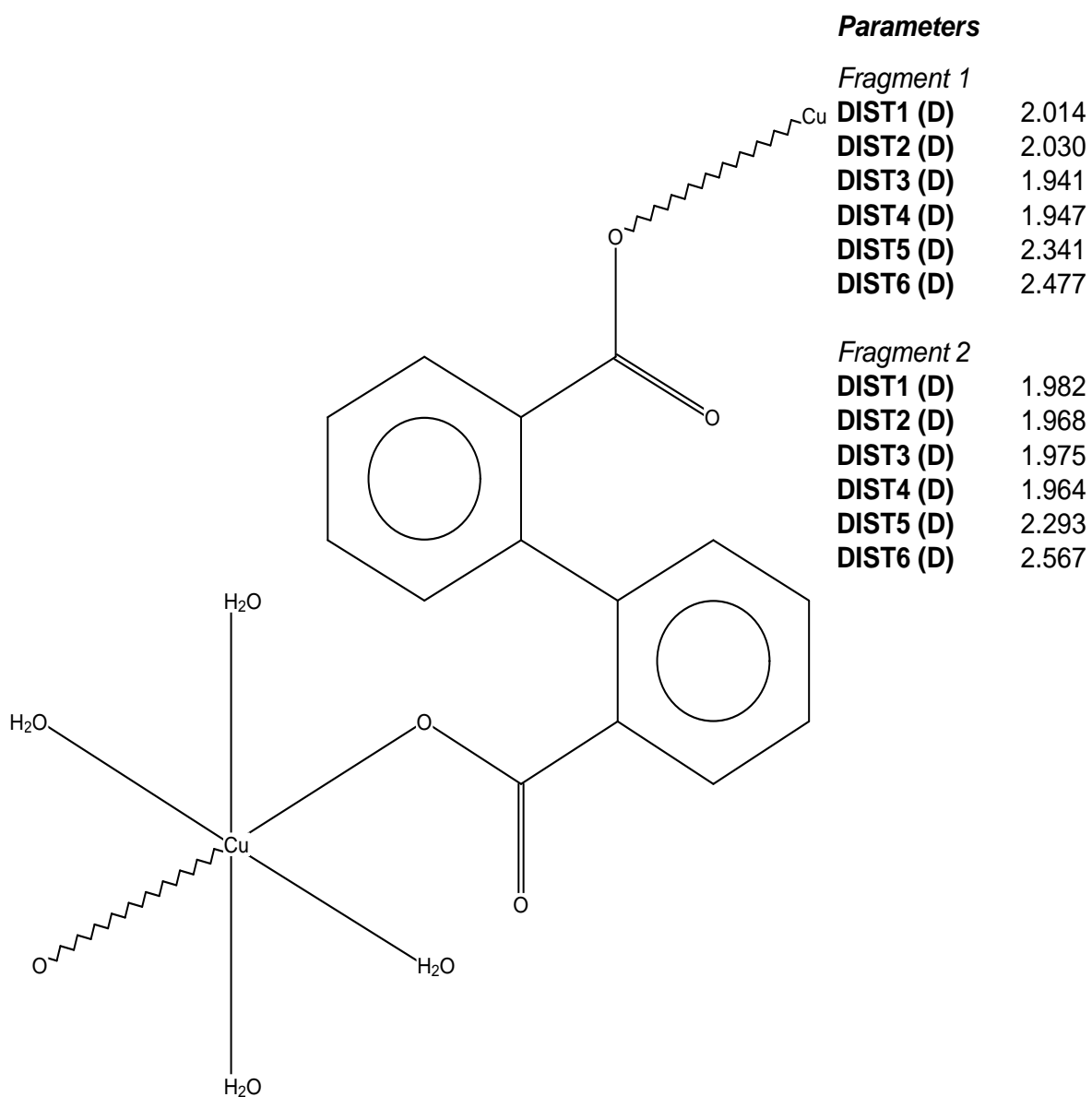
Reference: Z.S.Sahin, O.Sahin, Ozge Dagli, D.A.Kose (2016)
Polyhedron, **117**,214

Formula: (C₁₄ H₁₆ Cu₁ O₈)_n

Compound Name: catena-((μ-biphenyl-2,2'-dicarboxylato)-tetra-aqua-copper)

Space Group: P21 **Cell:** **a** 14.076(5) **b** 7.612(4) **c** 15.597(5)
Space Group No.: 4 **(Å, °)** **α** 90.00 **β** 114.25(0) **γ** 90.00

R-Factor (%): 2.89 **Temperature(K):** 296 **Density(g/cm³):** 1.638



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 67

FILDAH

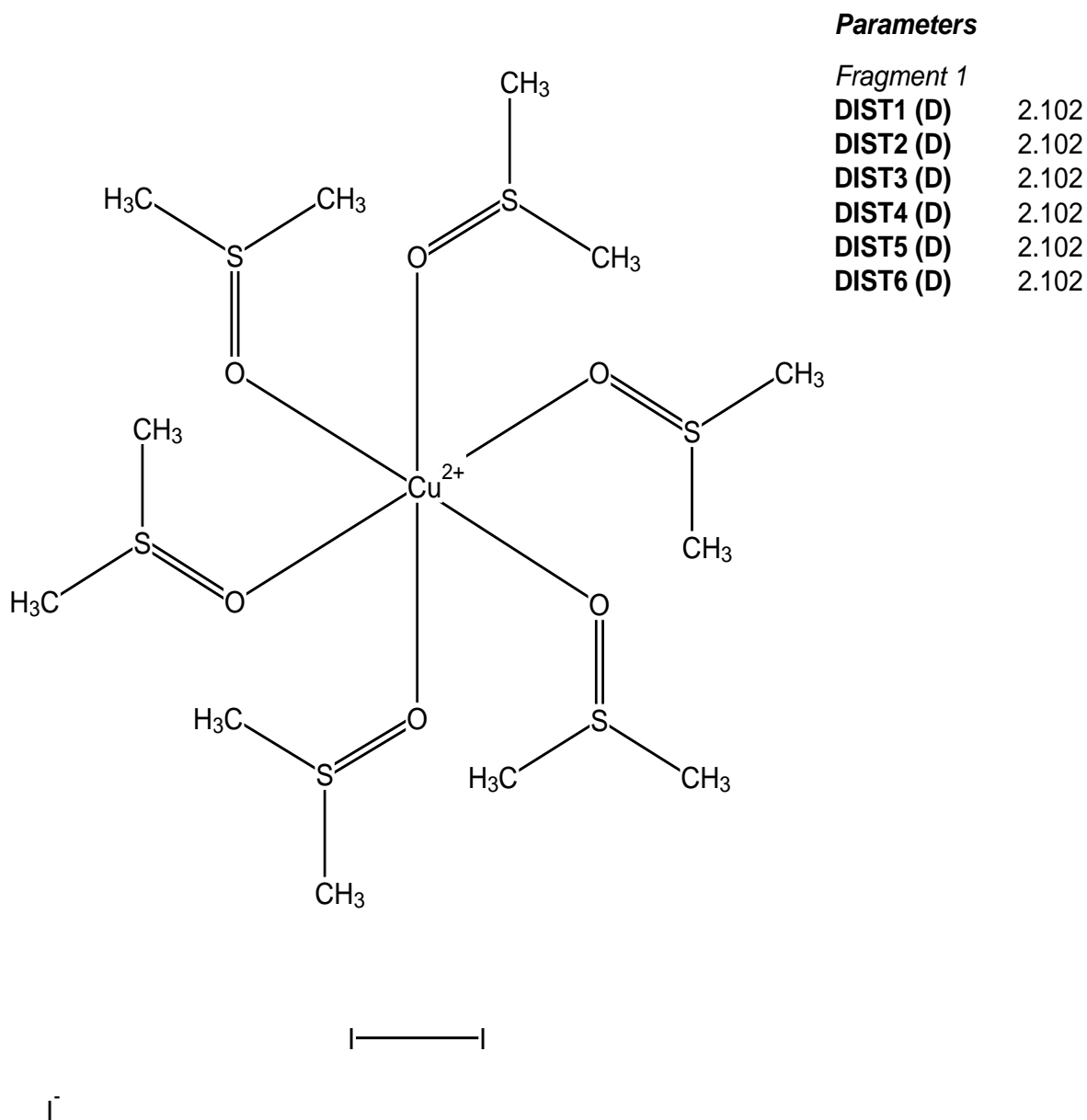
Reference: L.Garzon-Tovar, A.Duarte-Ruiz, K.Wurst (2013)
Inorg.Chem.Commun. ,**32**,64

Formula: C₁₂ H₃₆ Cu₁ O₆ S₆²⁺, I₂, 2(I₁¹⁻)

Compound Name: hexakis(Dimethylsulfoxide)-copper(ii) bis(iodide) di-iodine

Space Group: R-3 **Cell:** **a** 11.841(0) **b** 11.841(0) **c** 19.830(5)
Space Group No.: 148 **(Å, °)** α 90.00 β 90.00 γ 120.00

R-Factor (%): 2.68 **Temperature(K):** 296 **Density(g/cm³):** 2.151



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 68

FOFSUQ

Reference: E.Brana, C.Mendoza, P.Vitoria, J.Gonzalez-Platas, S.Dominguez, C.Kremer (2014) *Inorg.Chim.Acta* ,417,192

Formula: $(C_{18} H_{31} Cu_3 N_5 O_{24}^{2-})_n, 2n(H_3 O_1^{1+})$

Compound Name: catena-[(μ_3 -3,3',3''-nitrilotripropanoato)-(μ_3 -3,3',3''-ammoniotripropanoato)-tris(μ_2 -nitrate)-trihydroxy-tri-copper dioxonium]

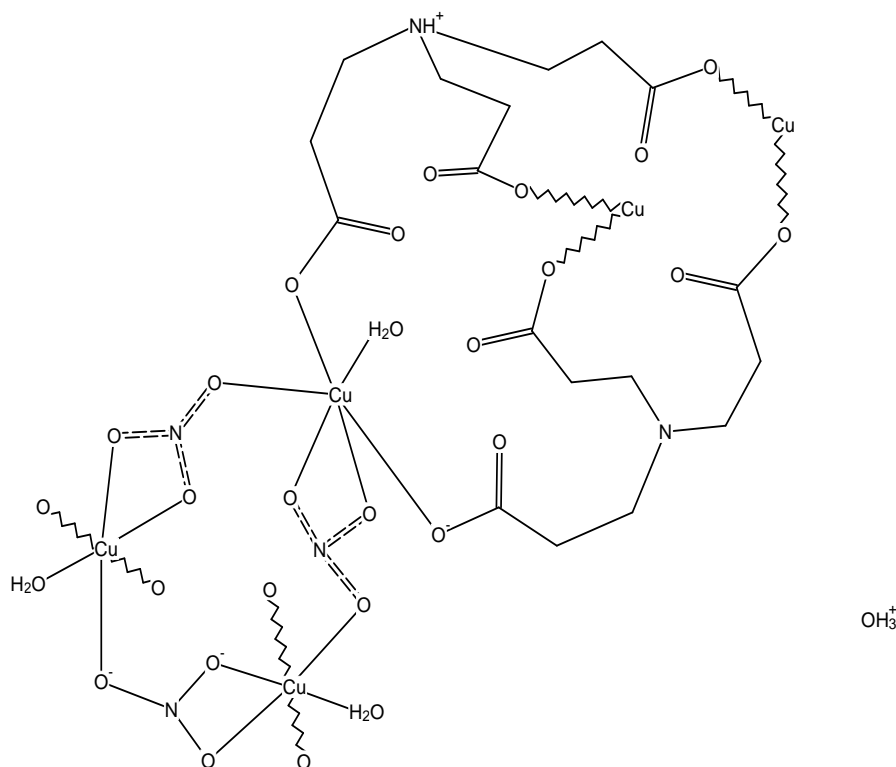
Space Group: P63/m **Cell:** **a** 11.040(0) **b** 11.040(0) **c** 14.698(0)
Space Group No.: 176 **(Å, °)** α 90.00 β 90.00 γ 120.00

R-Factor (%): 2.17 **Temperature(K):** 100 **Density(g/cm³):** 1.991

Parameters

Fragment 1

DIST1 (D) 1.943
DIST2 (D) 1.921
DIST3 (D) 2.000
DIST4 (D) 1.943
DIST5 (D) 2.640
DIST6 (D) 2.381



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 69

FUDPOK

Reference: Ming-Yang He, Sheng-Chun Chen, Zhi-Hui Zhang, Kun-Lin Huang, Fang-Hua Yin, Qun Chen (2009) *Inorg.Chim.Acta* ,**362**, 2569

Formula: (C₁₂ H₁₂ Cl₄ Cu₁ O₈)_n,n(C₄ H₈ O₂)

Compound Name: catena-((μ₂-1,4-dioxane)-(μ₂-2,3,4-tetrachloro-1,4-benzenedicarboxylato)-diaqua-copper(ii) 1,4-dioxane solvate)

Space Group: P-1 **Cell:** **a** 7.583(3) **b** 7.936(4) **c** 10.134(5)

Space Group No.: 2 **(Å, °)** **α** 76.49(0) **β** 76.10(0) **γ** 70.86(0)

R-Factor (%): 2.66 **Temperature(K):** 296 **Density(g/cm³):** 1.740

Parameters

Fragment 1

DIST1 (D) 1.979

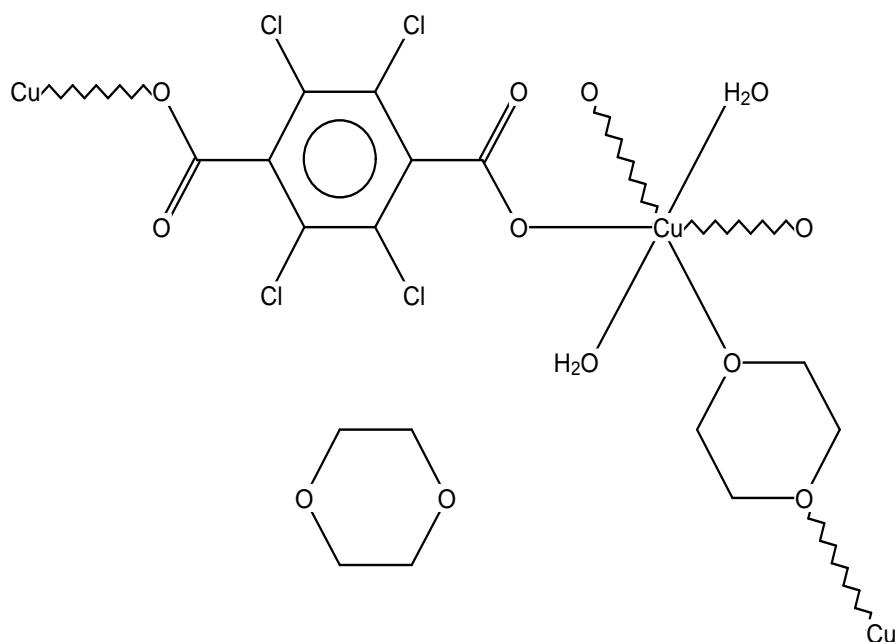
DIST2 (D) 1.979

DIST3 (D) 1.942

DIST4 (D) 1.942

DIST5 (D) 2.575

DIST6 (D) 2.575



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 70

GACJAX

Reference: T.K.Prasad, M.V.Rajasekharan (2010) *Inorg.Chim.Acta*, **363**,2971

Formula: $(C_{42} H_{34} Ce_2 Cu_2 N_6 O_{32})_n, 16n(H_2 O)_1$

Compound Name: catena-(tetrakis(μ_2 -pyridine-2,6-dicarboxylato)-bis(pyridine-2,6-dicarboxylato)-octaaqua-di-cerium-di-copper hexadecahydrate)

Space Group: P-1 **Cell:** **a** 10.238(0) **b** 12.410(0) **c** 13.790(1)
Space Group No.: 2 (**Å, °**) α 84.33(0) β 89.56(0) γ 68.32(0)

R-Factor (%): 2.50 **Temperature(K):** 100 **Density(g/cm³):** 1.877

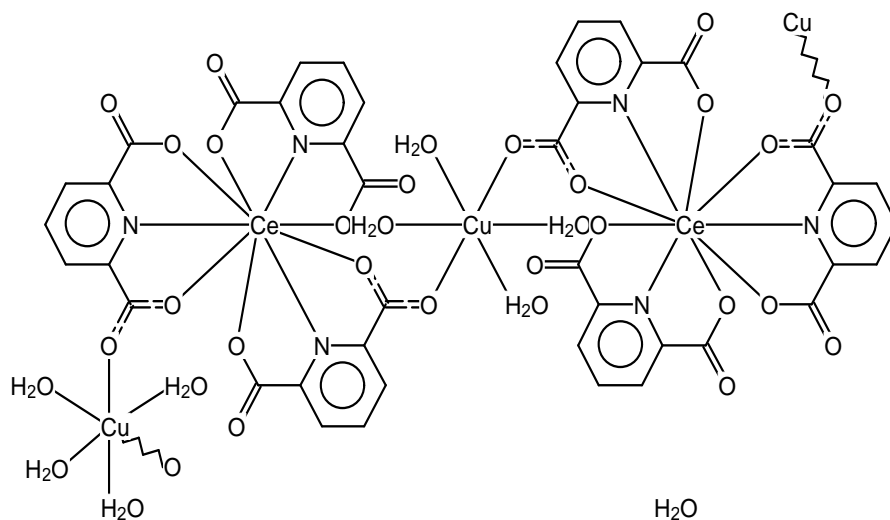
Parameters

Fragment 1

DIST1 (D) 1.953
DIST2 (D) 1.953
DIST3 (D) 1.987
DIST4 (D) 1.987
DIST5 (D) 2.369
DIST6 (D) 2.369

Fragment 2

DIST1 (D) 1.997
DIST2 (D) 1.955
DIST3 (D) 1.997
DIST4 (D) 1.955
DIST5 (D) 2.353
DIST6 (D) 2.353



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 72

GEKRUL

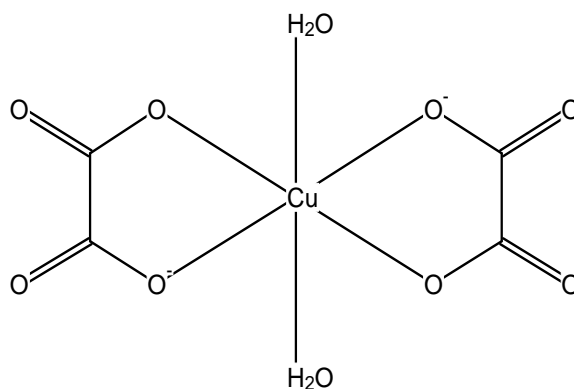
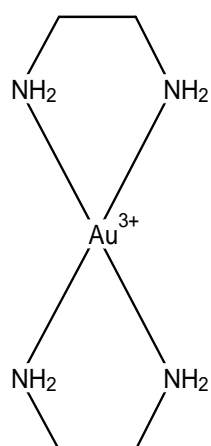
Reference: E.V.Makotchenko, E.A.Bykova, E.Yu.Semitut, Yu.V.Shubin, P.V.Snytnikov, P.E.Plyusnin (2011) *Zh.Strukt.Khim.(Russ.)(J.Struct.Chem.)*, **52**,952

Formula: $2(\text{C}_4\text{H}_{16}\text{Au}_1\text{N}_4^{3+}), \text{C}_4\text{H}_4\text{Cu}_1\text{O}_{10}^{2-}, 2(\text{C}_4\text{H}_2\text{Cu}_1\text{O}_9^{2-}), 4(\text{H}_2\text{O}_1)$

Compound Name: bis(Ethylenediamine-N,N')-gold(iii) bis(aqua-bis(oxalato-O,O')-copper(ii)) diaqua-bis(oxalato)-copper(ii) tetrahydrate

Space Group: P21/c **Cell:** **a** 9.176(0) **b** 16.975(0) **c** 13.447(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 104.33(0) γ 90.00

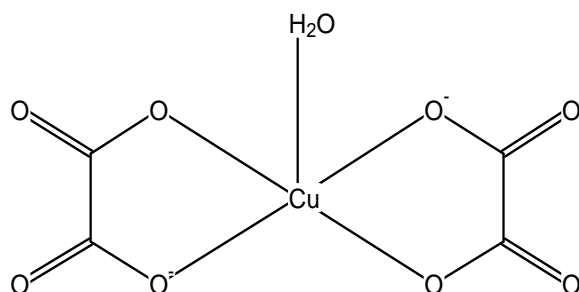
R-Factor (%): 1.51 **Temperature(K):** 150 **Density(g/cm³):** 2.450



Parameters

Fragment 1

DIST1 (D) 1.988
DIST2 (D) 1.957
DIST3 (D) 1.988
DIST4 (D) 1.957
DIST5 (D) 2.356
DIST6 (D) 2.356



H₂O

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 73

GELMUH

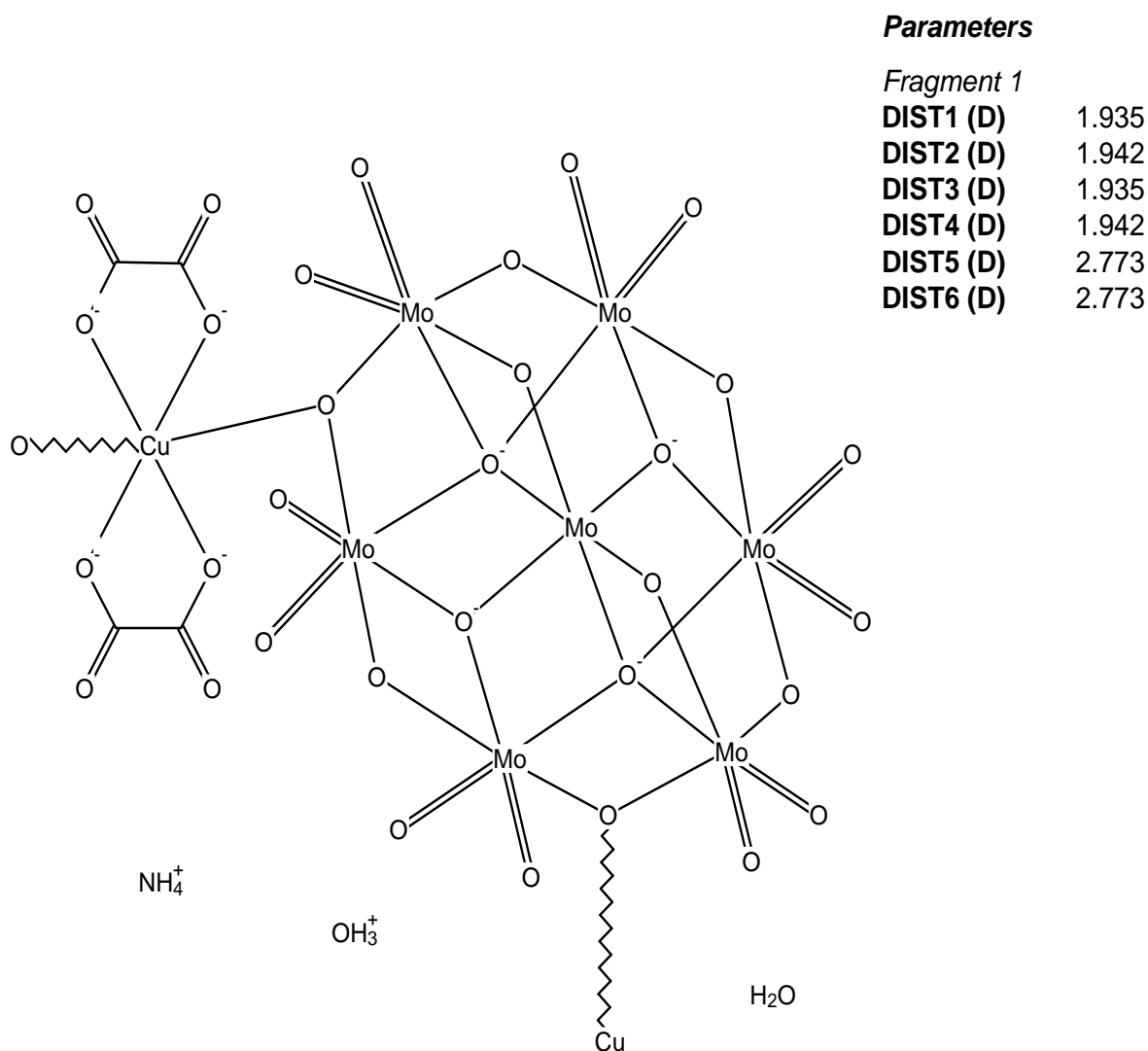
Reference: J.Li, Y.Liu, J.Luo, J.W.Zhao, P.T.Ma, J.Y.Niu (2011)
Koord.Khim.(Russ.)(Coord.Chem.), **37**,852

Formula: $(\text{H}_4 \text{N}_1^{1+})_6n, 2n(\text{H}_3 \text{O}_1^{1+}), n(\text{C}_4 \text{Cu}_1 \text{Mo}_7 \text{O}_{32}^{8-}), 7n(\text{H}_2 \text{O}_1)$

Compound Name: catena-(Hexaammonium bis(oxonium) bis(μ_4 -oxo)-tetrakis(μ_3 -oxo)-hexakis(μ_2 -oxo)-bis(oxalato)-dodecaoxo-heptamolybdenum(iv)-copper(ii) heptahydrate)

Space Group: P21/m **Cell:** **a** 10.146(0) **b** 18.262(0) **c** 10.499(0)
Space Group No.: 11 (**Å, °**) α 90.00 β 94.34(0) γ 90.00

R-Factor (%): 2.68 **Temperature(K):** 295 **Density(g/cm³):** 2.684



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 74

GIKMAP

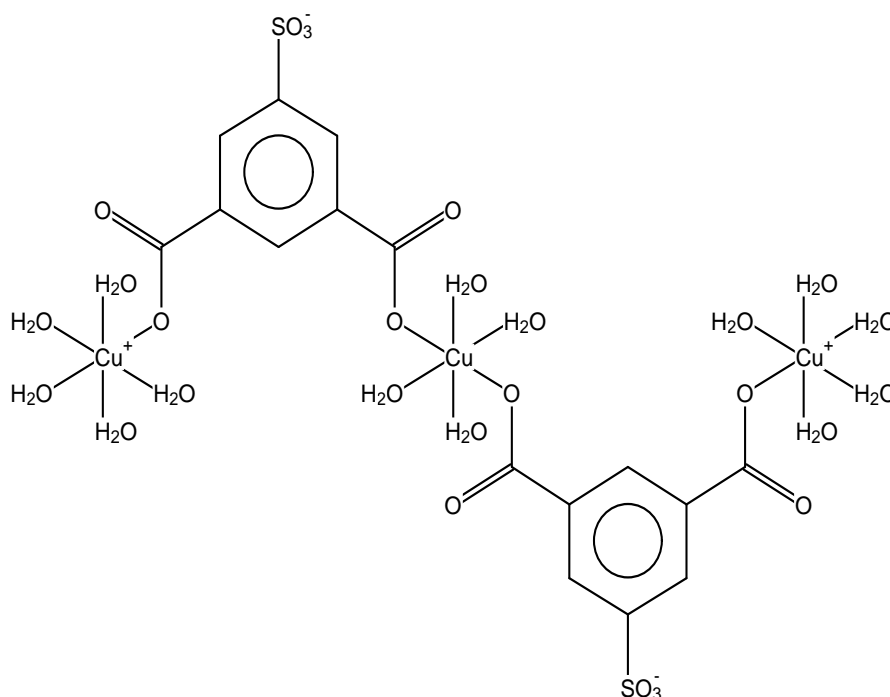
Reference: Qing-Yan Liu, Da-Qiang Yuan, Li Xu (2007)
Cryst. Growth Des., **7**, 1832

Formula: C₁₆ H₃₄ Cu₃ O₂₈ S₂

Compound Name: bis(μ_2 -5-Sulfoisophthalato)-tetradecaaqua-tri-copper(ii)

Space Group: P-1 **Cell:** **a** 6.614(1) **b** 10.699(2) **c** 12.180(3)
Space Group No.: 2 **(Å, °)** α 71.61(0) β 74.76(0) γ 75.41(0)

R-Factor (%): 2.38 **Temperature(K):** 293 **Density(g/cm³):** 1.989



Parameters

Fragment 1

DIST1 (D)	1.948
DIST2 (D)	1.987
DIST3 (D)	1.987
DIST4 (D)	1.948
DIST5 (D)	2.588
DIST6 (D)	2.588

Fragment 2

DIST1 (D)	1.938
DIST2 (D)	1.999
DIST3 (D)	1.948
DIST4 (D)	1.934
DIST5 (D)	2.397
DIST6 (D)	2.473

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 75

GIKMET

Reference: Qing-Yan Liu, Da-Qiang Yuan, Li Xu (2007)
Cryst. Growth Des., **7**, 1832

Formula: $(C_{16} H_{22} Cu_2 O_{22} S_2^{2-})_n \cdot n(C_2 H_{10} N_2^{2+})$

Compound Name: catena-(bis(μ_2 -5-Sulfoisophthalato)-octaaqua-di-copper(ii) 1,2-ethylenediammonium clathrate)

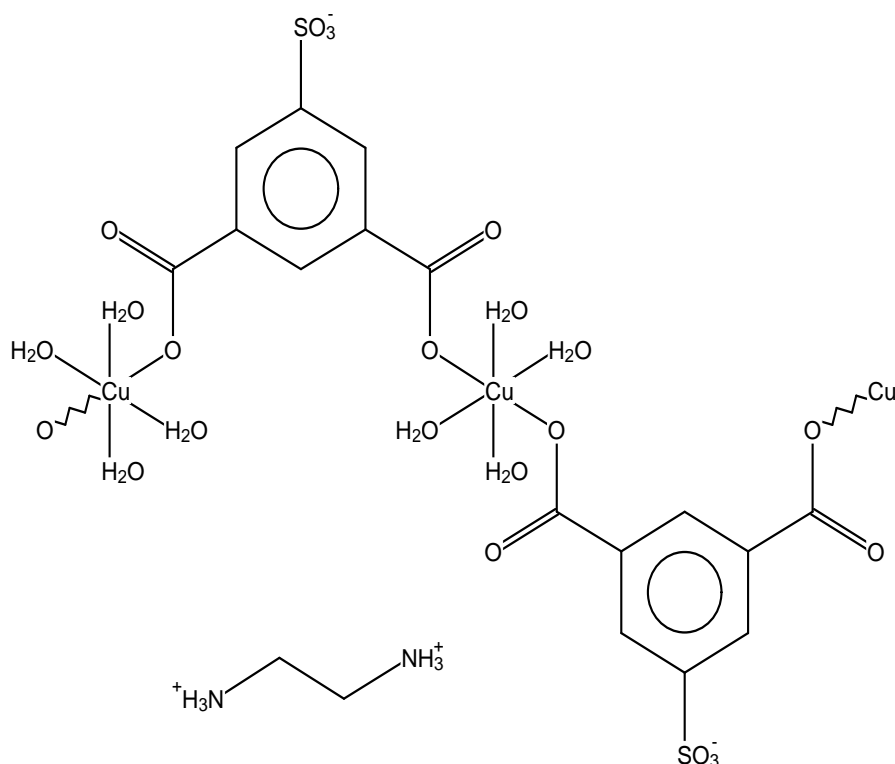
Space Group: P21/n **Cell:** **a** 6.953(1) **b** 16.301(4) **c** 13.265(3)
Space Group No.: 14 **(Å, °)** α 90.00 β 101.84(0) γ 90.00

R-Factor (%): 2.27 **Temperature(K):** 293 **Density(g/cm³):** 1.850

Parameters

Fragment 1

DIST1 (D)	1.949
DIST2 (D)	2.007
DIST3 (D)	1.975
DIST4 (D)	1.968
DIST5 (D)	2.427
DIST6 (D)	2.531



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 76

GURZID

Reference: B.Dey, A.Das, S.R.Choudhury, A.D.Jana, Li-Ping Lu, Miao-Li Zhu, S.Mukhopadhyay (2010) *Inorg.Chim.Acta* ,363,981

Formula: $(C_6 H_{12} Cd_1 Cu_1 O_{12})_n$

Compound Name: catena-(bis(μ_3 -malonato)-tetraaqua-cadmium(ii)-copper(ii))

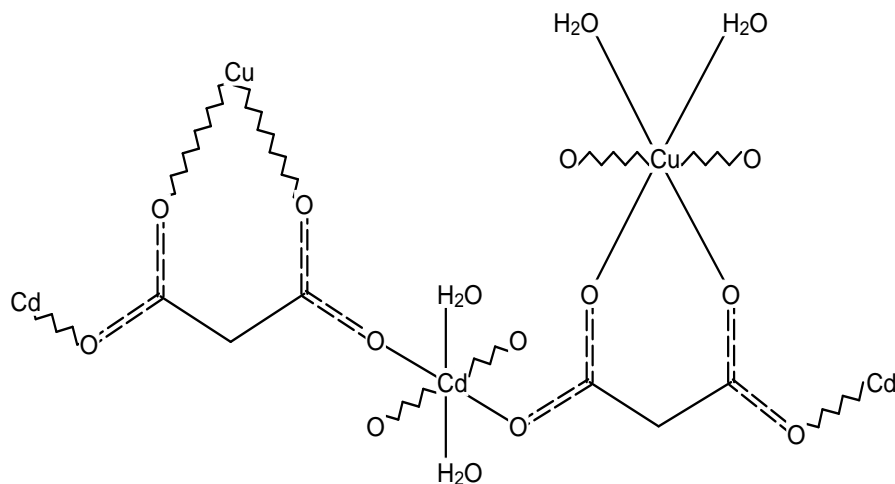
Space Group: Pbcn **Cell:** **a** 6.626(1) **b** 13.958(2) **c** 13.052(2)
Space Group No.: 60 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.25 **Temperature(K):** 298 **Density(g/cm³):** 2.488

Parameters

Fragment 1

DIST1 (D)	1.947
DIST2 (D)	1.909
DIST3 (D)	1.947
DIST4 (D)	1.909
DIST5 (D)	2.538
DIST6 (D)	2.538



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 77

GURZID01

Reference: V.S.Dhanya, M.R.Sudarsana Kumar, M.R.P.Kurup, M.Sithambaresan, S.M.Eapen, S.M.Roy (2014) *Inorg.Chim.Acta* ,**409**, 367

Formula: $(C_6 H_{12} Cd_1 Cu_1 O_{12})_n$

Compound Name: catena-[bis(μ_3 -malonato)-tetrakis(aqua)-cadmium-copper]

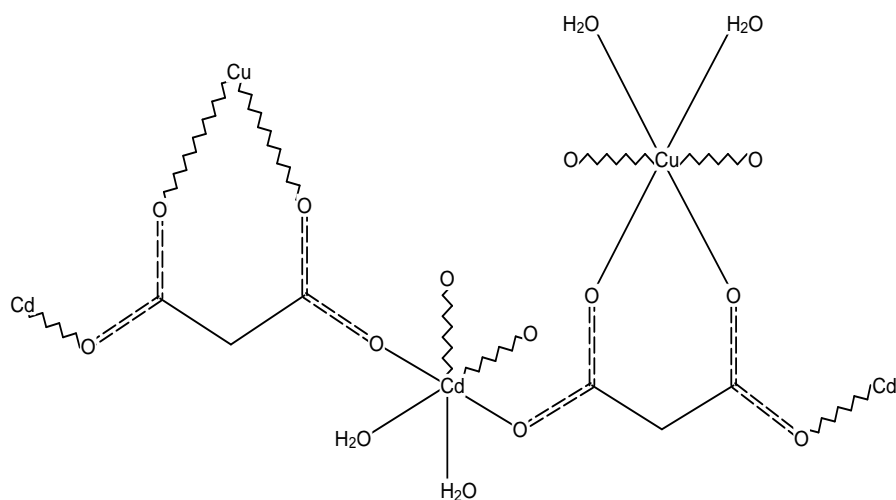
Space Group: Pbcn **Cell:** **a** 6.622(0) **b** 13.977(0) **c** 13.041(0)
Space Group No.: 60 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 1.62 **Temperature(K):** 296 **Density(g/cm³):** 2.488

Parameters

Fragment 1

DIST1 (D)	1.908
DIST2 (D)	1.945
DIST3 (D)	1.908
DIST4 (D)	1.945
DIST5 (D)	2.540
DIST6 (D)	2.540



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 78

HABHEY

Reference: K.Slepokura, A.Piatkowska, T.Lis (2002) *Z.Kristallogr.*, 217,614

Formula: C₄ H₁₂ Cu₁ O₁₂ P₂

Compound Name: Diaqua-bis(phosphonoacetato-O,O')-copper(ii)

Space Group: P-1 **Cell:** **a** 6.556(2) **b** 8.828(3) **c** 10.560(3)
Space Group No.: 2 **(Å, °)** α 79.00(3) β 84.09(3) γ 89.35(3)

R-Factor (%): 2.15 **Temperature(K):** 150 **Density(g/cm³):** 2.102

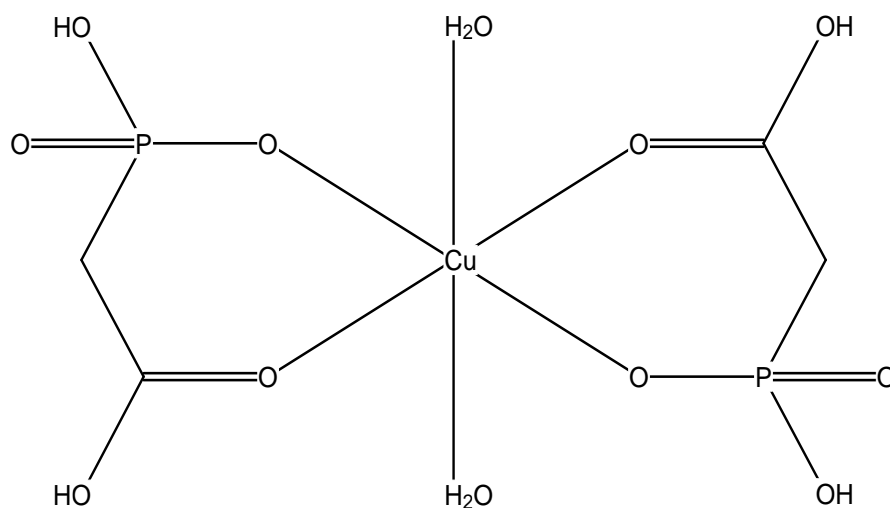
Parameters

Fragment 1

DIST1 (D) 2.011
DIST2 (D) 1.929
DIST3 (D) 1.929
DIST4 (D) 2.011
DIST5 (D) 2.398
DIST6 (D) 2.398

Fragment 2

DIST1 (D) 2.008
DIST2 (D) 1.928
DIST3 (D) 1.928
DIST4 (D) 2.008
DIST5 (D) 2.439
DIST6 (D) 2.439



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 79

HACGEZ

Reference: R.A.Allao, A.K.Jordao, J.A.L.C.Resende, A.C.Cunha, V.F.Ferreira, M.A.Novak, C.Sangregorio, L.Sorace, M.G.F.Vaz (2011) *Dalton Trans.* ,**40**,10843

Formula: (C₃₈ H₃₈ Cu₂ F₂₄ N₈ O₁₀)_n

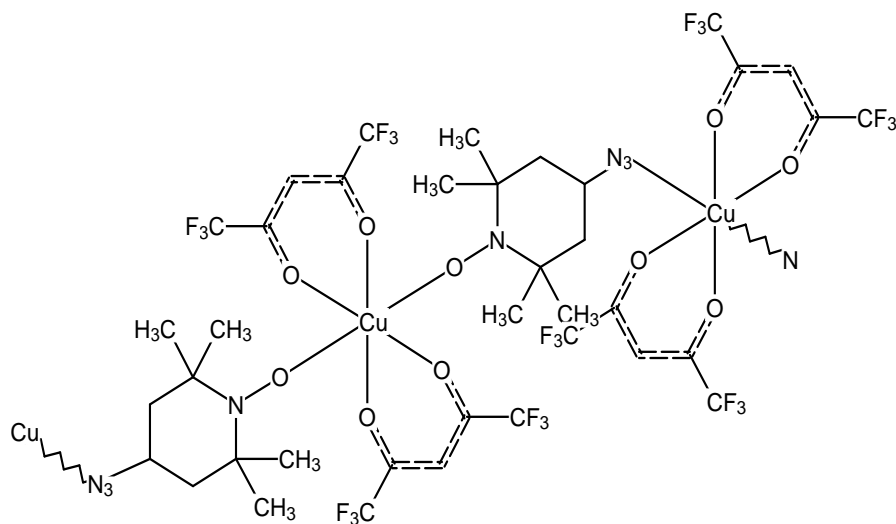
Compound Name: catena-(bis(μ₂-4-azido-2,2,6,6-tetramethylpiperidine-1-oxyl)-tetrakis(hexafluoroacetylacetonato)-di-copper)

Space Group: P-1 **Cell:** **a** 8.654(0) **b** 12.129(0) **c** 12.755(3)
Space Group No.: 2 **(Å, °)** **α** 77.66(0) **β** 85.33(0) **γ** 74.22(0)
R-Factor (%): 2.53 **Temperature(K):** 153 **Density(g/cm³):** 1.781

Parameters

Fragment 1

DIST1 (D) 1.937
DIST2 (D) 1.941
DIST3 (D) 1.937
DIST4 (D) 1.941
DIST5 (D) 2.509
DIST6 (D) 2.509



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 80

HAJRAM

Reference: F.S.Delgado, J.Sanchiz, C.Ruiz-Perez, F.Lloret, M.Julve (2004) *CrystEngComm*, **6**,443

Formula: (C₆ H₆ Cu₁ O₈)_n

Compound Name: catena-(bis(μ_2 -malonato)-copper(ii))

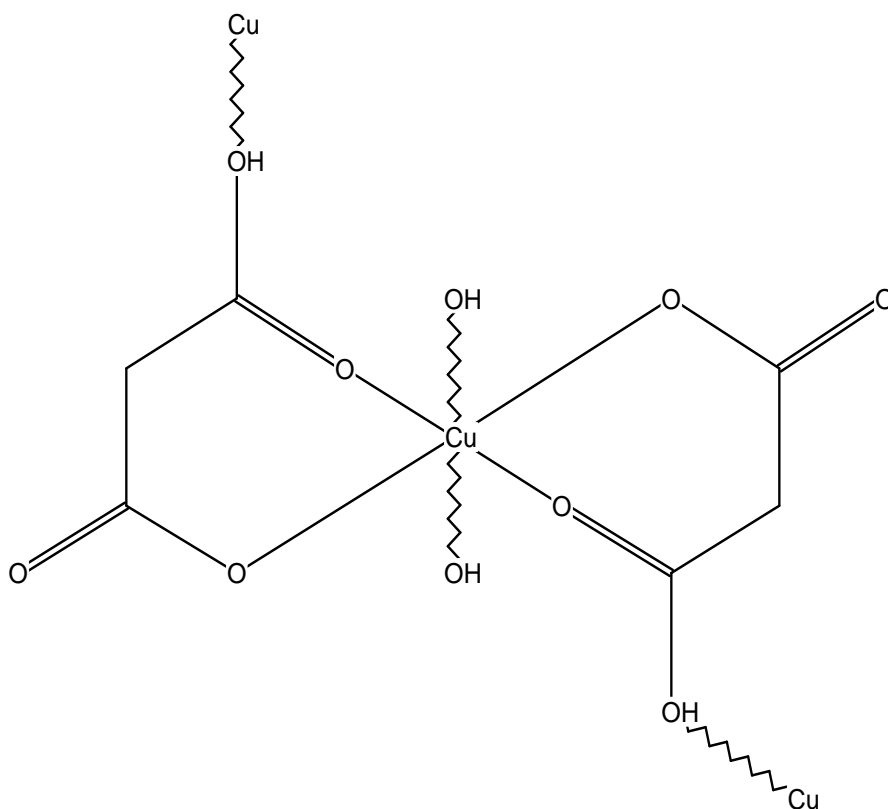
Space Group: Pbc_a **Cell:** **a** 6.742(0) **b** 9.382(0) **c** 12.452(1)
Space Group No.: 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.78 **Temperature(K):** 293 **Density(g/cm³):** 2.274

Parameters

Fragment 1

DIST1 (D)	1.944
DIST2 (D)	1.932
DIST3 (D)	1.932
DIST4 (D)	1.944
DIST5 (D)	2.543
DIST6 (D)	2.543



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 81

HESKIZ

Reference: S.Kawata, S.Kitagawa, M.Kondo, I.Furuchi, M.Munakata (1994) *Angew.Chem.,Int.Ed.* ,**33**,1759

Formula: (C₈ H₈ Cl₂ Cu₁ O₆)_n

Compound Name: catena-((μ_2 -3,6-Dichloro-2,5-dihydroxy-p-benzoquinonato)-bis(methanol-O)-copper(ii))

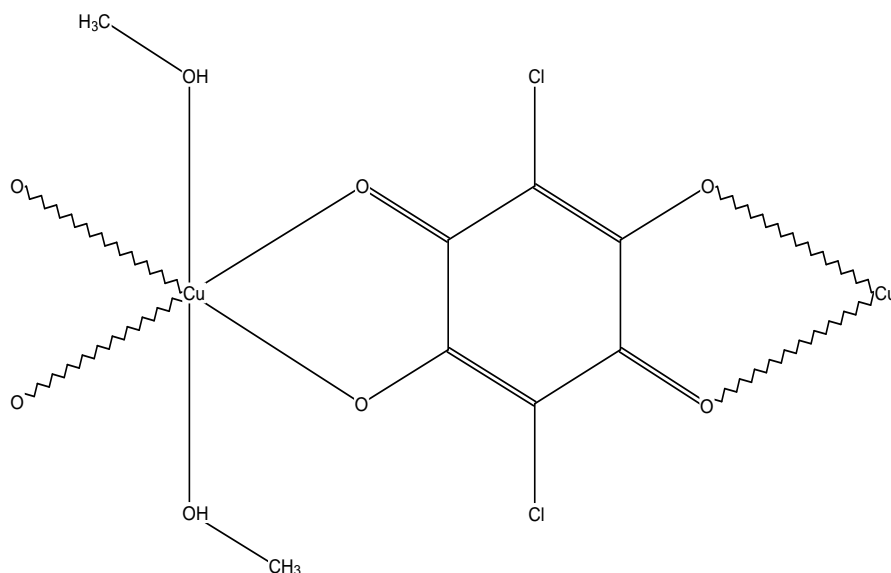
Space Group: P-1 **Cell:** **a** 7.672(0) **b** 7.780(2) **c** 5.108(0)
Space Group No.: 2 **(Å, °)** α 99.89(2) β 98.41(1) γ 100.25(2)

R-Factor (%): 2.90 **Temperature(K):** 295 **Density(g/cm³):** 1.912

Parameters

Fragment 1

DIST1 (D)	1.963
DIST2 (D)	1.963
DIST3 (D)	2.005
DIST4 (D)	2.005
DIST5 (D)	2.279
DIST6 (D)	2.279



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 82

HINWEH

Reference: S.Balboa, A.Castineiras, P.S.Herle, J.Strahle (2007)
Z.Anorg.Allg.Chem. ,**633**,2420

Formula: (C₆ H₁₀ Cu₁ O₆)_n

Compound Name: catena-(bis(μ_2 -Lactato-O,O',O'')-copper(ii))

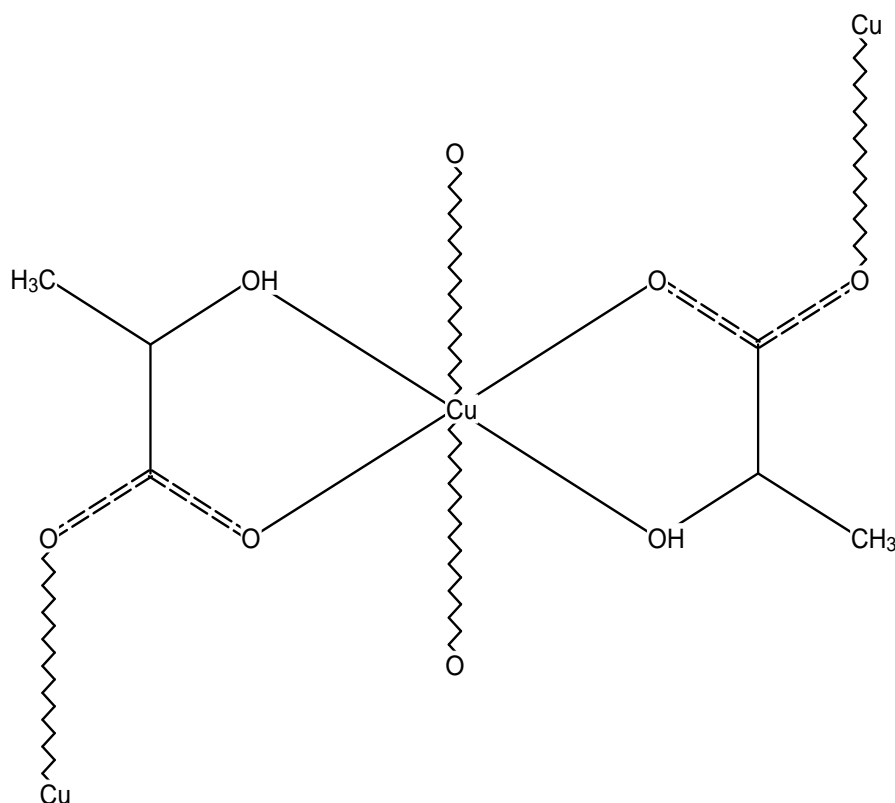
Space Group: P21/c **Cell:** **a** 5.185(1) **b** 8.362(1) **c** 8.841(4)
Space Group No.: 14 **(Å, °)** α 90.00 β 110.86(3) γ 90.00

R-Factor (%): 2.63 **Temperature(K):** 208 **Density(g/cm³):** 2.241

Parameters

Fragment 1

DIST1 (D) 1.947
DIST2 (D) 1.926
DIST3 (D) 1.926
DIST4 (D) 1.947
DIST5 (D) 2.499
DIST6 (D) 2.499



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 83

HOWFEE

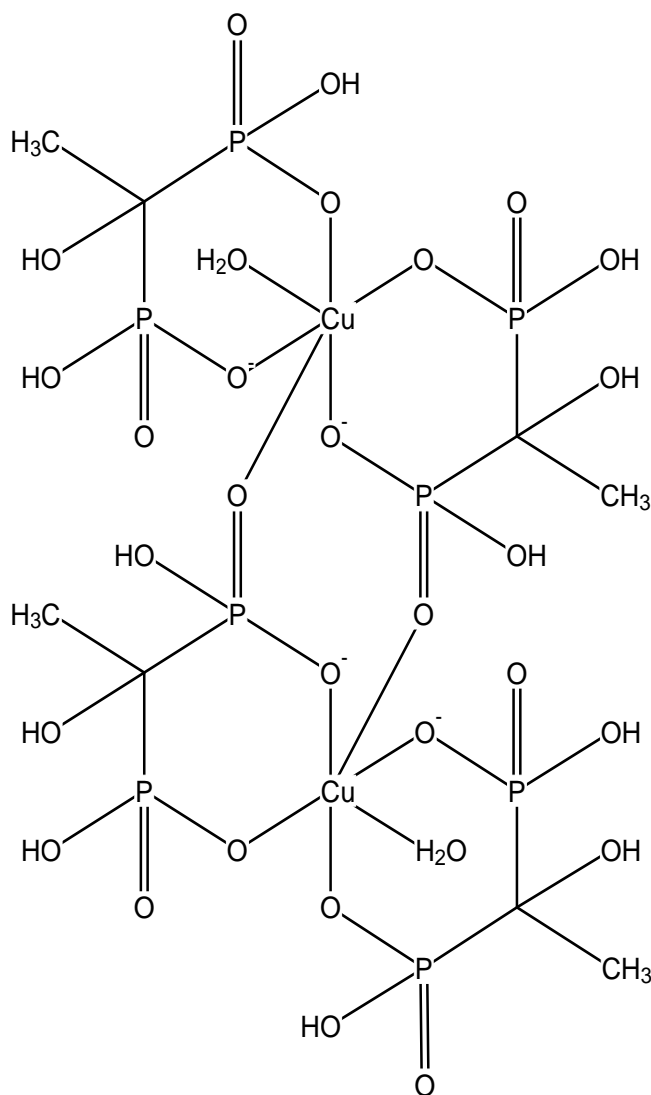
Reference: V.S.Sergienko, G.G.Aleksandrov, E.G.Afonin (1999)
Koord.Khim.(Russ.)(Coord.Chem.), **25**,451

Formula: C₈ H₂₈ Cu₂ O₃₀ P₈⁴⁻·4(K₁¹⁺),4(H₂O₁)

Compound Name: Tetra-potassium bis(aqua-(μ₂-(1-hydroxyethane-1,1-diphosphonato-O, O'))-(1-hydroxyethane-1,1-diphosphonato-O,O)-copper(ii)) tetrahydrate

Space Group: P21/c **Cell:** **a** 12.530(1) **b** 12.143(1) **c** 12.787(1)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 108.95(1) **γ** 90.00

R-Factor (%): 2.45 **Temperature(K):** 295 **Density(g/cm³):** 2.180



Parameters

Fragment 1

DIST1 (D)	1.984
DIST2 (D)	1.960
DIST3 (D)	1.985
DIST4 (D)	2.033
DIST5 (D)	2.359
DIST6 (D)	2.327

H₂O

K⁺

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 84

HULMAC

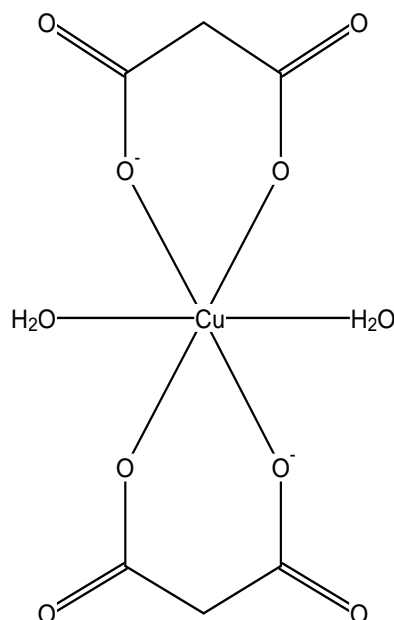
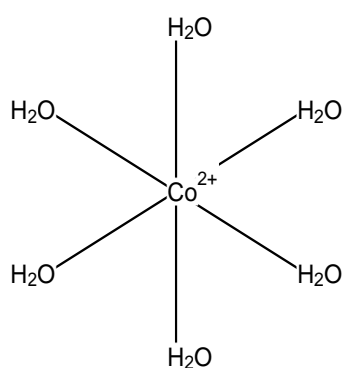
Reference: Y.Rodriguez-Martin, J.Sanchiz, C.Ruiz-Perez, F.Lloret, M.Julve (2002) *CrystEngComm* ,4,631

Formula: $H_{12} Co_1 O_6^{2+}, C_6 H_8 Cu_1 O_{10}^{2-}$

Compound Name: Hexa-aqua-cobalt(ii) diaqua-bis(malonato-O,O')-copper(ii)

Space Group: P-1 **Cell:** **a** 5.266(1) **b** 7.495(1) **c** 10.332(2)
Space Group No.: 2 **(Å, °)** α 107.14(0) β 98.99(0) γ 96.17(0)

R-Factor (%): 2.88 **Temperature(K):** 293 **Density(g/cm³):** 2.058



Parameters

Fragment 1

DIST1 (D)	1.946
DIST2 (D)	1.947
DIST3 (D)	1.946
DIST4 (D)	1.947
DIST5 (D)	2.459
DIST6 (D)	2.459

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 85

HULMEG

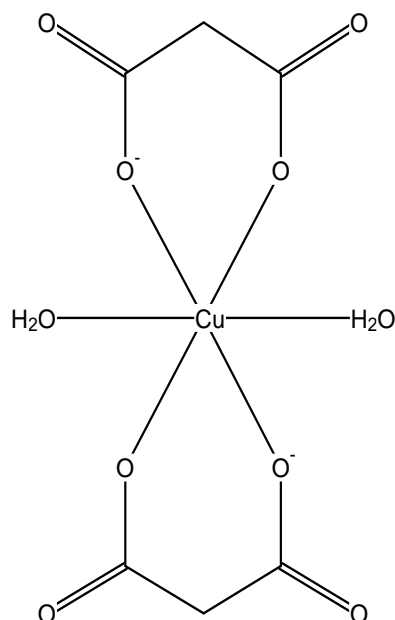
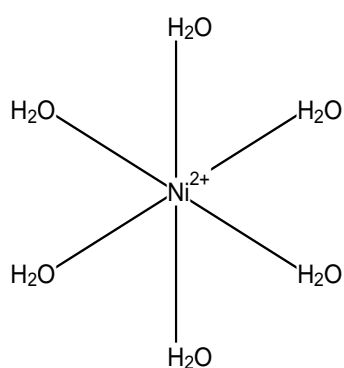
Reference: Y.Rodriguez-Martin, J.Sanchiz, C.Ruiz-Perez, F.Lloret, M.Julve (2002) *CrystEngComm* ,4,631

Formula: $\text{H}_{12} \text{Ni}_1 \text{O}_6^{2+}, \text{C}_6 \text{H}_8 \text{Cu}_1 \text{O}_{10}^{2-}$

Compound Name: Hexa-aqua-nickel(ii) diaqua-bis(malonato-O,O')-copper(ii)

Space Group: P-1 **Cell:** **a** 5.242(1) **b** 7.480(3) **c** 10.278(4)
Space Group No.: 2 **(Å, °)** α 107.15(3) β 98.77(3) γ 96.34(3)

R-Factor (%): 2.73 **Temperature(K):** 293 **Density(g/cm³):** 2.081



Parameters

Fragment 1

DIST1 (D)	1.946
DIST2 (D)	1.947
DIST3 (D)	1.946
DIST4 (D)	1.947
DIST5 (D)	2.445
DIST6 (D)	2.445

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 86

HUXWAY

Reference: B.Barja, R.Baggio, M.T.Garland, P.F.Aramendia, O.Pena, M.Perec (2003) *Inorg.Chim.Acta* ,**346**,187

Formula: (C₂₄ H₃₆ Cu₃ O₃₆ Tb₂)_n,12n(H₂ O₁)

Compound Name: catena-[hexakis(μ₃-2,2'-Oxydiacetato)-hexa-aqua-tri-copper(ii)-diterbium(iii) dodecahydrate]

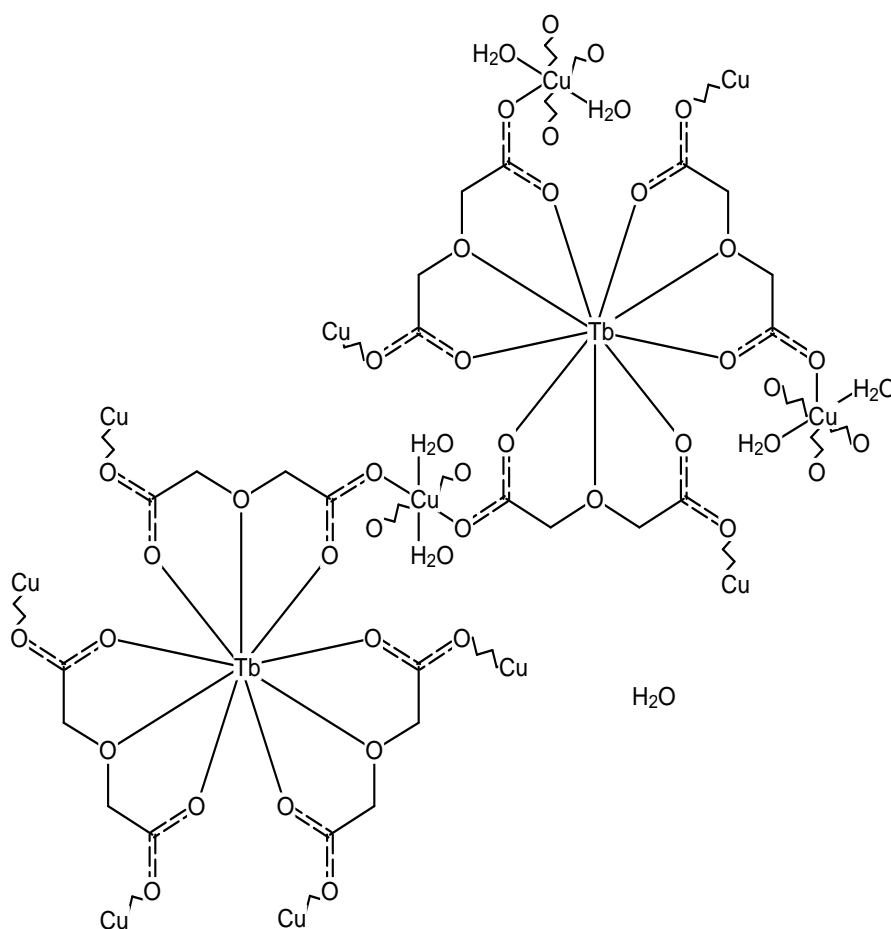
Space Group: P6/mcc **Cell:** **a** 14.693(2) **b** 14.693(2) **c** 15.125(2)
Space Group No.: 192 **(Å, °)** α 90.00 β 90.00 γ 120.00

R-Factor (%): 2.74 **Temperature(K):** 293 **Density(g/cm³):** 1.909

Parameters

Fragment 1

DIST1 (D)	1.951
DIST2 (D)	1.951
DIST3 (D)	1.951
DIST4 (D)	1.951
DIST5 (D)	2.500
DIST6 (D)	2.500



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 87

ICAMOQ

Reference: Wei Chen, Jinfeng Chu, I.Mutikainen, J.Reedijk, U.Turpeinen, Yu-Fei Song (2011) *CrystEngComm* ,13,7299

Formula: $C_{26} H_{32} Cu_2 N_{12} O_2^{4+}, 2(H_2 O_1), C_4 Cl_2 Cu_1 O_{16}^{4-}$

Compound Name: bis(ethanedioato)-bis(perchlorato)-copper bis(μ_2 -1,1-bis(1H-imidazol-2-yl)-N-((pyridin-2-yl)methyl)methanamine)-diaqua-di-copper dihydrate

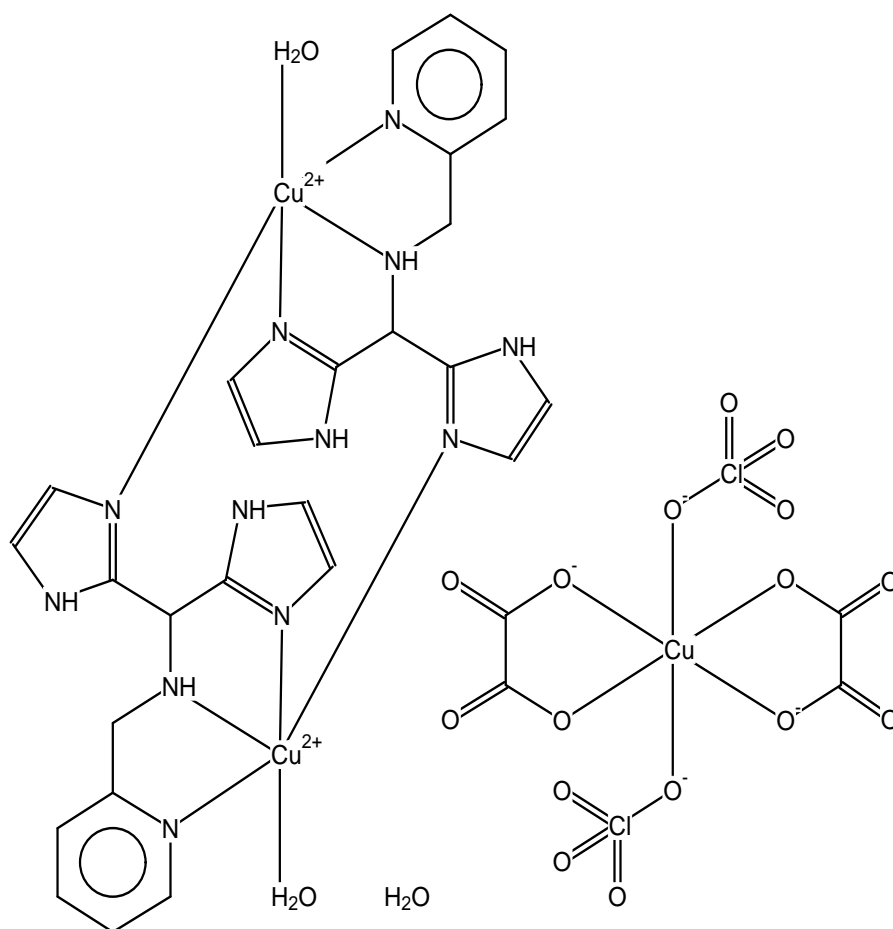
Space Group: P21/n **Cell:** **a** 10.145(1) **b** 16.441(2) **c** 13.180(2)
Space Group No.: 14 **(Å, °)** α 90.00 β 109.54(0) γ 90.00

R-Factor (%): 2.89 **Temperature(K):** 93 **Density(g/cm³):** 1.838

Parameters

Fragment 1

DIST1 (D)	1.968
DIST2 (D)	1.926
DIST3 (D)	1.968
DIST4 (D)	1.926
DIST5 (D)	2.463
DIST6 (D)	2.463



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 89

IKIPEX02

Reference: M.A.Ershov, V.G.Skvortsov, Y.Yu.Pilchikova,
O.V.Koltsova, K.Yu.Suponitsky (2006)
Acta Crystallogr., Sect.E: Struct.Rep.Online ,62,m3073

Formula: C₆ H₁₂ Cu₁ N₆ O₁₀

Compound Name: bis(malonamide-κ²O,O')bis(nitrato-κO)copper(ii)

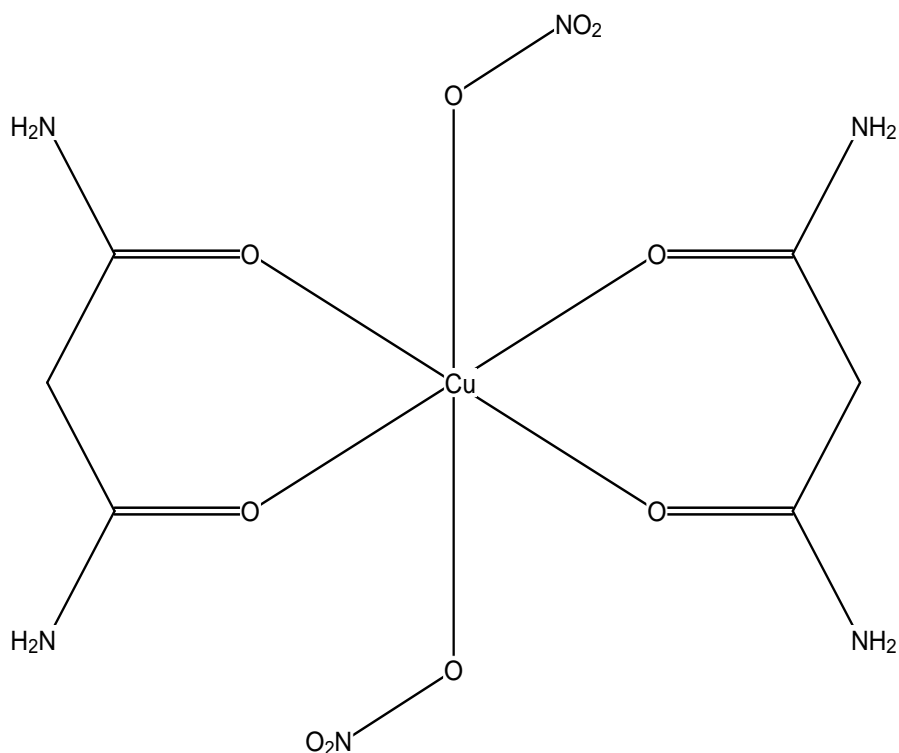
Space Group: P-1 **Cell:** **a** 6.852(0) **b** 7.070(0) **c** 7.461(0)
Space Group No.: 2 (**Å, °**) **α** 89.66(0) **β** 69.49(0) **γ** 73.48(0)

R-Factor (%): 2.41 **Temperature(K):** 120 **Density(g/cm³):** 2.015

Parameters

Fragment 1

DIST1 (D)	1.973
DIST2 (D)	1.934
DIST3 (D)	1.973
DIST4 (D)	1.934
DIST5 (D)	2.396
DIST6 (D)	2.396



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 90

ININID

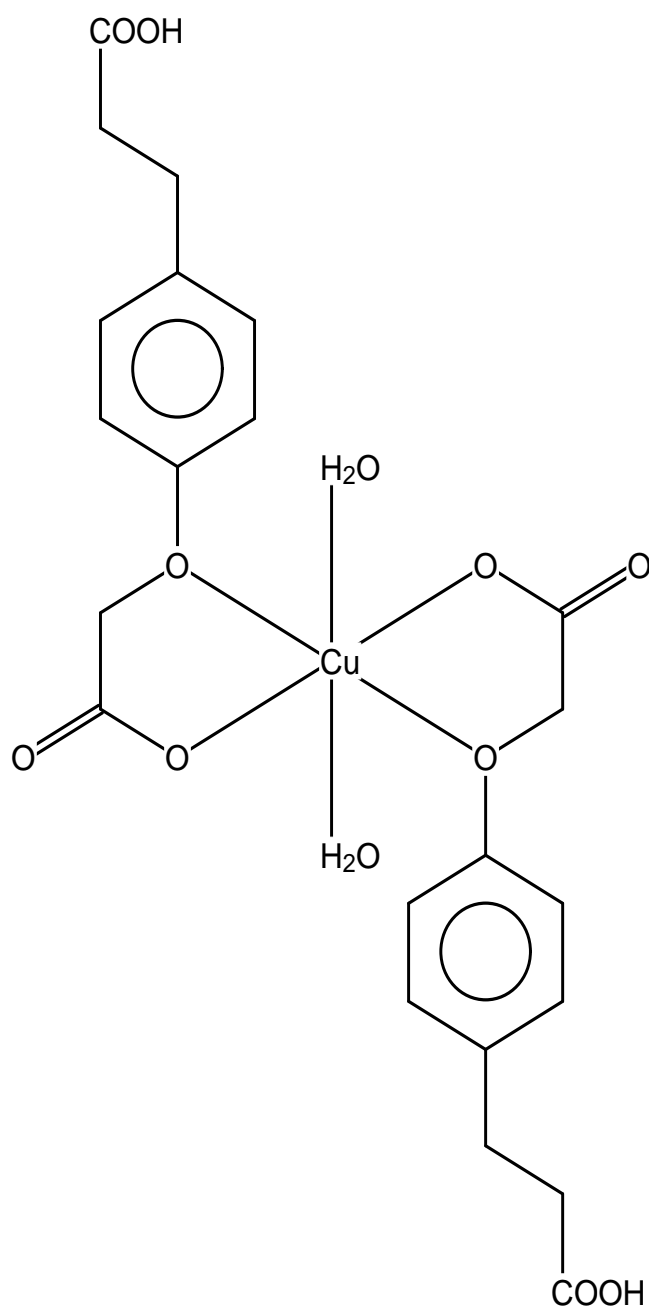
Reference: Chong-Bo Liu, Hui-Liang Wen, Yun-Nan Gong,
Xiao-Ming Liu, Sheng-Shui Tan (2011) *Z.Anorg.Allg.Chem.* ,637,122

Formula: C₂₂ H₂₆ Cu₁ O₁₂

Compound Name: Diaqua-bis(2-(4-(2-carboxyethoxy)phenoxy)acetato)-copper(ii)

Space Group: P-1 **Cell:** **a** 5.337(1) **b** 6.710(1) **c** 16.386(3)
Space Group No.: 2 **(Å, °)** α 87.15(0) β 82.17(0) γ 73.13(0)

R-Factor (%): 2.53 **Temperature(K):** 291 **Density(g/cm³):** 1.630



Parameters

Fragment 1

DIST1 (D)	1.947
DIST2 (D)	1.963
DIST3 (D)	1.963
DIST4 (D)	1.947
DIST5 (D)	2.420
DIST6 (D)	2.420

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 91

IPOWOA

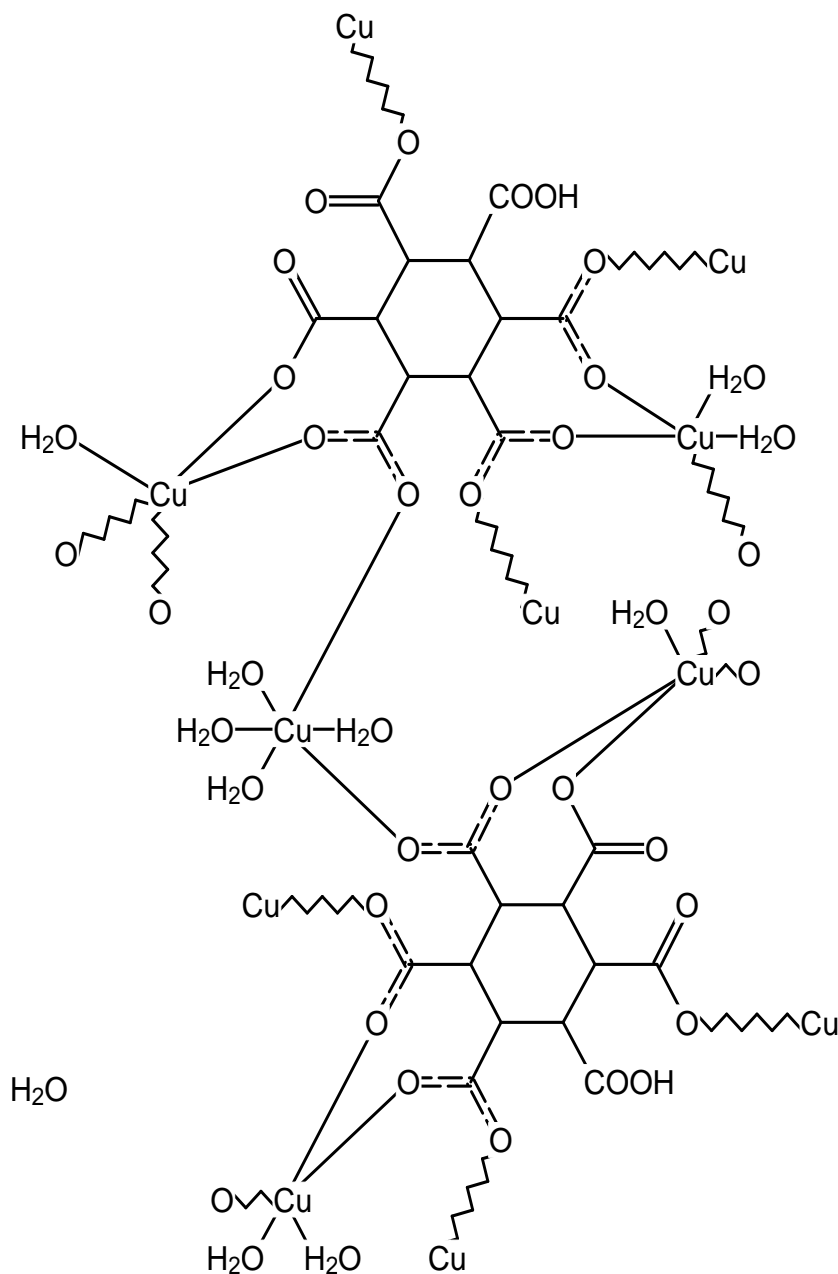
Reference: Yue-Qing Zheng, Xia-Xia Guo, Xiao-Yan Han, Jia-Hui Xu (2011) *Inorg.Chim.Acta* ,**370**,36

Formula: $(C_{24} H_{34} Cu_5 O_{34})_n \cdot 4n(H_2 O)_1$

Compound Name: catena(-bis(μ_6 -6-Carboxyl-benzene-1,2,3,4,5-pentacarboxylato)-deca-aqua-penta-copper tetrahydrate)

Space Group: C2/c **Cell:** **a** 17.101(3) **b** 8.397(1) **c** 27.654(6)
Space Group No.: 15 (**Å, °**) α 90.00 β 104.63(3) γ 90.00

R-Factor (%): 2.65 **Temperature(K):** 293 **Density(g/cm³):** 2.172



Parameters

Fragment 1

DIST1 (D)	1.953
DIST2 (D)	1.950
DIST3 (D)	1.950
DIST4 (D)	1.935
DIST5 (D)	2.408
DIST6 (D)	2.408

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 92

JEGNOZ

Reference: Zhu-Yan Zhang, Shan Gao, Li-Hua Huo, Hui Zhao,
Jing-Gui Zhao (2006)
Wuji Huaxue Xuebao(Chin.)(Chin.J.Inorg.Chem.) ,**22**,905

Formula: (C₁₄ H₁₂ Cu₁ N₂ O₆)_n

Compound Name: catena-(bis(μ₂-(4-Oxo-4H-pyridin-1-yl)acetato-O,O',O'')-copper(ii))

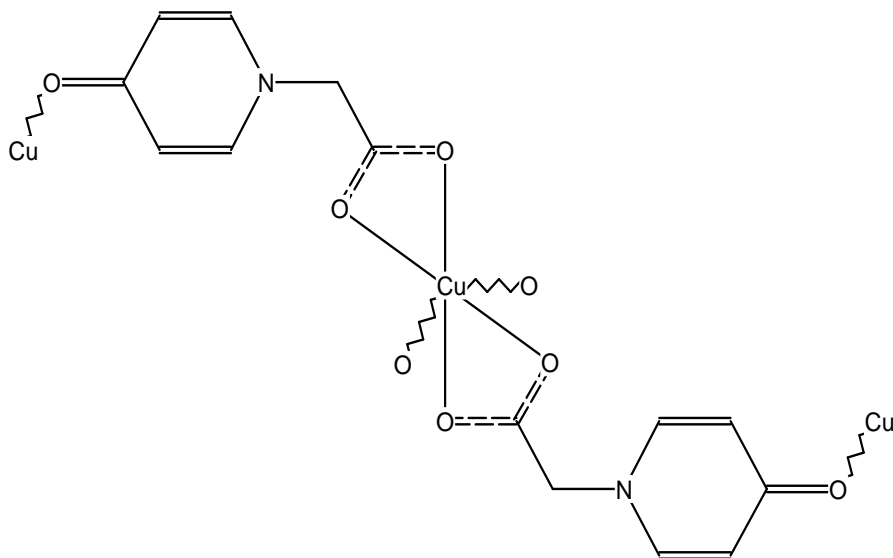
Space Group: P-1 **Cell:** **a** 7.132(1) **b** 7.398(1) **c** 7.530(1)
Space Group No.: 2 **(Å, °)** **α** 91.46(3) **β** 109.14(3) **γ** 111.31(3)

R-Factor (%): 2.86 **Temperature(K):** 295 **Density(g/cm³):** 1.771

Parameters

Fragment 1

DIST1 (D)	1.941
DIST2 (D)	1.960
DIST3 (D)	1.960
DIST4 (D)	1.941
DIST5 (D)	2.716
DIST6 (D)	2.716



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 93

JUFXOZ

Reference: W.Clegg, J.M.Holcroft, N.C.Martin (2015) *CrystEngComm*, **17**,2857

Formula: (C₁₀ H₈ Cu₁ K₂ O₁₁)_n,H₂ O₁

Compound Name: catena-[(μ-benzene-1,2,4,5-tetracarboxylato)-bis(μ-aqua)-aqua-di-potassium-copper monohydrate]

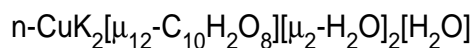
Space Group: P-1 **Cell:** **a** 7.739(1) **b** 10.600(1) **c** 10.616(1)
Space Group No.: 2 (**Å, °**) α 112.87(1) β 90.41(1) γ 104.19(1)

R-Factor (%): 2.85 **Temperature(K):** 295 **Density(g/cm³):** 1.994

Parameters

Fragment 1

DIST1 (D) 1.991
DIST2 (D) 1.948
DIST3 (D) 1.935
DIST4 (D) 1.977
DIST5 (D) 2.601
DIST6 (D) 2.611



H₂O

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 94

JUFXUF

Reference: W.Clegg, J.M.Holcroft, N.C.Martin (2015) *CrystEngComm*, 17,2857

Formula: (C₁₀ H₁₀ Cu₁ Na₂ O₁₂)_n

Compound Name: catena-[(μ-benzene-1,2,4,5-tetracarboxylato)-tri-aqua-copper-di-sodium]

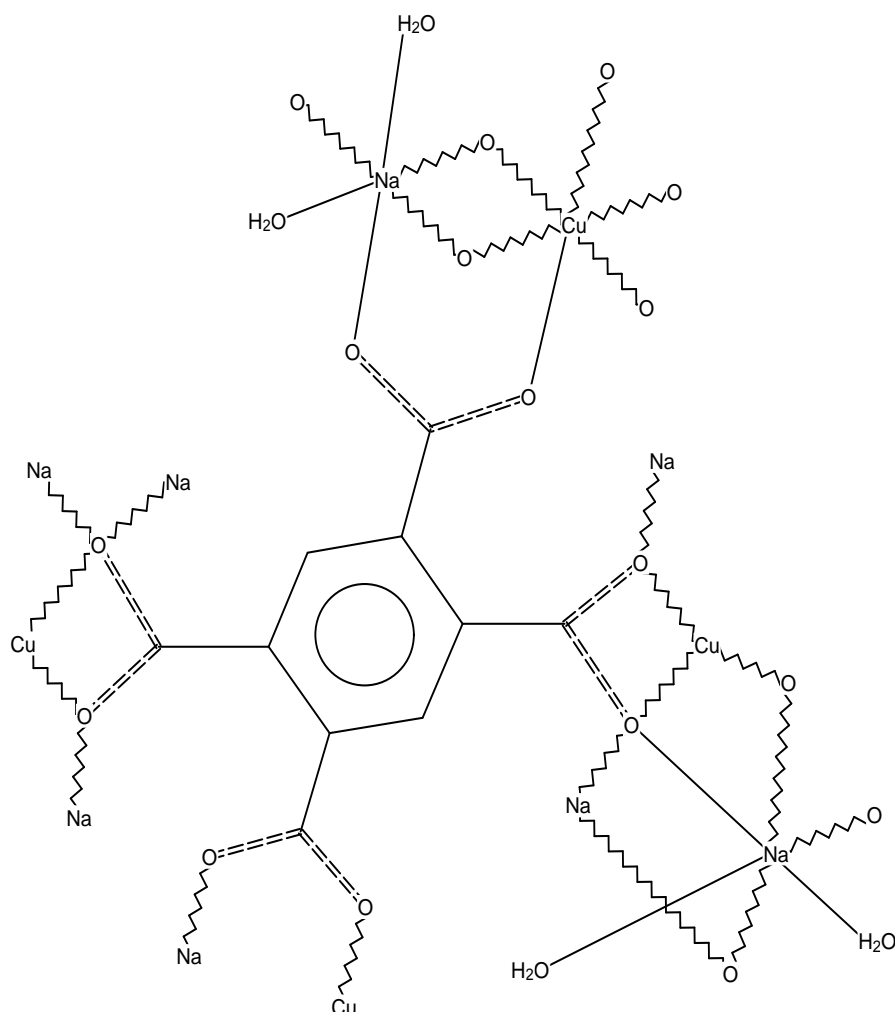
Space Group: C2/c **Cell:** **a** 6.894(0) **b** 16.338(1) **c** 12.938(0)
Space Group No.: 15 **(Å, °)** **α** 90.00 **β** 99.67(0) **γ** 90.00

R-Factor (%): 2.05 **Temperature(K):** 160 **Density(g/cm³):** 1.996

Parameters

Fragment 1

DIST1 (D)	1.940
DIST2 (D)	1.955
DIST3 (D)	1.940
DIST4 (D)	1.955
DIST5 (D)	2.767
DIST6 (D)	2.767



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 95

JUQNEO

Reference: E.V.Karpova, A.I.Boltalin, M.A.Zakharov, N.I.Sorokina,
Y.M.Korenev, S.I.Troyanov (1998) *Z.Anorg.Allg.Chem.* ,**624**,741

Formula: C₄ H₈ Cu₁ F₆ O₈

Compound Name: Tetra-aqua-bis(trifluoroacetato-O)-copper(ii)

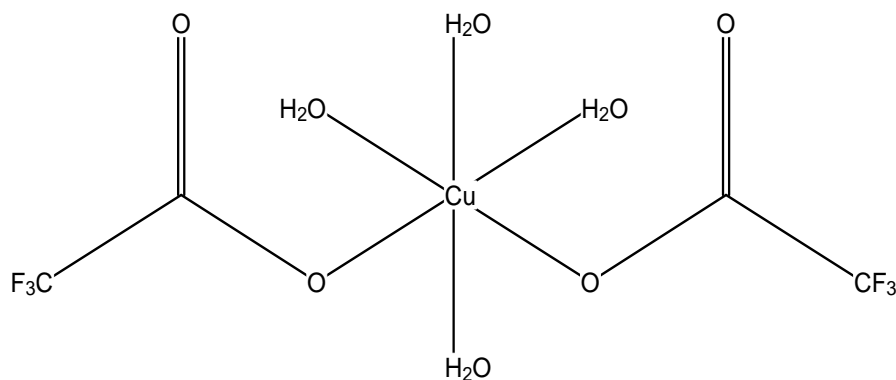
Space Group: P21 **Cell:** **a** 5.064(1) **b** 12.091(2) **c** 9.537(2)
Space Group No.: 4 **(Å, °)** α 90.00 β 99.10(3) γ 90.00

R-Factor (%): 2.50 **Temperature(K):** 295 **Density(g/cm³):** 2.083

Parameters

Fragment 1

DIST1 (D)	1.943
DIST2 (D)	1.967
DIST3 (D)	2.003
DIST4 (D)	1.931
DIST5 (D)	2.436
DIST6 (D)	2.459



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 96

KCUOXD02

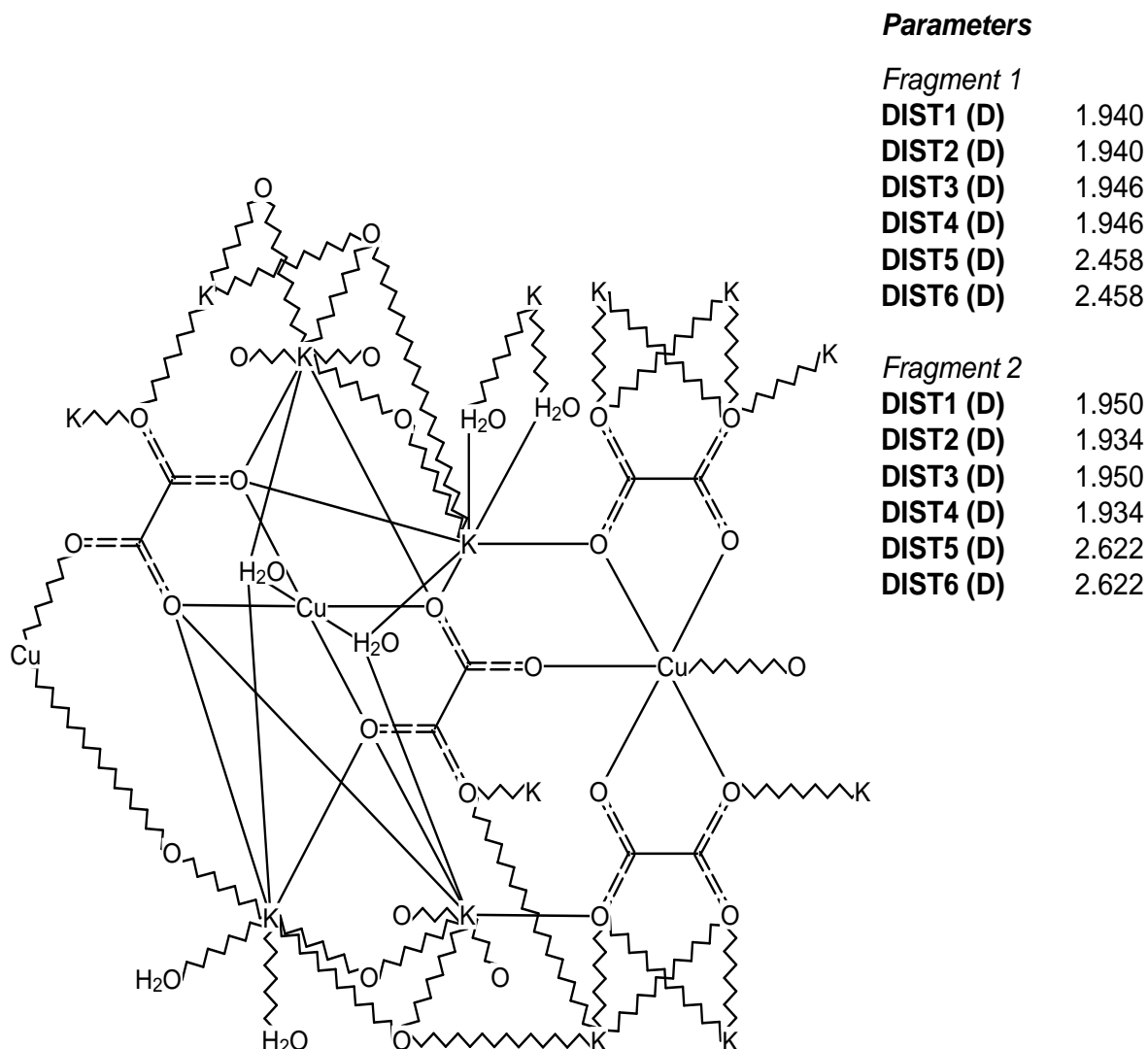
Reference: Jian Wu, Jian-Qing Liu (2010)
Synth.React.Inorg.,Met.-Org.,Nano-Met.Chem. ,**40**,237

Formula: (C₈ H₈ Cu₂ K₄ O₂₀)_n

Compound Name: catena-[bis(μ₈-Oxalato)-bis(μ₅-oxalato)-bis(μ₃-aqua)-bis(μ₂-aqua)-di-copper(ii)-tetra-potassium(i)]

Space Group: P-1 **Cell:** **a** 6.938(2) **b** 8.703(3) **c** 9.022(3)
Space Group No.: 2 **(Å, °)** α 108.25(0) β 99.96(0) γ 97.19(0)

R-Factor (%): 2.25 **Temperature(K):** 296 **Density(g/cm³):** 2.350



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 97

KCUOXD03

Reference: B.Zhang, Y.Zhang, J.Zhang, X.Yan, D.Zhu (2016)
CrystEngComm ,18,5062

Formula: (C₈ H₈ Cu₂ K₄ O₂₀)_n

Compound Name: catena-[tetrakis(μ-Oxalato)-tetrakis(μ-aqua)-di-copper-tetra-potassium]

Space Group: P-1 **Cell:** **a** 6.904(2) **b** 8.660(3) **c** 8.929(3)
Space Group No.: 2 **(Å, °)** α 107.95(0) β 99.64(0) γ 97.64(0)

R-Factor (%): 2.83 **Temperature(K):** 173 **Density(g/cm³):** 2.394

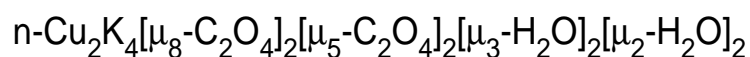
Parameters

Fragment 1

DIST1 (D) 1.942
DIST2 (D) 1.941
DIST3 (D) 1.942
DIST4 (D) 1.941
DIST5 (D) 2.424
DIST6 (D) 2.424

Fragment 2

DIST1 (D) 1.931
DIST2 (D) 1.951
DIST3 (D) 1.931
DIST4 (D) 1.951
DIST5 (D) 2.583
DIST6 (D) 2.583



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 98

KOHXAH

Reference: Junwei Ye, Jingying Zhang, Ling Ye, Dong Xie, Tao Xu, Gang Li, Guiling Ning (2008) *Dalton Trans.* ,5342

Formula: $(C_{48} H_{28} Cu_2 La_2 N_6 O_{40})_n \cdot 4n(H_2 O)_1$

Compound Name: catena-(bis(μ_4 -5-Nitroisophthalato-O,O',O'',O''')-bis(μ_3 -5-nitroisophthalato-O,O',O'',O''')-bis(μ_3 -hydrogen 5-nitroisophthalato-O,O',O'',O''')-bis(μ_2 -aqua)-diaqua-di-copper(ii)-di-lanthanum(iii) tetrahydrate)

Space Group: P-1 **Cell:** **a** 10.845(2) **b** 12.041(2) **c** 13.634(3)

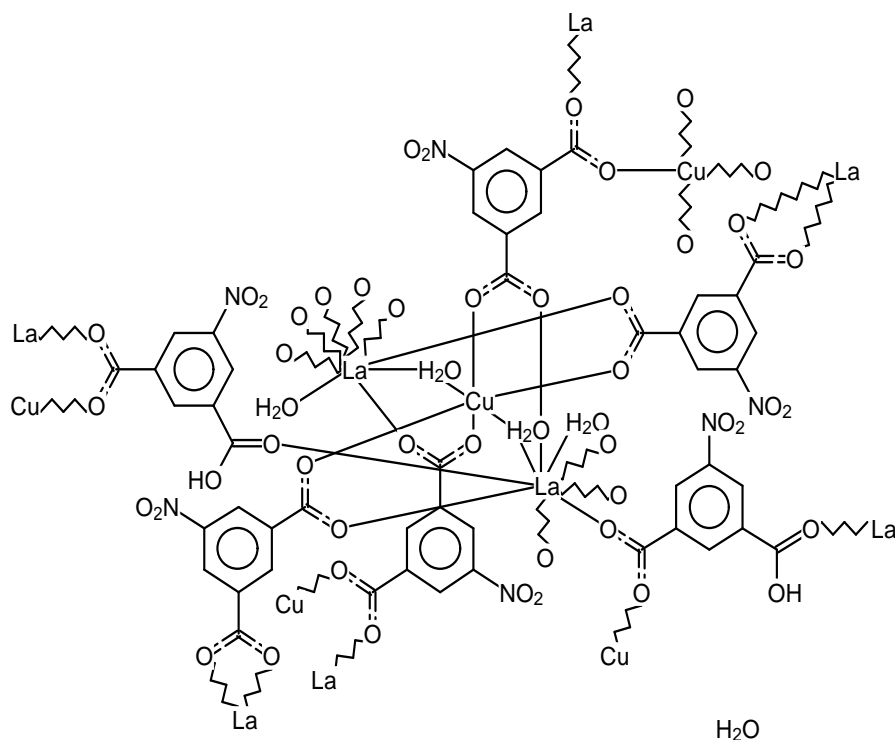
Space Group No.: 2 **(Å, °)** α 108.07(3) β 108.82(3) γ 103.88(3)

R-Factor (%): 2.22 **Temperature(K):** 293 **Density(g/cm³):** 2.021

Parameters

Fragment 1

DIST1 (D)	1.967
DIST2 (D)	1.920
DIST3 (D)	1.967
DIST4 (D)	1.920
DIST5 (D)	2.696
DIST6 (D)	2.696



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 99

LAJPEU

Reference: Wenqi Zhao, Zhanhua Su, Zhifeng Zhao, Bowen Cong, Lin Xia, Baibin Zhou (2015) *J.Inorg.Organomet.Polym.Mater.* ,**25**,1373

Formula: $(C_{28} H_{40} As_6 Cu_5 Mo_6 N_{24} O_{30})_n \cdot 2n(H_2 O)_1$

Compound Name: catena-(bis(μ_7 - 1,3,5,2,4,6-Trioxatriarsinane-2,4,6-triolato)-tetrakis(μ_2 -1,1'-propane-1,3-diylbis(1H-1,2,4-triazole))-decakis(μ_2 -oxo)-octa-oxo-penta-copper-hexa-molybdenum dihydrate)

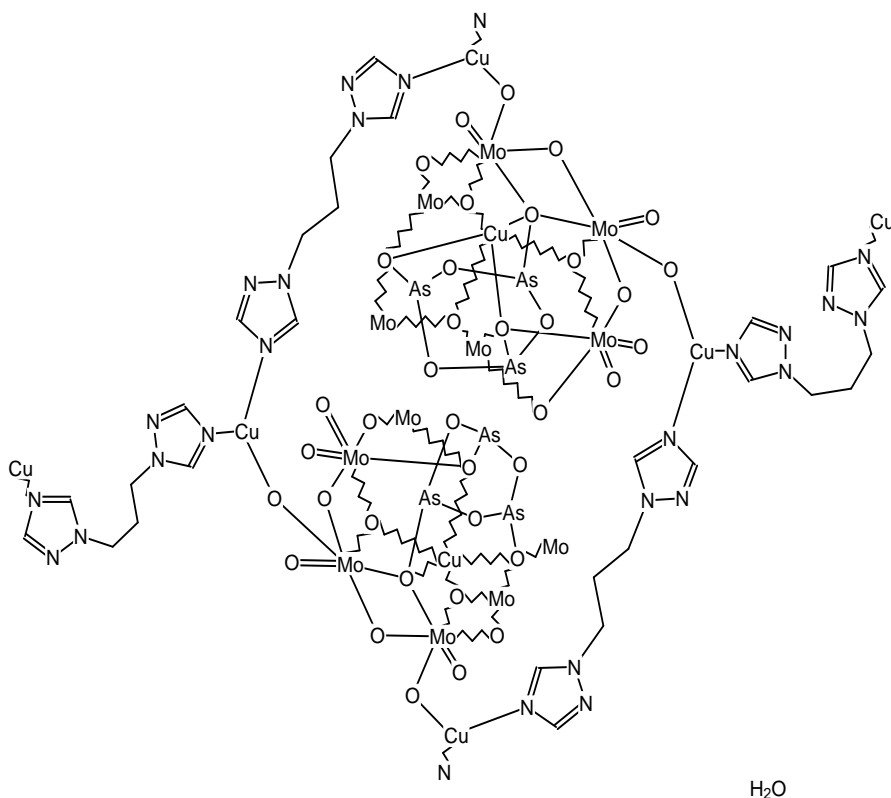
Space Group: P-1 **Cell:** **a** 9.335(0) **b** 13.093(0) **c** 14.644(0)
Space Group No.: 2 (**Å**, °) α 100.94 β 90.73 γ 109.56

R-Factor (%): 2.69 **Temperature(K):** 296 **Density(g/cm³):** 2.588

Parameters

Fragment 1

DIST1 (D)	2.178
DIST2 (D)	2.034
DIST3 (D)	2.178
DIST4 (D)	2.034
DIST5 (D)	2.025
DIST6 (D)	2.025



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 100

LICNAN

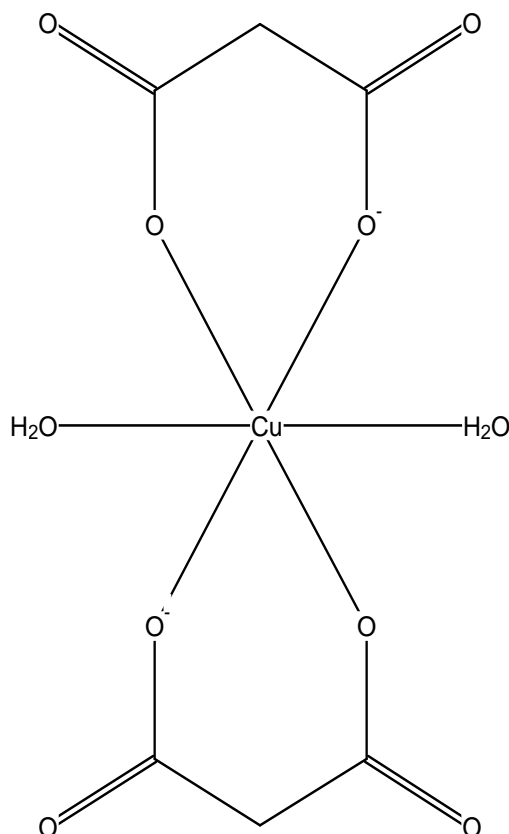
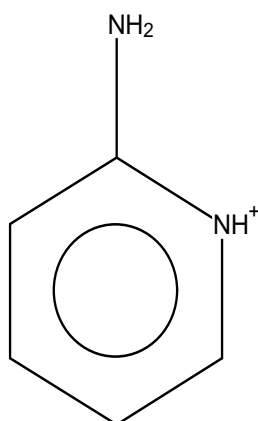
Reference: S.R.Choudhury, J.Bhattacharyya, S.Das, B.Dey, S.Mukhopadhyay, Li-Ping Lu, Miao-Li Zhu (2007) *Acta Crystallogr., Sect.E: Struct.Rep.Online* ,**63**,m1331

Formula: $2(\text{C}_5\text{H}_7\text{N}_2^+), \text{C}_6\text{H}_8\text{Cu}_1\text{O}_{10}^{2-}$

Compound Name: bis(2-Aminopyridinium) diaqua-bis(malonato- $\kappa^2\text{O},\text{O}'$)-copper(ii)

Space Group: P-1 **Cell:** **a** 7.043(1) **b** 7.912(1) **c** 9.577(1)
Space Group No.: 2 (**Å, °**) α 96.10(0) β 107.87(0) γ 103.74(0)

R-Factor (%): 2.75 **Temperature(K):** 298 **Density(g/cm³):** 1.694



Parameters

Fragment 1

DIST1 (D)	1.929
DIST2 (D)	1.934
DIST3 (D)	1.934
DIST4 (D)	1.929
DIST5 (D)	2.665
DIST6 (D)	2.665

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 101

LICNAN01

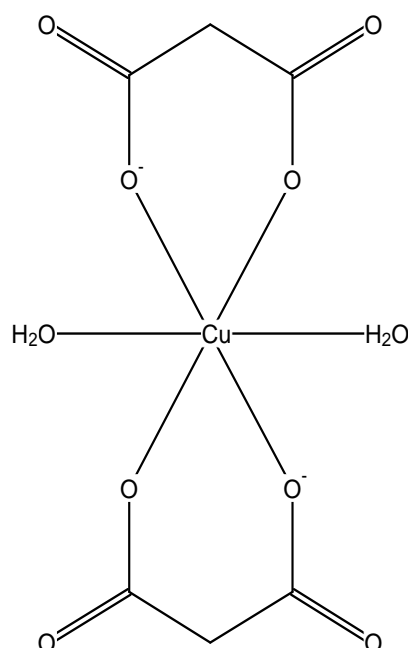
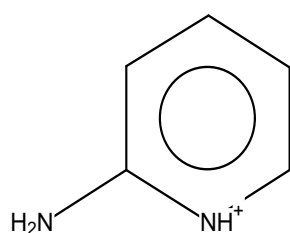
Reference: S.R.Choudhury, P.Gamez, A.Robertazzi,
Chih-Yuan Chen, Hon Man Lee, S.Mukhopadhyay (2008)
Cryst.Growth Des. ,**8**,3773

Formula: $2(\text{C}_5\text{H}_7\text{N}_2^+), \text{C}_6\text{H}_8\text{Cu}_1\text{O}_{10}^{2-}$

Compound Name: bis(2-Aminopyridinium) trans-diaqua-bis(malonato)-copper(ii)

Space Group: P-1 **Cell:** **a** 6.995(0) **b** 7.887(0) **c** 9.556(1)
Space Group No.: 2 (**Å, °**) α 96.30(0) β 108.47(0) γ 104.09(0)

R-Factor (%): 2.15 **Temperature(K):** 150 **Density(g/cm³):** 1.727



Parameters

Fragment 1

DIST1 (D)	1.937
DIST2 (D)	1.933
DIST3 (D)	1.937
DIST4 (D)	1.933
DIST5 (D)	2.621
DIST6 (D)	2.621

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 102

LIKZAI

Reference: Shujuan An, Bing Yin, Ping Liu, Xiangnan Li, Chen Li, Jianli Li, Zhen Shi (2013) *Synthesis* ,45,2525

Formula: (C₁₆ H₁₂ Cu₁ O₆)_n

Compound Name: catena-[bis(μ₂-oxido(phenyl)acetato)-copper]

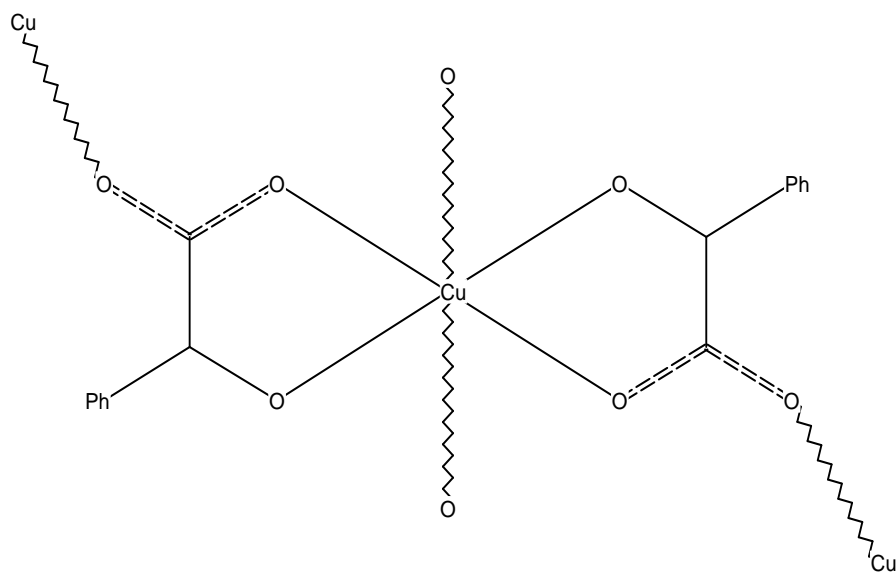
Space Group: P21/c **Cell:** **a** 15.619(3) **b** 4.954(1) **c** 9.548(1)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 102.76(0) **γ** 90.00

R-Factor (%): 2.75 **Temperature(K):** 296 **Density(g/cm³):** 1.677

Parameters

Fragment 1

DIST1 (D)	1.936
DIST2 (D)	2.005
DIST3 (D)	2.005
DIST4 (D)	1.936
DIST5 (D)	2.452
DIST6 (D)	2.452



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 103

LUCWAJ

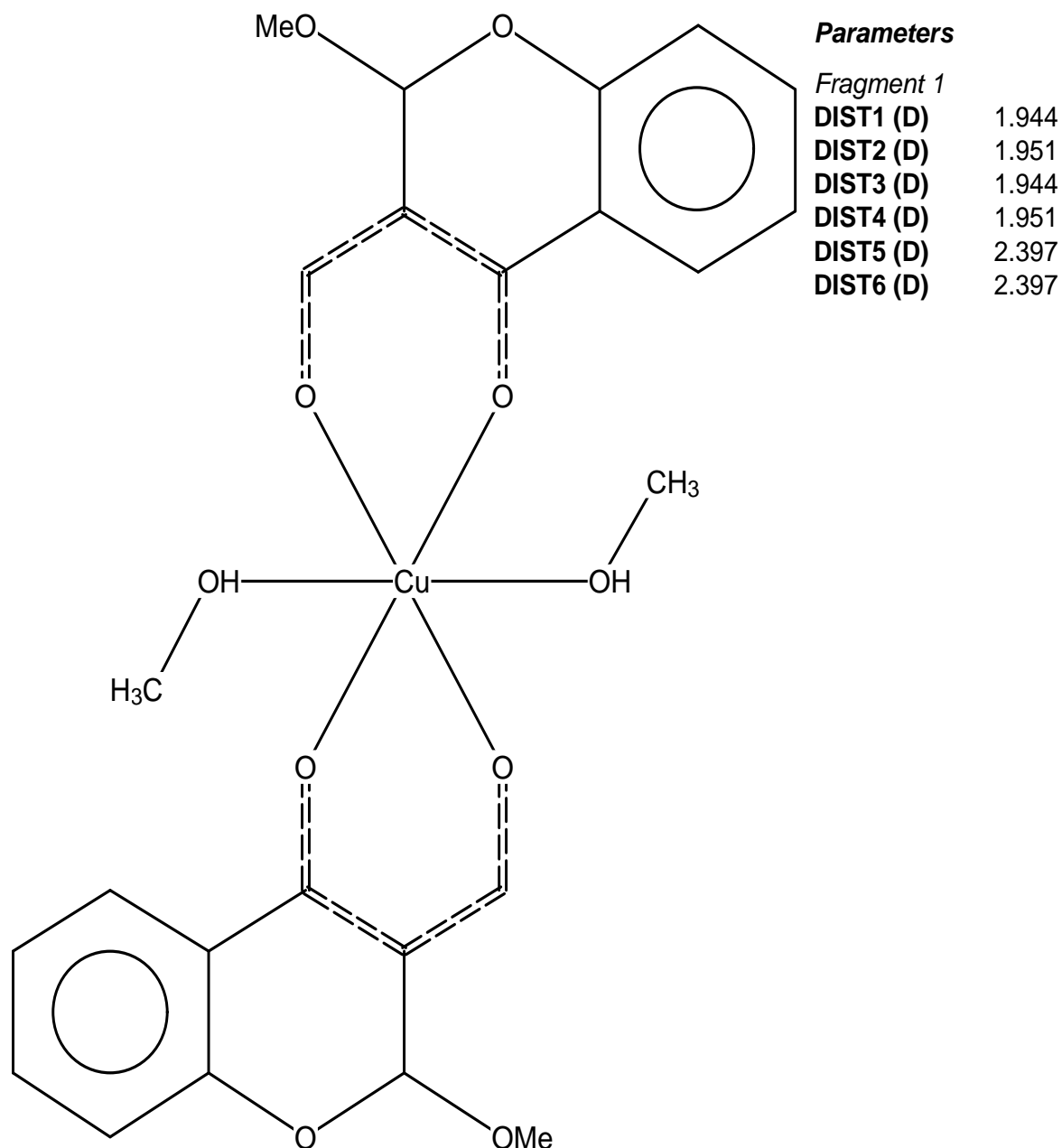
Reference: I.Yousuf, F.Arjmand, S.Tabassum, L.Toupet, R.A.Khan, M.A.Siddiqui (2015) *Dalton Trans.* ,44,10330

Formula: C₂₄ H₂₆ Cu₁ O₁₀

Compound Name: bis(Methanol)-bis(3-(oxymethylene)-2-methoxy-2,3-dihydro-4H-chromen-4-one)-copper(ii)

Space Group: P21/c **Cell:** **a** 8.751(0) **b** 5.077(0) **c** 26.223(0)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 96.30(0) **γ** 90.00

R-Factor (%): 2.84 **Temperature(K):** 140 **Density(g/cm³):** 1.543



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 104

LUTTEA

Reference: Yue-Qing Zheng, Xiao-Yan Han, Hong-Lin Zhu (2010)
Polyhedron ,29,911

Formula: (C₈ H₁₆ Cu₁ Na₂ O₁₅)_n

Compound Name: catena-[(μ₈-Tetrahydrofuran-2,3,4,5-tetracarboxylato)-(μ₂-aqua)-pentaqua-copper(ii)-di-sodium]

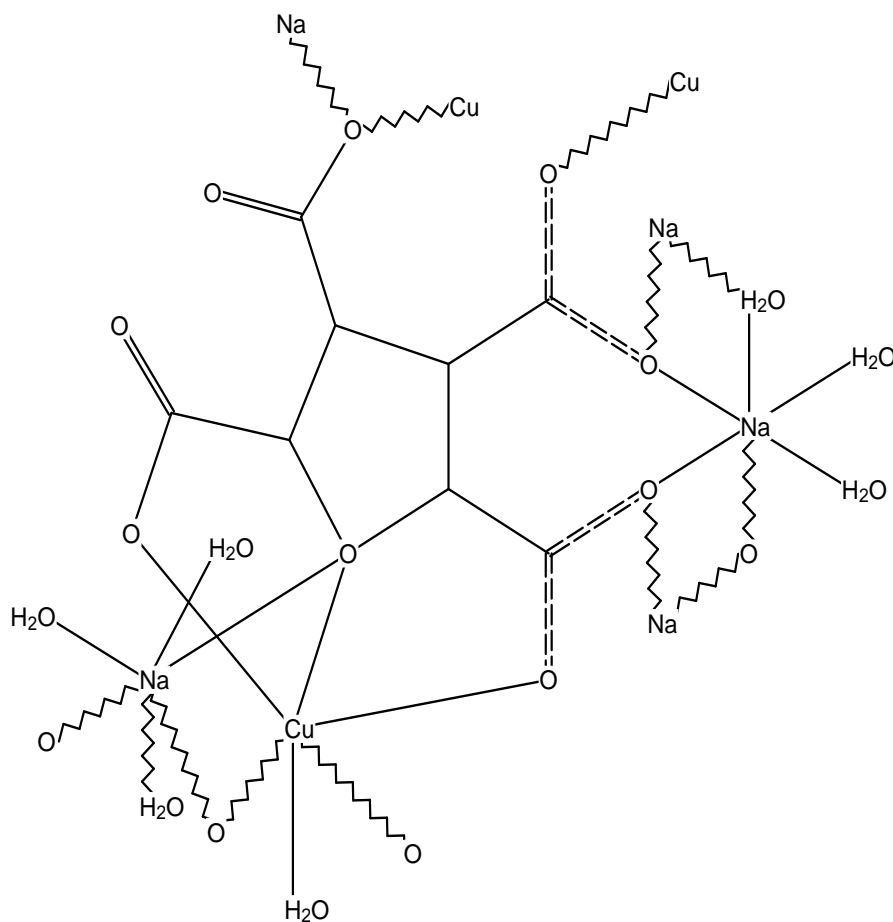
Space Group: P21/c **Cell:** **a** 8.276(1) **b** 12.727(3) **c** 15.090(3)
Space Group No.: 14 **(Å, °)** α 90.00 β 90.08(3) γ 90.00

R-Factor (%): 2.72 **Temperature(K):** 293 **Density(g/cm³):** 1.930

Parameters

Fragment 1

DIST1 (D)	1.979
DIST2 (D)	1.976
DIST3 (D)	1.966
DIST4 (D)	1.924
DIST5 (D)	2.426
DIST6 (D)	2.544



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 105

LUVMUL01

Reference: B.Demoro, F.Caruso, M.Rossi, D.Benitez, M.Gonzalez, H.Cerecetto, B.Parajan-Costa, J.Castiglioni, M.Galizzi, R.Docampo, L.Otero, D.Gambino (2010) *J.Inorg.Biochem.* ,**104**,1252

Formula: C₁₄ H₂₀ Cu₁ N₂ O₁₄ P₄,4(H₂ O₁)

Compound Name: bis(dihydrogen 1-hydroxy-2-(3-pyridinio)ethane-1,1-diyl)diphosphonate)-copper(ii) tetrahydrate

Synonym: bis(risedronato)-copper(ii) tetrahydrate

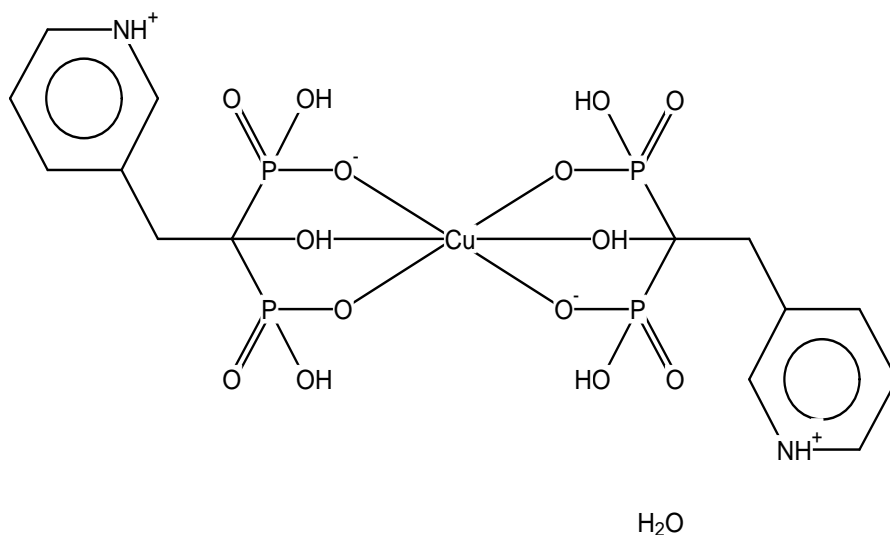
Space Group: P-1 **Cell:** **a** 7.651(0) **b** 8.587(0) **c** 10.279(0)
Space Group No.: 2 **(Å, °)** α 65.95(0) β 84.97(0) γ 78.88(0)

R-Factor (%): 2.43 **Temperature(K):** 125 **Density(g/cm³):** 1.921

Parameters

Fragment 1

DIST1 (D)	1.946
DIST2 (D)	1.960
DIST3 (D)	1.946
DIST4 (D)	1.960
DIST5 (D)	2.655
DIST6 (D)	2.655



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 106

LUVZUY

Reference: T.E.Knight, J.K.McCusker (2010) *J.Am.Chem.Soc.* , **132**, 2208

Formula: C₄₈ H₃₆ Cu₁ F₆ N₆ O₁₆ Re₂ S₂, 2(C₂ H₃ N₁)

Compound Name: bis(μ_2 -3-(4-Pyridyl)acetylacetonato)-bis(2,2'-bipyridine)-hexacarbonyl-bis(trifluoromethanesulfonato)-copper(ii)-di-rhenium(ii) acetonitrile solvate

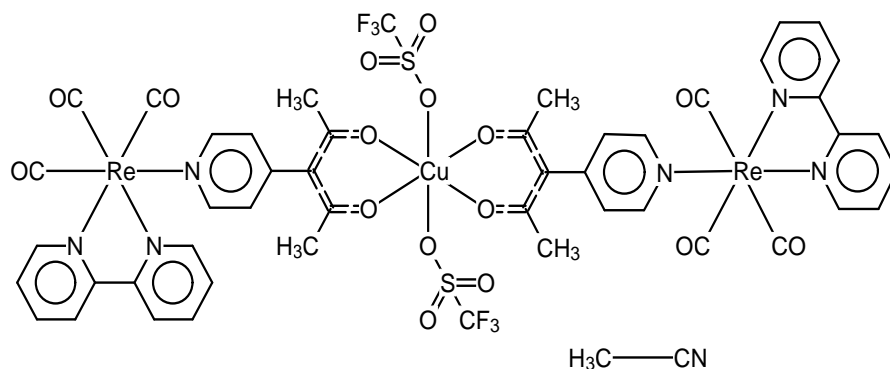
Space Group: P21/c **Cell:** **a** 10.321(1) **b** 24.532(3) **c** 12.161(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 104.03(0) γ 90.00

R-Factor (%): 1.89 **Temperature(K):** 173 **Density(g/cm³):** 1.833

Parameters

Fragment 1

DIST1 (D) 1.920
DIST2 (D) 1.914
DIST3 (D) 1.920
DIST4 (D) 1.914
DIST5 (D) 2.705
DIST6 (D) 2.705



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 107

MACUFR

Reference: E.Sletten, L.H.Jensen (1973)
Acta Crystallogr., Sect. B: Struct. Crystallogr. Cryst. Chem., **29**, 1752

Formula: $(C_3 H_3 Cu_1 O_6^{1-})_n, n(C_2 H_8 N_1^{1+})$

Compound Name: catena-(dimethylammonium tris(μ_2 -formate)-copper(ii))

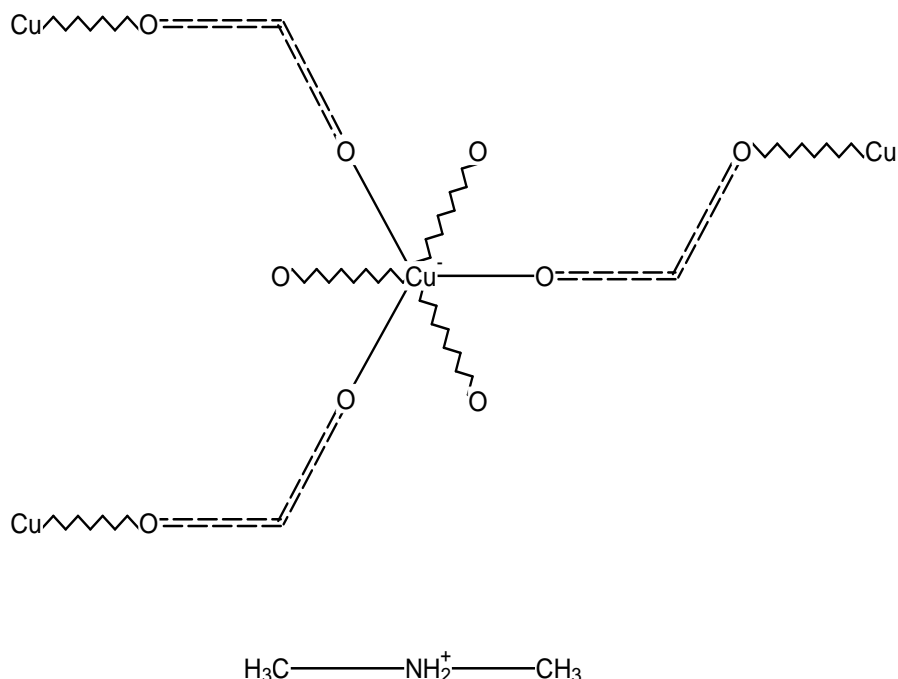
Space Group: I2/c **Cell:** **a** 11.420(0) **b** 8.714(0) **c** 8.850(0)
Space Group No.: 15 **(Å, °)** α 90.00 β 96.25(0) γ 90.00

R-Factor (%): 1.70 **Temperature(K):** 295 **Density(g/cm³):** 1.856

Parameters

Fragment 1

DIST1 (D)	1.971
DIST2 (D)	1.969
DIST3 (D)	1.971
DIST4 (D)	1.969
DIST5 (D)	2.491
DIST6 (D)	2.491



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 108

MACUFR01

Reference: Deyuan Kong, J.Zon, J.McBee, A.Clearfield (2006)
Inorg.Chem. ,**45**,977

Formula: $(C_3 H_3 Cu_1 O_6^{1-})_n, n(C_2 H_8 N_1^{1+})$

Compound Name: catena-(dimethylammonium tris(μ_2 -formato)-copper)

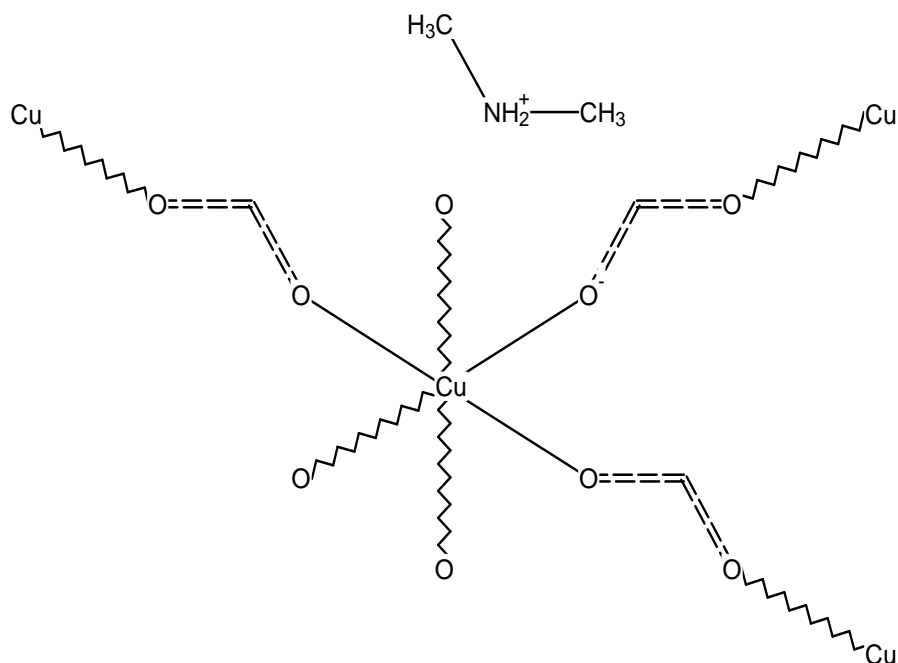
Space Group: C2/c **Cell:** **a** 13.733(12) **b** 8.659(8) **c** 8.808(8)
Space Group No.: 15 **(Å, °)** α 90.00 β 124.08(1) γ 90.00

R-Factor (%): 1.83 **Temperature(K):** 110 **Density(g/cm³):** 1.874

Parameters

Fragment 1

DIST1 (D)	1.975
DIST2 (D)	1.975
DIST3 (D)	1.978
DIST4 (D)	1.978
DIST5 (D)	2.456
DIST6 (D)	2.456



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 109

MACUFR03

Reference: F.R.Fronczek (2015)
CSD Communication(Private Communication) ,

Formula: $(C_3 H_3 Cu_1 O_6^{1-})_n, n(C_2 H_8 N_1^{1+})$

Compound Name: catena-[dimethylammonium tris(μ -formato)-copper]

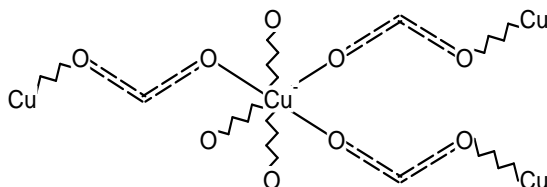
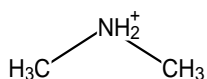
Space Group: C2/c **Cell:** **a** 13.695(0) **b** 8.632(0) **c** 8.769(0)
Space Group No.: 15 **(Å, °)** α 90.00 β 124.19(0) γ 90.00

R-Factor (%): 1.45 **Temperature(K):** 90 **Density(g/cm³):** 1.895

Parameters

Fragment 1

DIST1 (D)	1.967
DIST2 (D)	1.970
DIST3 (D)	1.967
DIST4 (D)	1.970
DIST5 (D)	2.447
DIST6 (D)	2.447



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 110

MAGMOZ

Reference: Ran Shang, Sa Chen, Bing-Wu Wang, Zhe-Ming Wang, Song Gao (2016) *Angew.Chem.,Int.Ed.* ,55,2097

Formula: $(C_3 H_3 Cu_1 O_6^{1-})_n, C_2 H_8 N_1^{1+}$

Compound Name: catena-[ethylammonium tris(μ_2 -formato)-copper]

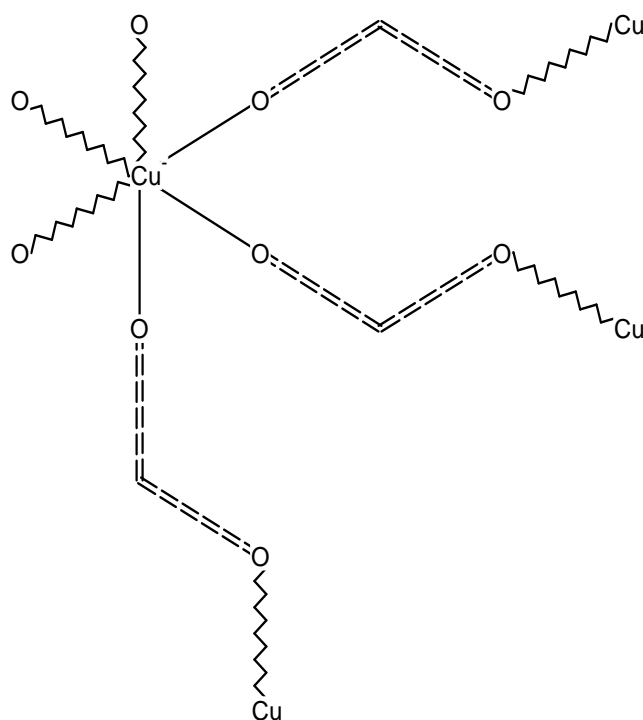
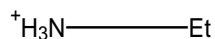
Space Group: Pna21 **Cell:** **a** 9.201(0) **b** 8.115(0) **c** 11.442(0)
Space Group No.: 33 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.09 **Temperature(K):** 291 **Density(g/cm³):** 1.902

Parameters

Fragment 1

DIST1 (D)	1.958
DIST2 (D)	2.015
DIST3 (D)	1.963
DIST4 (D)	2.009
DIST5 (D)	2.486
DIST6 (D)	2.407



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 111

MAGMOZ01

Reference: Ran Shang, Sa Chen, Bing-Wu Wang, Zhe-Ming Wang, Song Gao (2016) *Angew.Chem.,Int.Ed.* ,55,2097

Formula: $(C_3 H_3 Cu_1 O_6^{1-})_n, C_2 H_8 N_1^{1+}$

Compound Name: catena-[ethylammonium tris(μ_2 -formato)-copper]

Space Group: Pna21 **Cell:** **a** 9.216(0) **b** 8.118(0) **c** 11.459(0)
Space Group No.: 33 **(Å, °)** α 90.00 β 90.00 γ 90.00

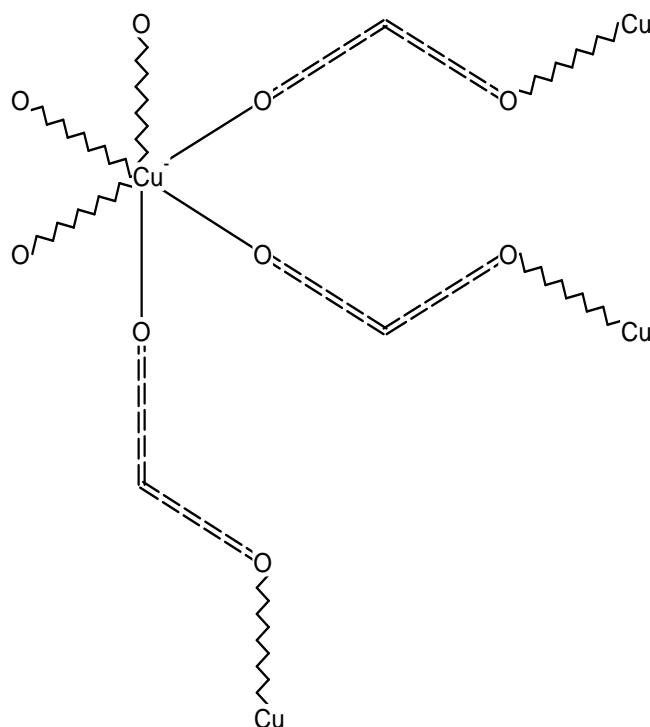
R-Factor (%): 2.65 **Temperature(K):** 320 **Density(g/cm³):** 1.896



Parameters

Fragment 1

DIST1 (D)	1.954
DIST2 (D)	2.020
DIST3 (D)	1.962
DIST4 (D)	2.008
DIST5 (D)	2.495
DIST6 (D)	2.416



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 112

MAGMOZ02

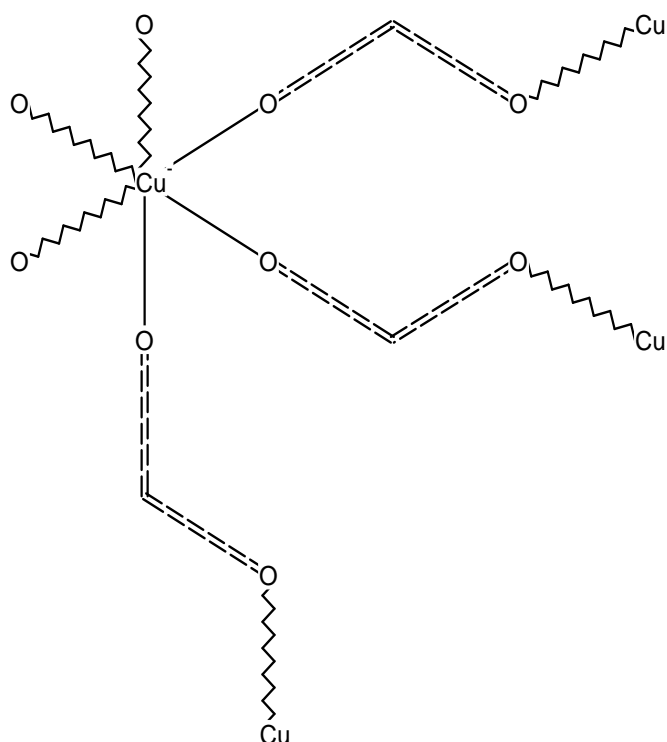
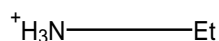
Reference: Ran Shang, Sa Chen, Bing-Wu Wang, Zhe-Ming Wang, Song Gao (2016) *Angew.Chem.,Int.Ed.* ,55,2097

Formula: $(C_3 H_3 Cu_1 O_6^{1-})_n, C_2 H_8 N_1^{1+}$

Compound Name: catena-[ethylammonium tris(μ_2 -formato)-copper]

Space Group: Pna21 **Cell:** **a** 9.209(0) **b** 8.110(0) **c** 11.445(0)
Space Group No.: 33 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.36 **Temperature(K):** 340 **Density(g/cm³):** 1.901



Parameters

Fragment 1

DIST1 (D)	1.951
DIST2 (D)	2.012
DIST3 (D)	1.956
DIST4 (D)	2.005
DIST5 (D)	2.491
DIST6 (D)	2.418

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 113

MAGMOZ03

Reference: Ran Shang, Sa Chen, Bing-Wu Wang, Zhe-Ming Wang, Song Gao (2016) *Angew.Chem.,Int.Ed.* ,55,2097

Formula: $(C_3 H_3 Cu_1 O_6^{1-})_n, C_2 H_8 N_1^{1+}$

Compound Name: catena-[ethylammonium tris(μ -formato)-copper]

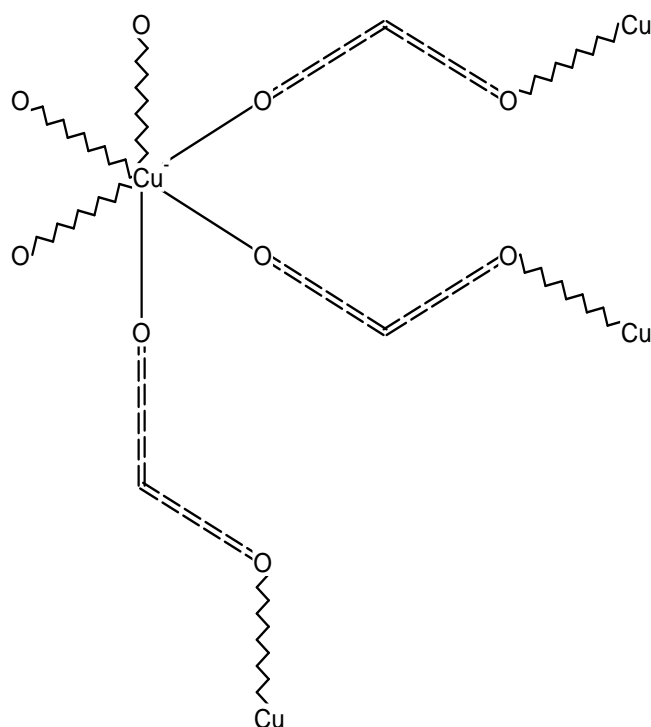
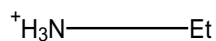
Space Group: Pna21 **Cell:** **a** 9.103(0) **b** 8.093(0) **c** 11.396(0)
Space Group No.: 33 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 1.87 **Temperature(K):** 93 **Density(g/cm³):** 1.936

Parameters

Fragment 1

DIST1 (D)	1.960
DIST2 (D)	2.017
DIST3 (D)	1.962
DIST4 (D)	2.008
DIST5 (D)	2.450
DIST6 (D)	2.366



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 114

MAGMOZ04

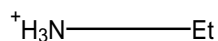
Reference: Ran Shang, Sa Chen, Bing-Wu Wang, Zhe-Ming Wang, Song Gao (2016) *Angew.Chem.,Int.Ed.* ,55,2097

Formula: $(C_3 H_3 Cu_1 O_6^{1-})_n, C_2 H_8 N_1^{1+}$

Compound Name: catena-[ethylammonium tris(μ -formato)-copper]

Space Group: Pna21 **Cell:** **a** 9.142(0) **b** 8.102(0) **c** 11.415(0)
Space Group No.: 33 **(Å, °)** α 90.00 β 90.00 γ 90.00

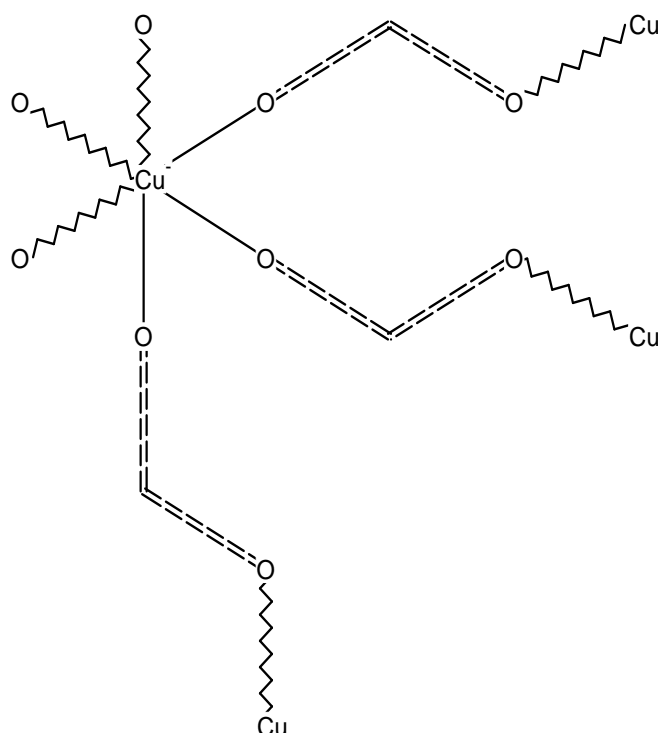
R-Factor (%): 1.96 **Temperature(K):** 180 **Density(g/cm³):** 1.922



Parameters

Fragment 1

DIST1 (D)	1.959
DIST2 (D)	2.017
DIST3 (D)	1.962
DIST4 (D)	2.009
DIST5 (D)	2.465
DIST6 (D)	2.382



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 115

MAGNEQ

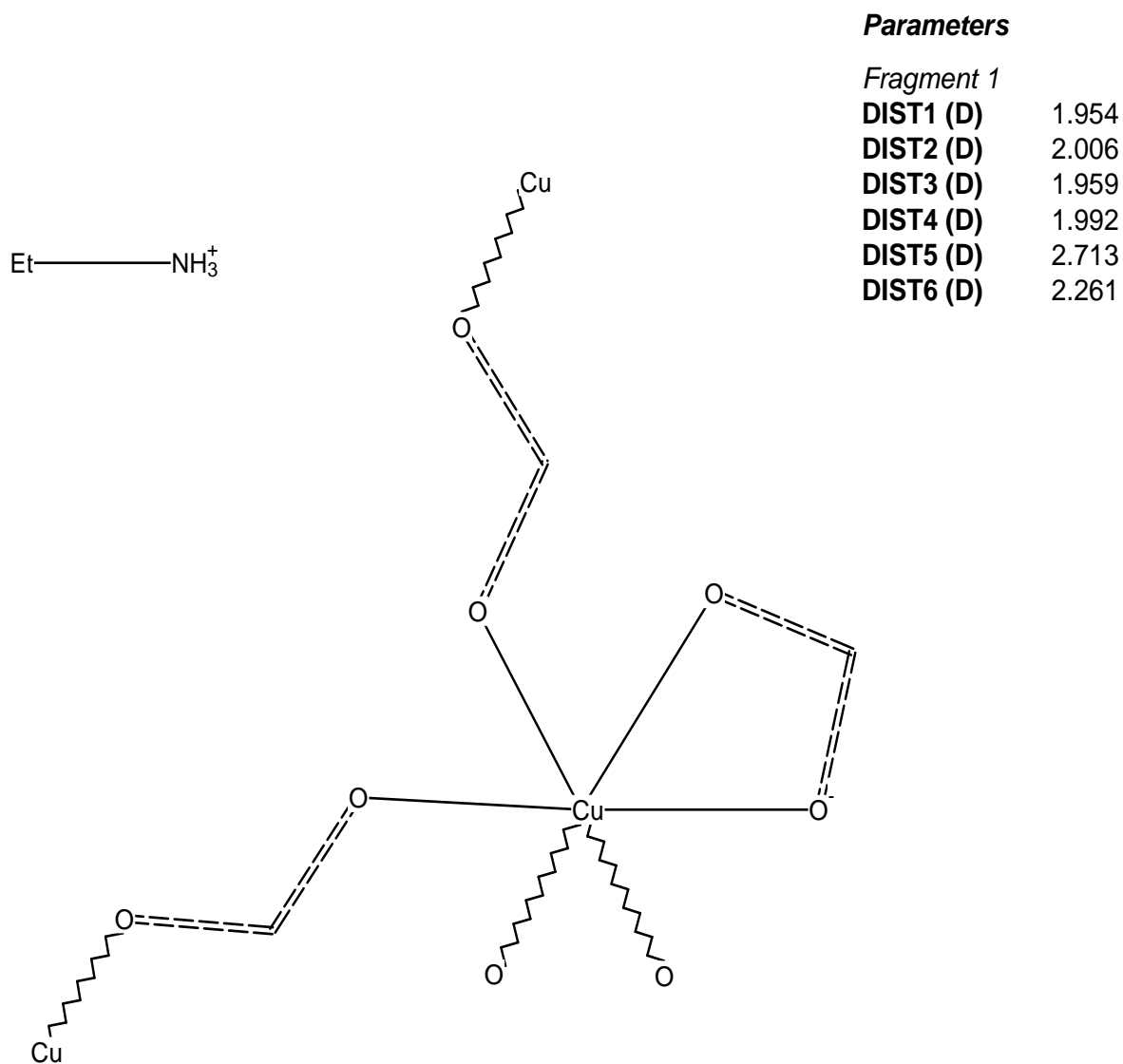
Reference: Ran Shang, Sa Chen, Bing-Wu Wang, Zhe-Ming Wang, Song Gao (2016) *Angew.Chem.,Int.Ed.* ,55,2097

Formula: $(C_3 H_3 Cu_1 O_6^{1-})_n, C_2 H_8 N_1^{1+}$

Compound Name: catena-[ethylammonium bis(μ_2 -formato)-(formato)-copper]

Space Group: P212121 **Cell:** **a** 10.034(0) **b** 8.283(0) **c** 11.158(0)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.86 **Temperature(K):** 100 **Density(g/cm³):** 1.753



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 116

MAGNEQ01

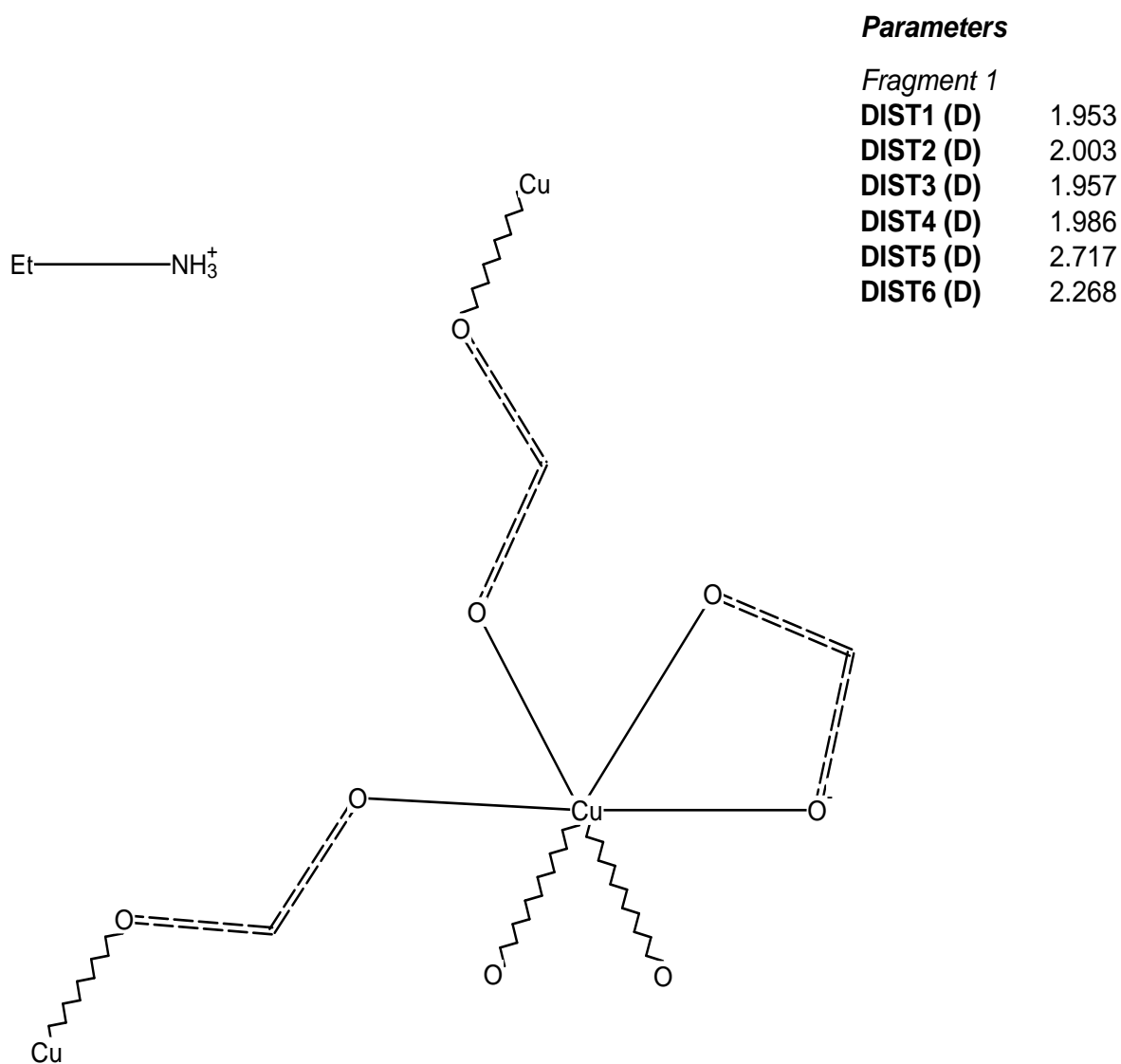
Reference: Ran Shang, Sa Chen, Bing-Wu Wang, Zhe-Ming Wang, Song Gao (2016) *Angew.Chem.,Int.Ed.* ,55,2097

Formula: $(C_3 H_3 Cu_1 O_6^{1-})_n, C_2 H_8 N_1^{1+}$

Compound Name: catena-[ethylammonium bis(μ_2 -formato)-(formato)-copper]

Space Group: P212121 **Cell:** **a** 10.073(0) **b** 8.279(0) **c** 11.154(0)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.58 **Temperature(K):** 180 **Density(g/cm³):** 1.747



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 117

MAGNEQ02

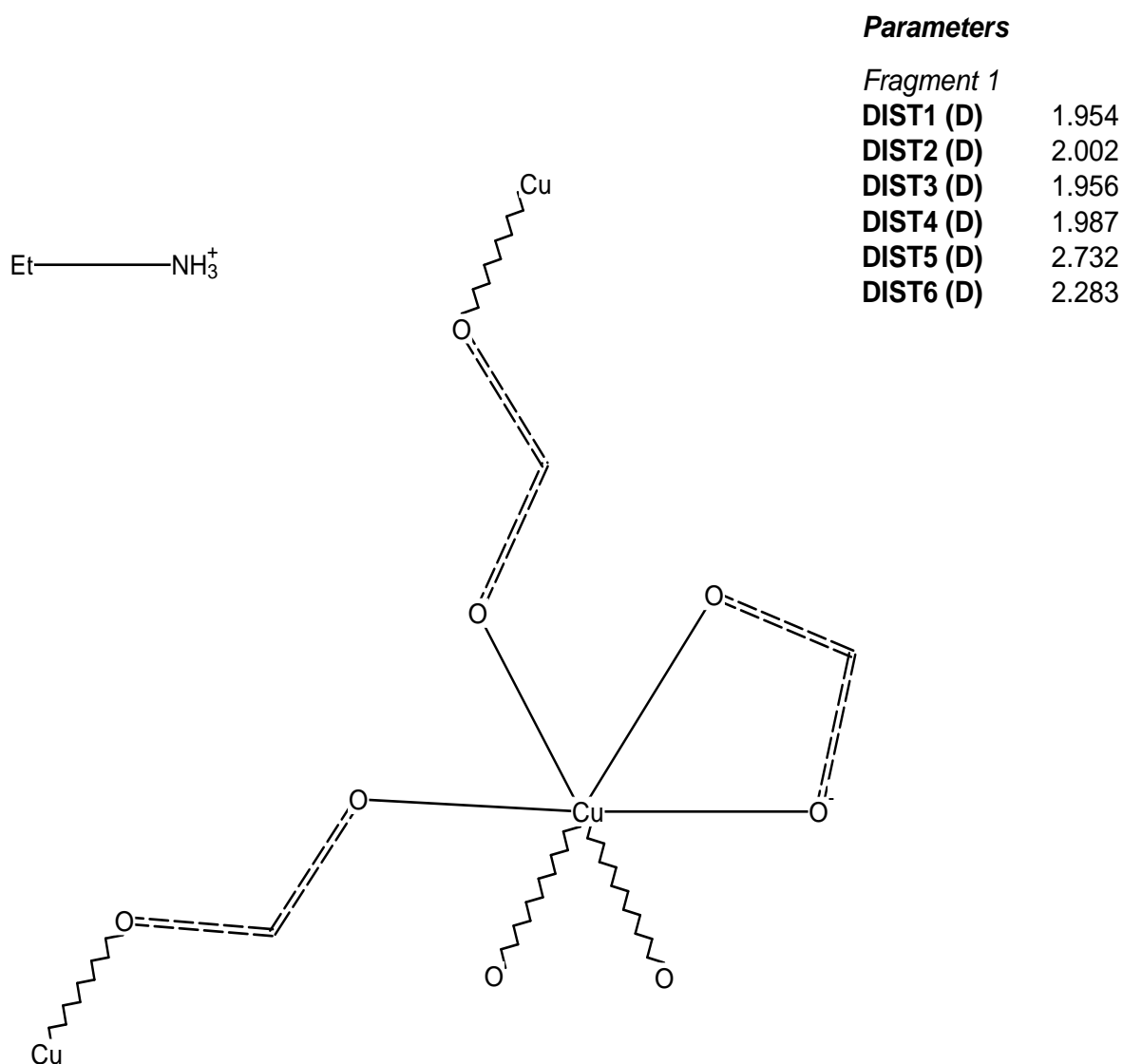
Reference: Ran Shang, Sa Chen, Bing-Wu Wang, Zhe-Ming Wang, Song Gao (2016) *Angew.Chem.,Int.Ed.* ,55,2097

Formula: $(C_3 H_3 Cu_1 O_6^{1-})_n, C_2 H_8 N_1^{1+}$

Compound Name: catena-[ethylammonium bis(μ_2 -formato)-(formato)-copper]

Space Group: P212121 **Cell:** **a** 10.144(0) **b** 8.289(0) **c** 11.160(0)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.86 **Temperature(K):** 290 **Density(g/cm³):** 1.732



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 118

MAGNEQ03

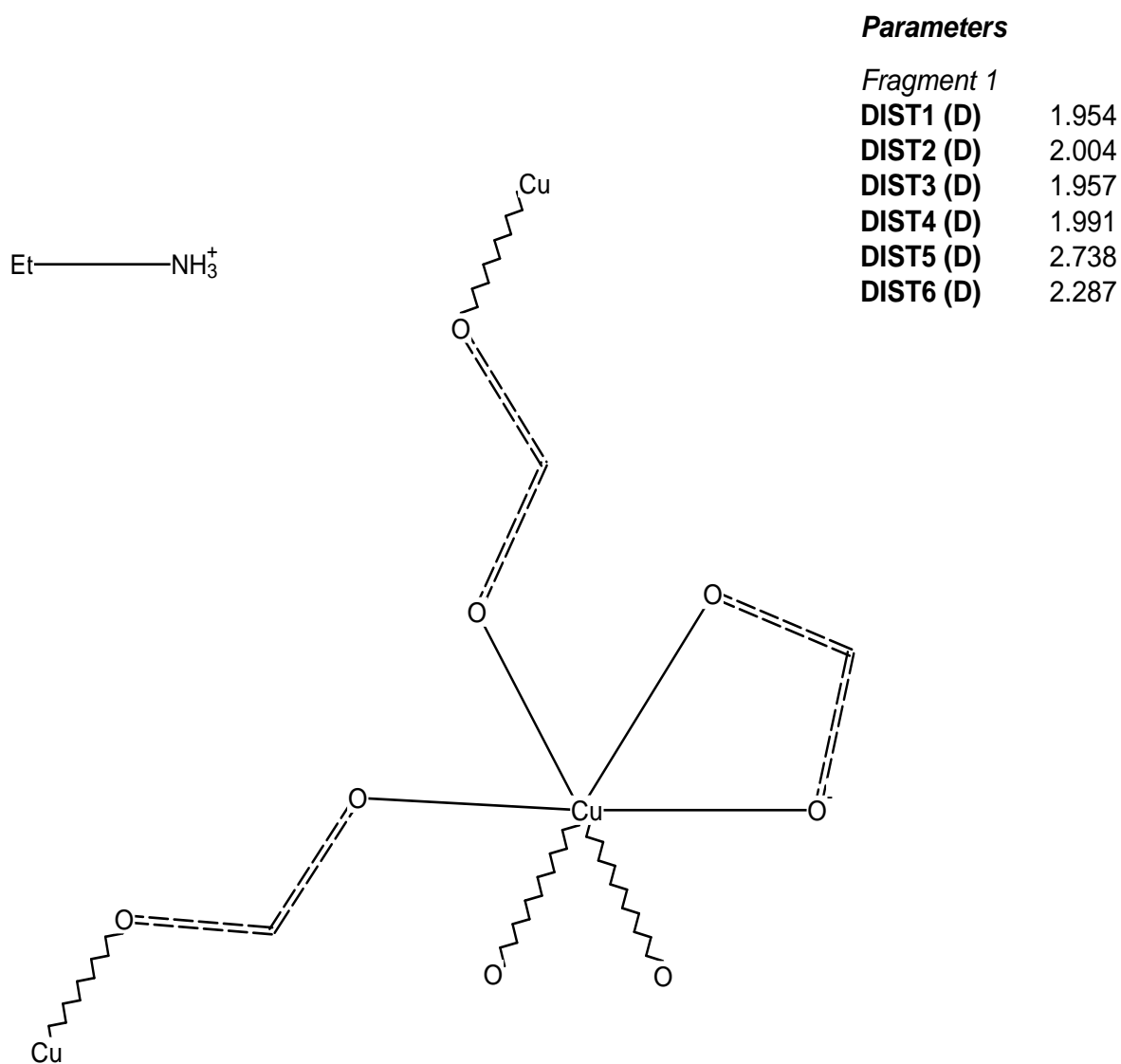
Reference: Ran Shang, Sa Chen, Bing-Wu Wang, Zhe-Ming Wang, Song Gao (2016) *Angew.Chem.,Int.Ed.* ,55,2097

Formula: $(C_3 H_3 Cu_1 O_6^{1-})_n, C_2 H_8 N_1^{1+}$

Compound Name: catena-[ethylammonium bis(μ_2 -formato)-(formato)-copper]

Space Group: P212121 **Cell:** **a** 10.165(0) **b** 8.296(0) **c** 11.181(0)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.90 **Temperature(K):** 320 **Density(g/cm³):** 1.724



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 119

MOHHIB

Reference: S.R.Choudhury, A.D.Jana, Chih-Yuan Chen, A.Dutta, E.Colacio, Hon Man Lee, G.Mostafa, S.Mukhopadhyay (2008) *CrystEngComm* ,10,1358

Formula: $(C_6 H_9 N_2^{1+})_2 n, n(C_6 H_4 Cu_1 O_8^{2-}), 2n(H_2 O_1)$

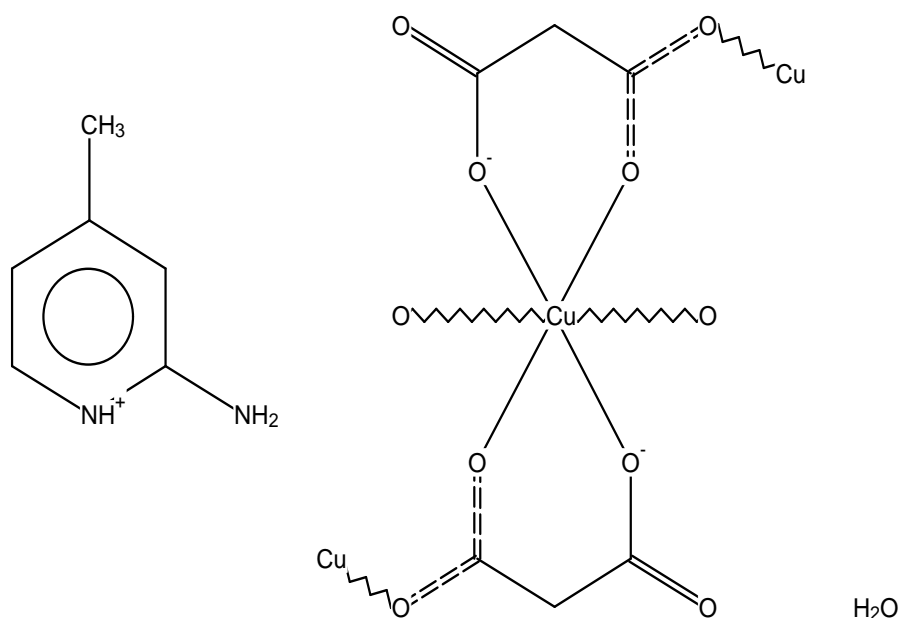
Compound Name: catena-(bis(2-Amino-4-methylpyridinium) bis(μ_2 -malonato)-copper(ii) dihydrate)

Space Group: P21/c **Cell:** **a** 15.491(0) **b** 9.638(0) **c** 7.451(0)
Space Group No.: 14 (**Å, °**) α 90.00 β 102.59(0) γ 90.00
R-Factor (%): 2.28 **Temperature(K):** 273 **Density(g/cm³):** 1.597

Parameters

Fragment 1

DIST1 (D) 1.922
DIST2 (D) 1.946
DIST3 (D) 1.946
DIST4 (D) 1.922
DIST5 (D) 2.614
DIST6 (D) 2.614



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 120

MOLHIG

Reference: A.Hori, K.Nakajima, Y.Akimoto, K.Naganuma, H.Yuge
(2014) *CrystEngComm*, **16**,8805

Formula: C₄₄ H₂₂ Cu₁ F₁₆ O₆

Compound Name: bis(1,3-dioxo-1,3-bis(2,3,5,6-tetrafluorophenyl)propan-2-ide)-
bis(methoxybenzene)-copper(ii)

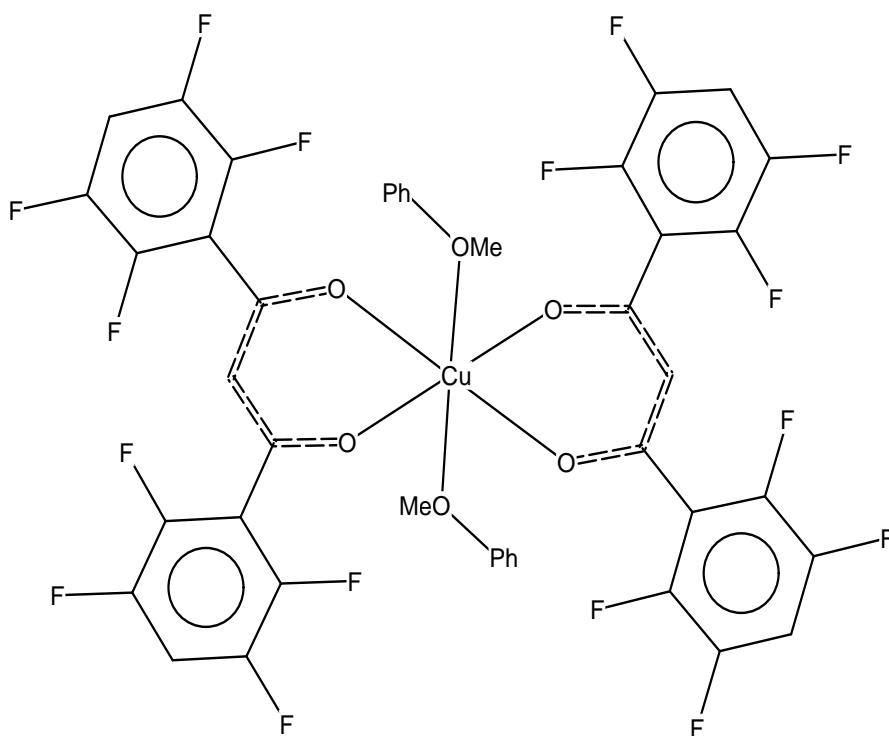
Space Group: P-1 **Cell:** **a** 7.728(2) **b** 11.089(3) **c** 12.681(4)
Space Group No.: 2 **(Å, °)** α 106.69(0) β 104.54(0) γ 92.43(0)

R-Factor (%): 2.69 **Temperature(K):** 100 **Density(g/cm³):** 1.684

Parameters

Fragment 1

DIST1 (D)	1.925
DIST2 (D)	1.923
DIST3 (D)	1.925
DIST4 (D)	1.923
DIST5 (D)	2.614
DIST6 (D)	2.614



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 121

MOLJUU

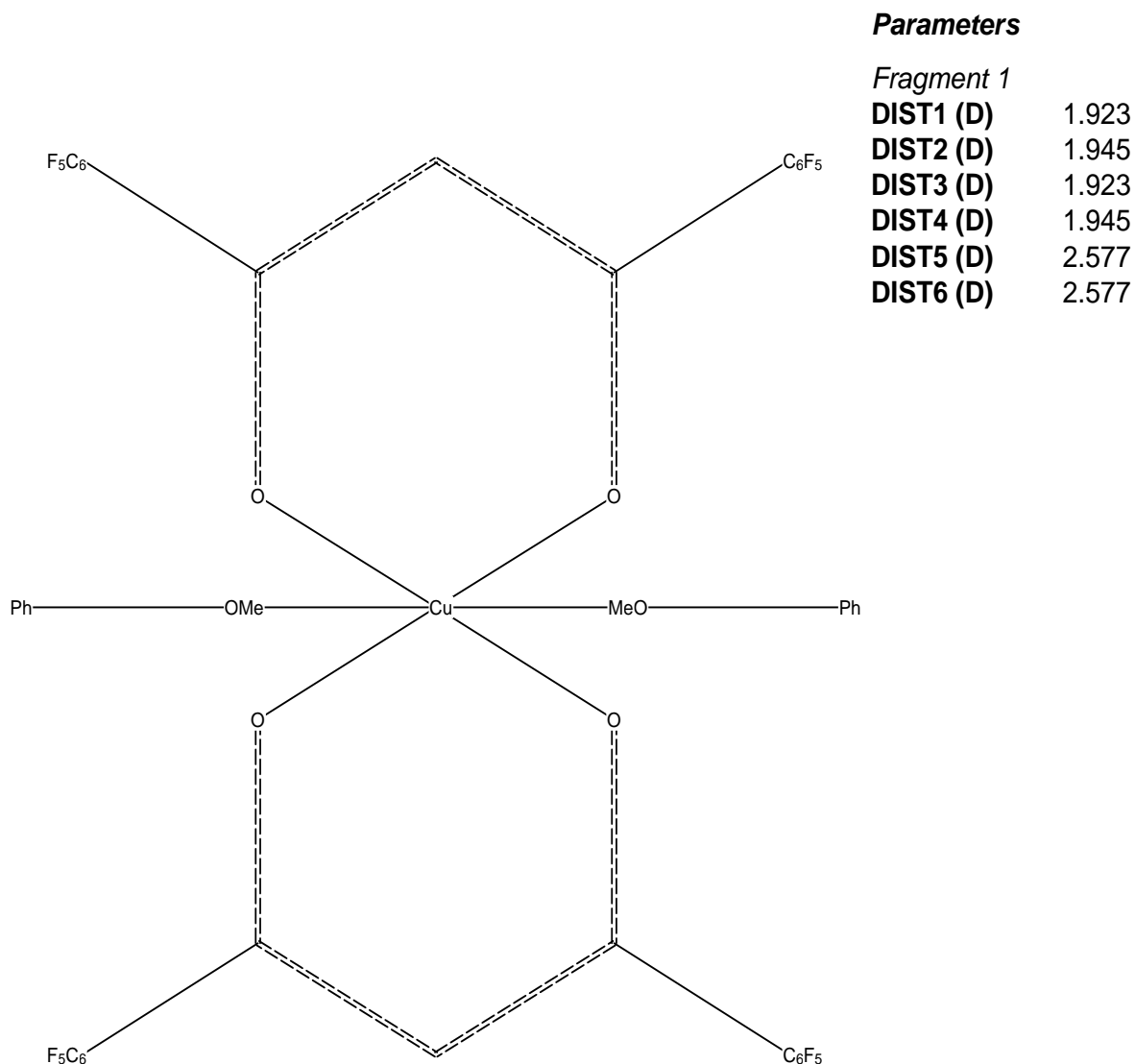
Reference: A.Hori, K.Nakajima, Y.Akimoto, K.Naganuma, H.Yuge
(2014) *CrystEngComm*, **16**,8805

Formula: C₄₄ H₁₈ Cu₁ F₂₀ O₆

Compound Name: bis(anisole)-bis(1,3-bis(pentafluorophenyl)propane-1,3-dionato)-
copper(ii)

Space Group: P-1 **Cell:** **a** 7.702(1) **b** 11.163(3) **c** 11.884(3)
Space Group No.: 2 **(Å, °)** α 106.86(0) β 92.79(0) γ 94.26(0)

R-Factor (%): 2.71 **Temperature(K):** 100 **Density(g/cm³):** 1.855



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 122

MUFDAU

Reference: N.V.Somov, F.F.Chausov (2015)
Kristallografiya(Russ.)(Crystallogr.Rep.) ,**60**,233

Formula: (C₃ H₁₆ Cu₁ N₁ O₁₂ P₃)_n

Compound Name: catena-[(μ -phosphono-N-((phosphono)methyl)-N-((phosphono)methyl) methanaminiumato)-trihydrato-copper]

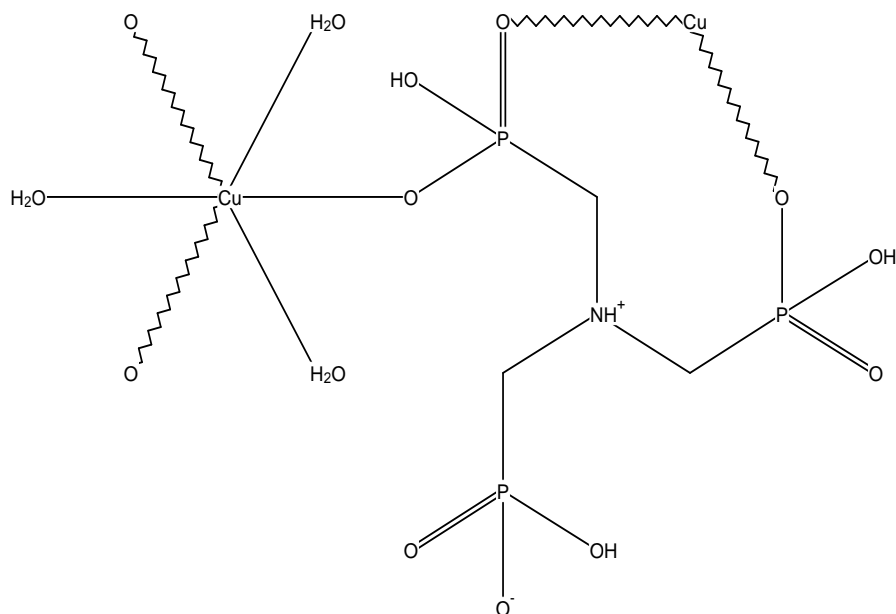
Space Group: P21/c **Cell:** **a** 9.251(0) **b** 15.982(0) **c** 9.547(0)
Space Group No.: 14 (**\AA , °**) α 90.00 β 113.70(0) γ 90.00

R-Factor (%): 1.97 **Temperature(K):** 293 **Density(g/cm³):** 2.131

Parameters

Fragment 1

DIST1 (D)	2.018
DIST2 (D)	2.049
DIST3 (D)	1.959
DIST4 (D)	1.948
DIST5 (D)	2.309
DIST6 (D)	2.297



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 123

NACSEP

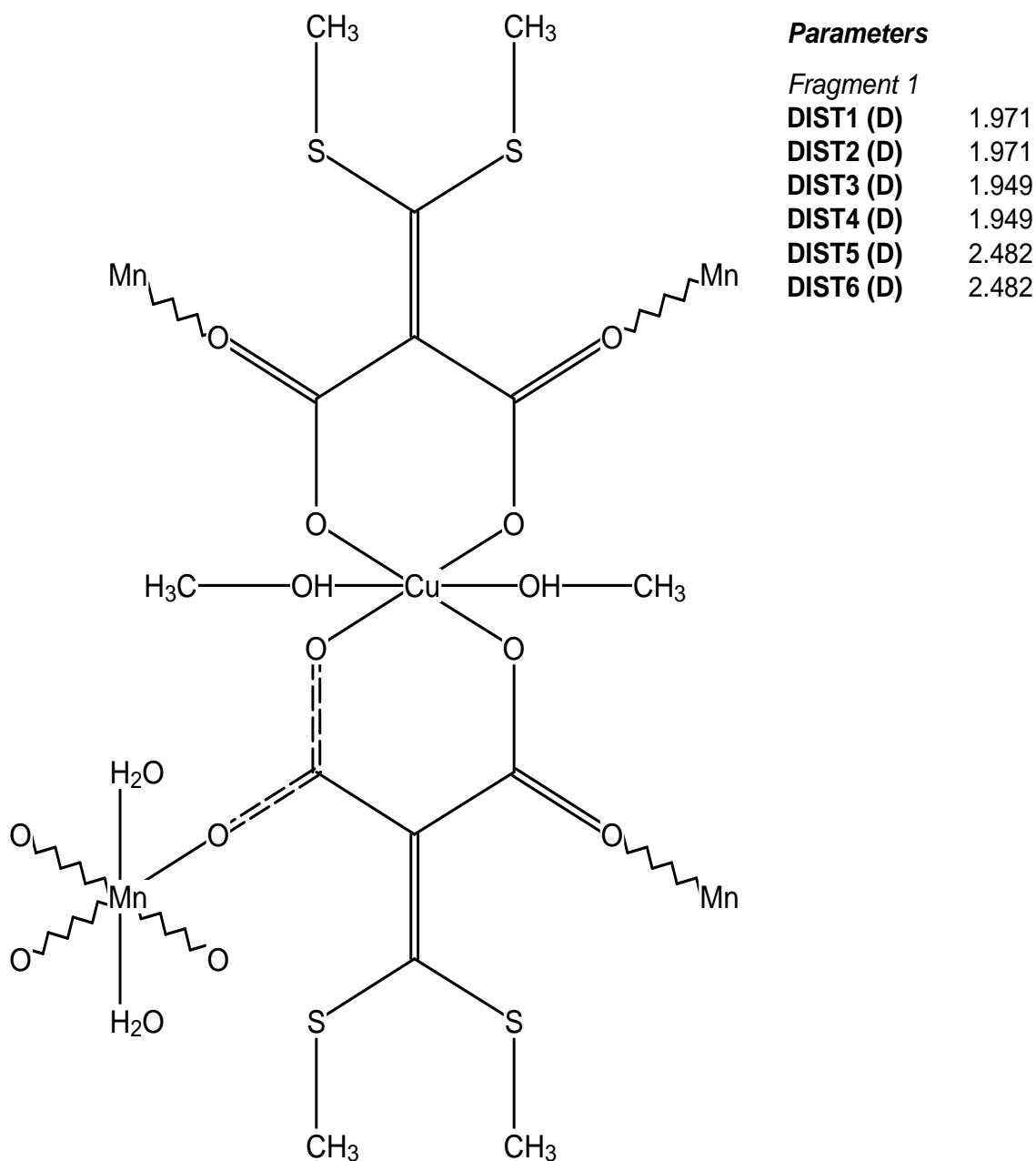
Reference: Jinkwon Kim, Jin Mook Lim, Yong-Kook Choi, Youngkyu Do (1996) *Angew.Chem.,Int.Ed.* ,**35**,998

Formula: (C₁₄ H₂₄ Cu₁ Mn₁ O₁₂ S₄)_n

Compound Name: catena-((bis(μ_3 -bis(Methylthio)methylene)malonato)-dimethanol-copper(ii)-diaqua-manganese(ii))

Space Group: P-1 **Cell:** **a** 7.278(0) **b** 7.338(2) **c** 11.392(0)
Space Group No.: 2 (**Å, °**) α 102.70(1) β 91.17(1) γ 93.37(1)

R-Factor (%): 2.14 **Temperature(K):** 295 **Density(g/cm³):** 1.770



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 124

NAFXAU

Reference: Shan Gao, Yu-Mei Yue, Dong-Sheng Ma, Jin-Sheng Gao, Peng-Fei Yan (2004) *Jiegou Huaxue(Chin.)(Chin.J.Struct.Chem.)*, **23**, 825

Formula: C₁₈ H₁₈ Cu₁ O₁₂

Compound Name: diaqua-bis(4-carboxyphenoxyacetato)-copper(ii)

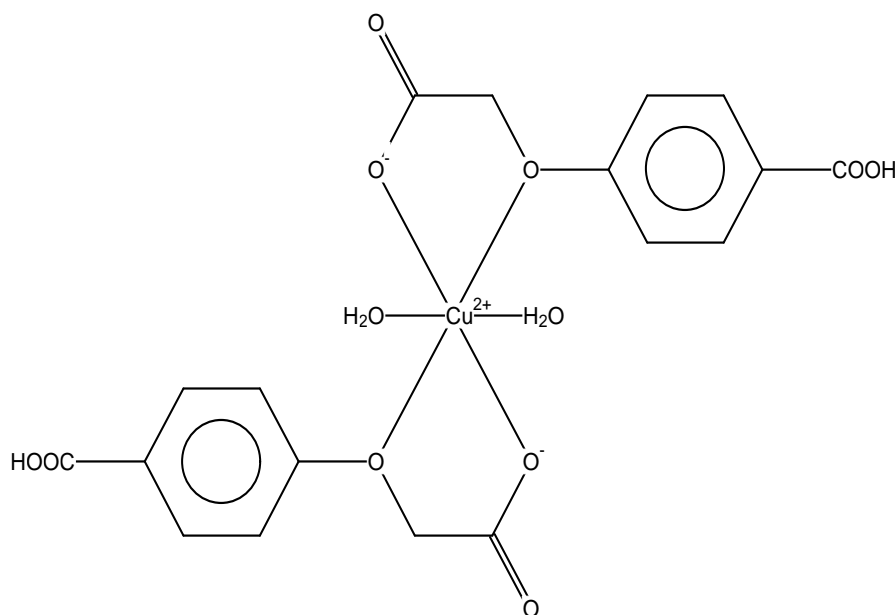
Space Group: C2/c **Cell:** **a** 12.298(3) **b** 7.380(1) **c** 21.413(4)
Space Group No.: 15 **(Å, °)** **α** 90.00 **β** 94.00(3) **γ** 90.00

R-Factor (%): 2.79 **Temperature(K):** 293 **Density(g/cm³):** 1.678

Parameters

Fragment 1

DIST1 (D)	1.920
DIST2 (D)	1.941
DIST3 (D)	1.941
DIST4 (D)	1.955
DIST5 (D)	2.382
DIST6 (D)	2.382



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 125

NAPCIR

Reference: E.V.Dikarev, Haitao Zhang, Bo Li (2005) *J.Am.Chem.Soc.* , 127,6156

Formula: C₄₀ H₈ Bi₂ Cu₁ F₄₈ O₁₆

Compound Name: bis(μ_2 -1,1,1,5,5,5-Hexafluoroacetylacetonato)-hexakis(1,1,1,5,5,5-hexafluoro-acetylacetonato)-di-bismuth(iii)-copper(ii)

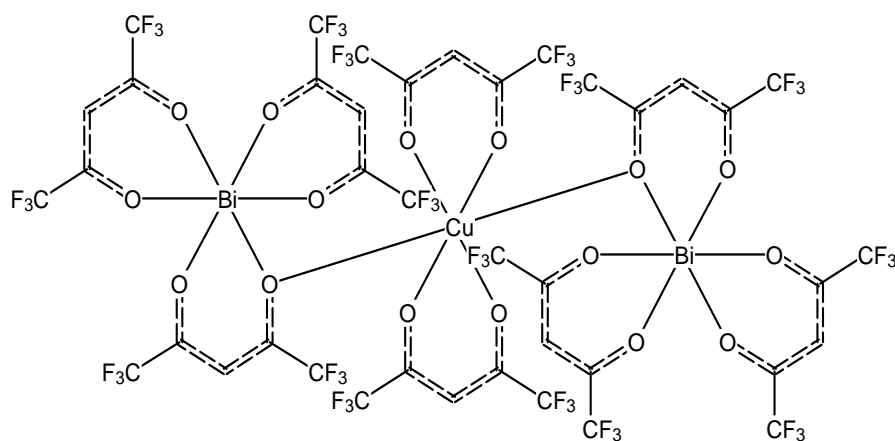
Space Group: P-1 **Cell:** **a** 8.696(0) **b** 11.243(0) **c** 16.877(0)
Space Group No.: 2 (**Å, °**) α 73.72(0) β 76.46(0) γ 69.63(0)

R-Factor (%): 2.10 **Temperature(K):** 90 **Density(g/cm³):** 2.419

Parameters

Fragment 1

DIST1 (D)	1.928
DIST2 (D)	1.928
DIST3 (D)	1.926
DIST4 (D)	1.926
DIST5 (D)	2.588
DIST6 (D)	2.588



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 126

NEDPAO

Reference: B.Kozlevcar, M.Humar, P.Strauch, I.Leban (2005)
Z.Naturforsch.,B:Chem.Sci. ,**60**,1273

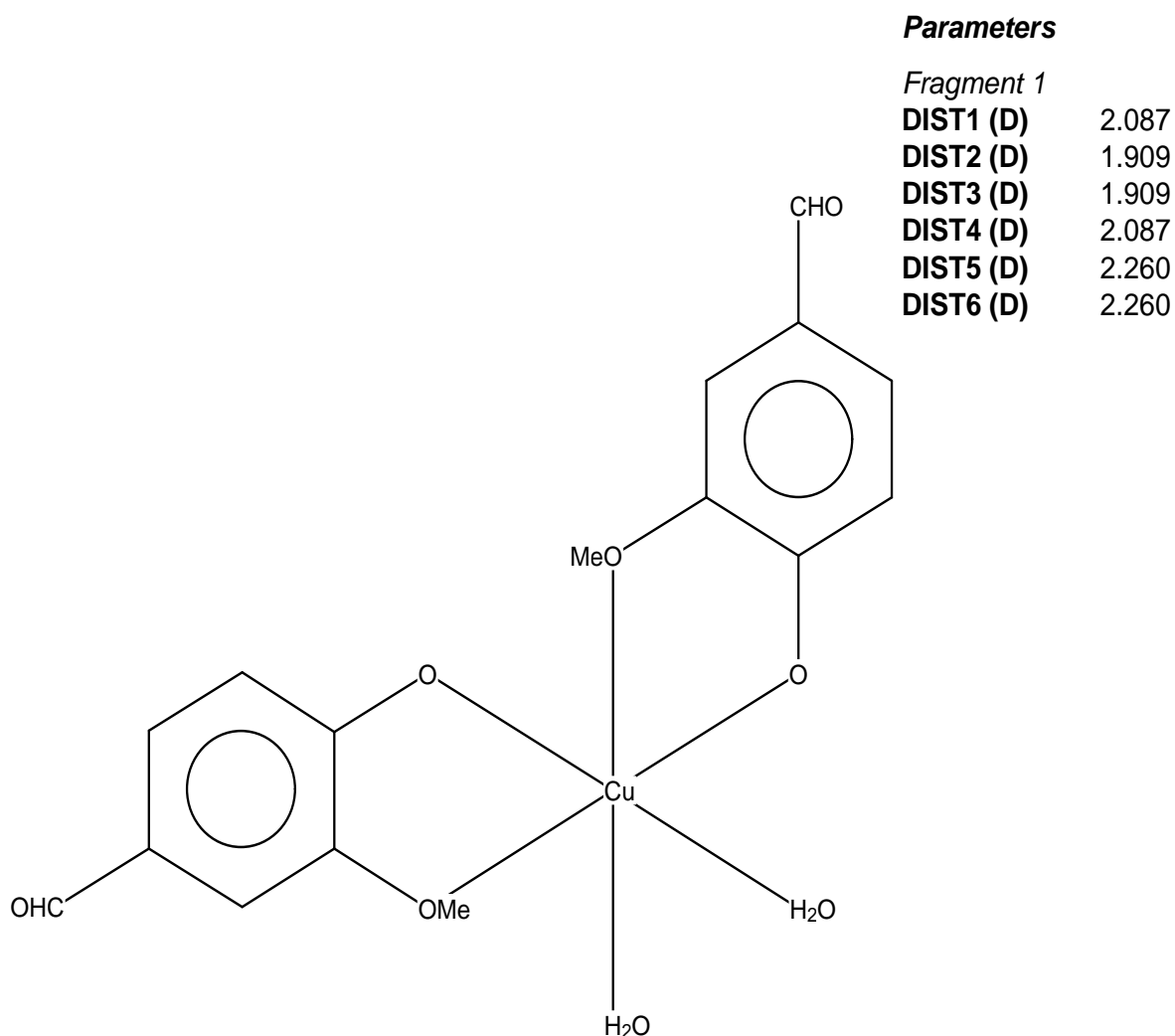
Formula: C₁₆ H₁₈ Cu₁ O₈

Compound Name: cis-Diaqua-bis(vanillinato)-copper(ii)

Synonym: cis-Diaqua-bis(4-formyl-2-methoxyphenolato)-copper(ii)

Space Group: C2/c **Cell:** **a** 22.042(0) **b** 10.689(0) **c** 7.667(0)
Space Group No.: 15 **(Å, °)** **α** 90.00 **β** 104.85(0) **γ** 90.00

R-Factor (%): 2.56 **Temperature(K):** 293 **Density(g/cm³):** 1.529



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 127

NEDPAO01

Reference: B.Kozlevcar, A.Golobic, P.Strauch (2006) *Polyhedron* ,**25**, 2824

Formula: C₁₆ H₁₈ Cu₁ O₈

Compound Name: cis-diaqua-bis(4-formyl-2-methoxyphenolato-O,O')-copper(ii)

Synonym: cis-diaqua-bis(vanillinato)-copper(ii)

Space Group: P21/c **Cell:** **a** 7.740(0) **b** 10.492(0) **c** 21.240(0)

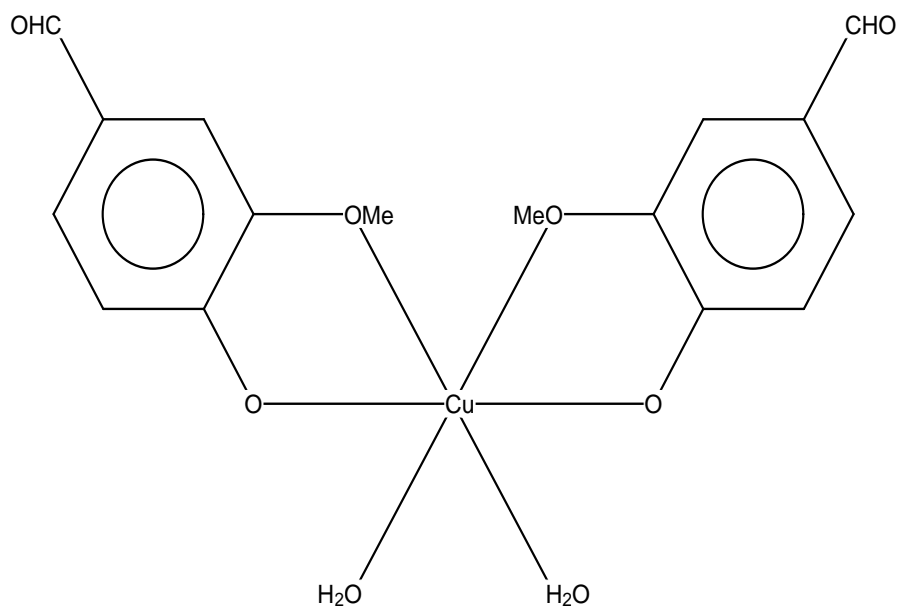
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 95.63(0) **γ** 90.00

R-Factor (%): 2.60 **Temperature(K):** 115 **Density(g/cm³):** 1.555

Parameters

Fragment 1

DIST1 (D)	1.919
DIST2 (D)	1.914
DIST3 (D)	2.151
DIST4 (D)	2.020
DIST5 (D)	2.354
DIST6 (D)	2.163



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 128

NENBEO

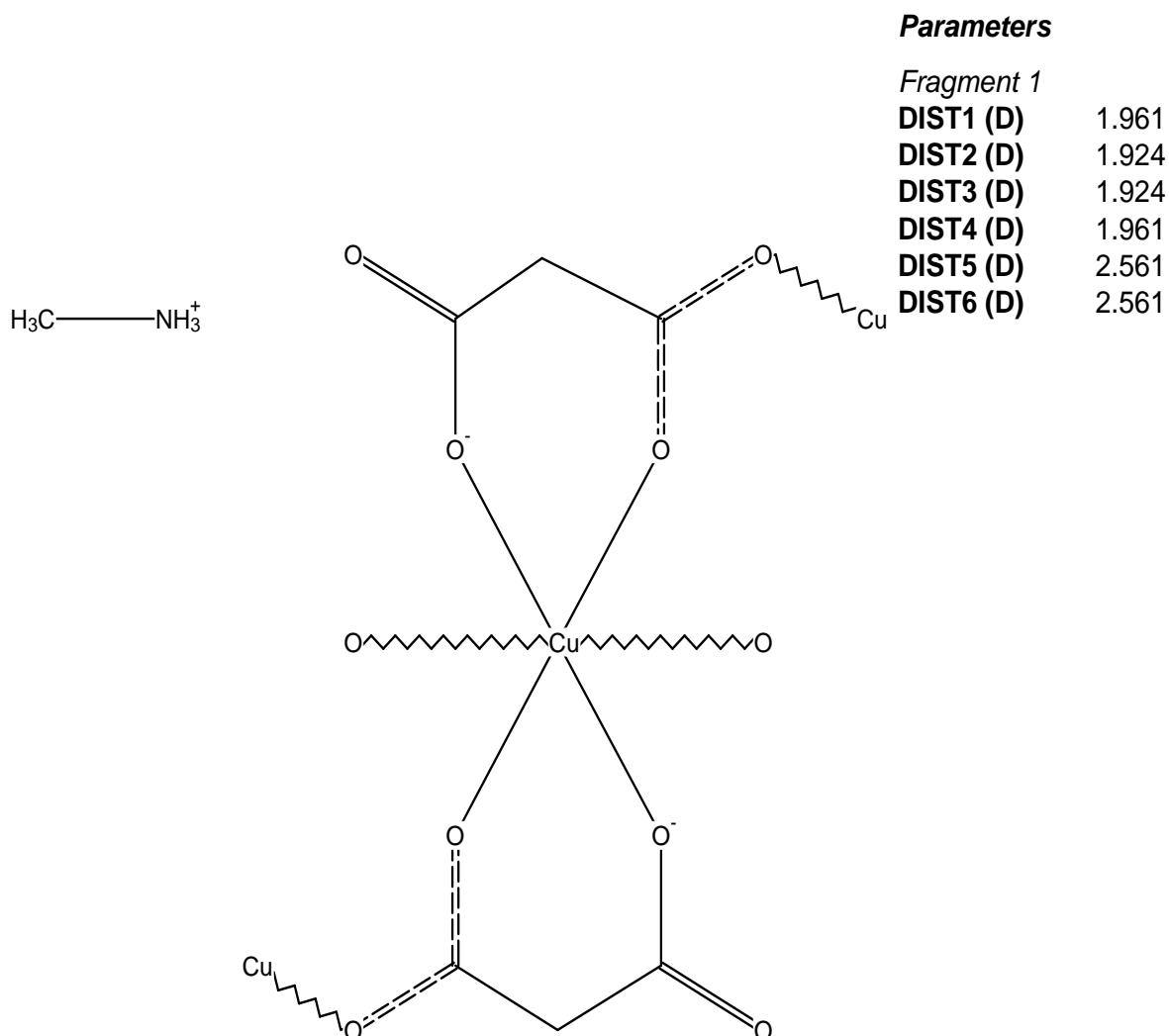
Reference: F.S.Delgado, C.Ruiz-Perez, J.Sanchiz, F.Lloret, M.Julve (2006) *CrystEngComm*, **8**,530

Formula: $(C_1 H_6 N_1^{1+})_2 n, n(C_6 H_4 Cu_1 O_8^{2-})$

Compound Name: catena-(bis(methylammonium) bis(μ_2 -malonato)-copper(ii))

Space Group: P21/c **Cell:** **a** 8.687(0) **b** 9.059(0) **c** 8.968(0)
Space Group No.: 14 (**Å, °**) α 90.00 β 115.20(0) γ 90.00

R-Factor (%): 2.28 **Temperature(K):** 293 **Density(g/cm³):** 1.726



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 129

NERKUQ

Reference: Bao-Qing Ma, Hao-Ling Sun, Song Gao, Guang-Xian Xu (2001) *Inorg.Chem.* ,**40**,6247

Formula: $2(\text{C}_{10}\text{H}_8\text{N}_2\text{O}_2), \text{H}_{12}\text{Cu}_1\text{O}_6^{2+}, 2(\text{Cl}_1^{-}), 2(\text{H}_2\text{O}_1)$

Compound Name: Hexa-aqua-copper(ii) dichloride (4,4'-bipyridine-N,N'-dioxide) solvate dihydrate

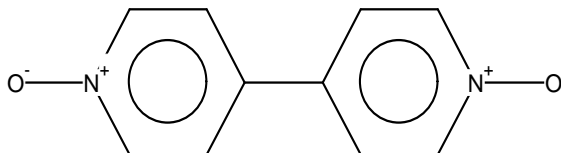
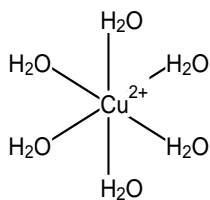
Space Group: P-1 **Cell:** **a** 6.732(0) **b** 10.254(1) **c** 10.423(4)
Space Group No.: 2 (**Å, °**) α 85.09(2) β 72.81(1) γ 89.23(1)

R-Factor (%): 2.88 **Temperature(K):** 293 **Density(g/cm³):** 1.588

Parameters

Fragment 1

DIST1 (D) 1.968
DIST2 (D) 1.968
DIST3 (D) 1.968
DIST4 (D) 1.968
DIST5 (D) 2.376
DIST6 (D) 2.376



Cl^-

H_2O

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 130

NERWAK

Reference: A.V.Pestov, P.A.Slepukhin, Yu.G.Yatluk (2012)
Koord.Khim.(Russ.)(Coord.Chem.) ,**38**,874

Formula: C₈ H₁₈ Cu₁ O₁₀

Compound Name: Diaqua-bis((2-hydroxyethoxy)acetato-O,O')-copper(ii)

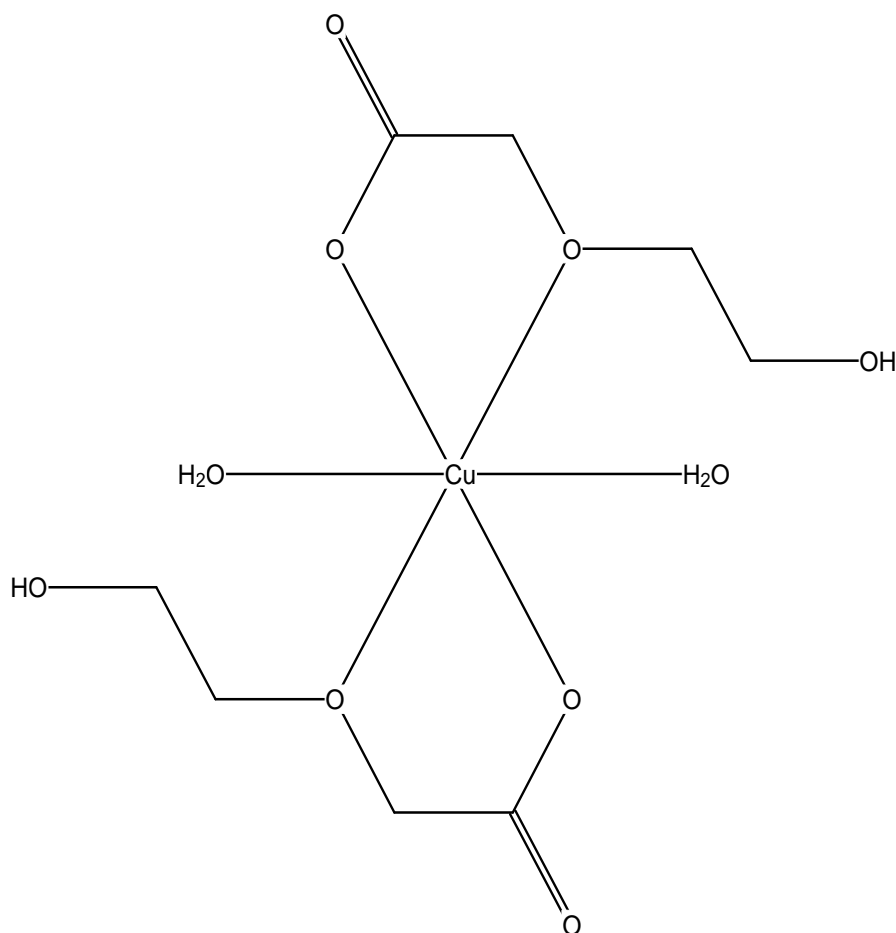
Space Group: P-1 **Cell:** **a** 6.957(0) **b** 7.277(0) **c** 7.309(0)
Space Group No.: 2 (**Å, °**) **α** 75.38(0) **β** 64.18(1) **γ** 75.09(0)

R-Factor (%): 2.35 **Temperature(K):** 295 **Density(g/cm³):** 1.766

Parameters

Fragment 1

DIST1 (D)	1.993
DIST2 (D)	1.952
DIST3 (D)	1.952
DIST4 (D)	1.993
DIST5 (D)	2.375
DIST6 (D)	2.375



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 131

NOMGAZ

Reference: Gui-lin Zhuang, Li Tan, Wu-lin Chen, Jun Zheng, Hong-zhou Yao, Xing Zhong, Jian-guo Wang (2014) *Inorg.Chem.Front.* ,1,526

Formula: (C₈ H₁₂ Cu₁ N₂ O₈)_n

Compound Name: catena-[(μ-2,2'-(2,5-dioxopiperazine-1,4-diyl)diacetato)-diaqua-copper]

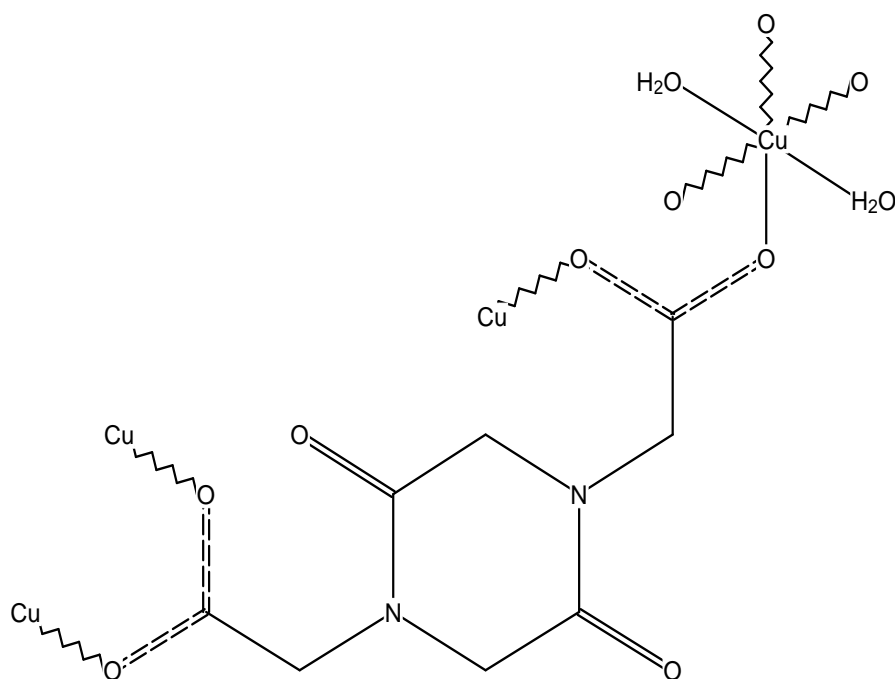
Space Group: C2/c **Cell:** **a** 20.548(0) **b** 4.657(0) **c** 13.977(0)
Space Group No.: 15 **(Å, °)** **α** 90.00 **β** 124.40(0) **γ** 90.00

R-Factor (%): 2.25 **Temperature(K):** 301 **Density(g/cm³):** 1.972

Parameters

Fragment 1

DIST1 (D) 1.957
DIST2 (D) 1.957
DIST3 (D) 1.950
DIST4 (D) 1.950
DIST5 (D) 2.615
DIST6 (D) 2.615



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 132

OFEJIU

Reference: Yan-Yan Jia, Bin Liu, Xue-Mei Liu, Jian-Hui Yang (2013)
CrystEngComm, 15, 7936

Formula: (C₄ H₄ Br₂ Cu₁ K₂ Li₁ O₁₉ Ru₂)_n

Compound Name: catena-[tetrakis(μ₄-carbonato)-bis(μ₄-bromo)-bis(μ₂-aqua)-pentakis(μ₂-oxo)-copper-di-potassium-lithium-di-ruthenium]

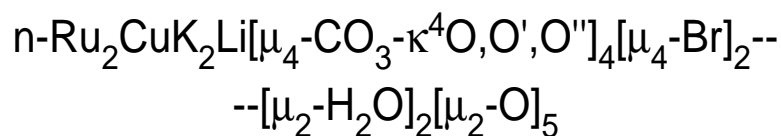
Space Group: Pccn **Cell:** **a** 10.976(0) **b** 11.284(1) **c** 17.248(1)
Space Group No.: 56 (**Å, °**) α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.41 **Temperature(K):** 296 **Density(g/cm³):** 2.695

Parameters

Fragment 1

DIST1 (D) 2.009
DIST2 (D) 2.009
DIST3 (D) 2.059
DIST4 (D) 2.059
DIST5 (D) 2.312
DIST6 (D) 2.312



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 133

OJUXUO

Reference: Junqing Zhang, Cun Li, Juanjuan Wang, Mei Zhu, Licun Li (2016) *Eur.J.Inorg.Chem.* ,1383

Formula: C₄₆ H₂₀ Cu₁ Dy₂ F₃₆ O₁₈

Compound Name: bis(μ -1,1,1,5,5,5-hexafluoroacetylacetonato)-bis(μ -2-oxy-4-methoxybenzaldehyde)-tetrakis(1,1,1,5,5,5-hexafluoroacetylacetonato)-copper-di-dysprosium

Space Group: P-1 **Cell:** **a** 9.883(2) **b** 11.104(2) **c** 15.995(3)

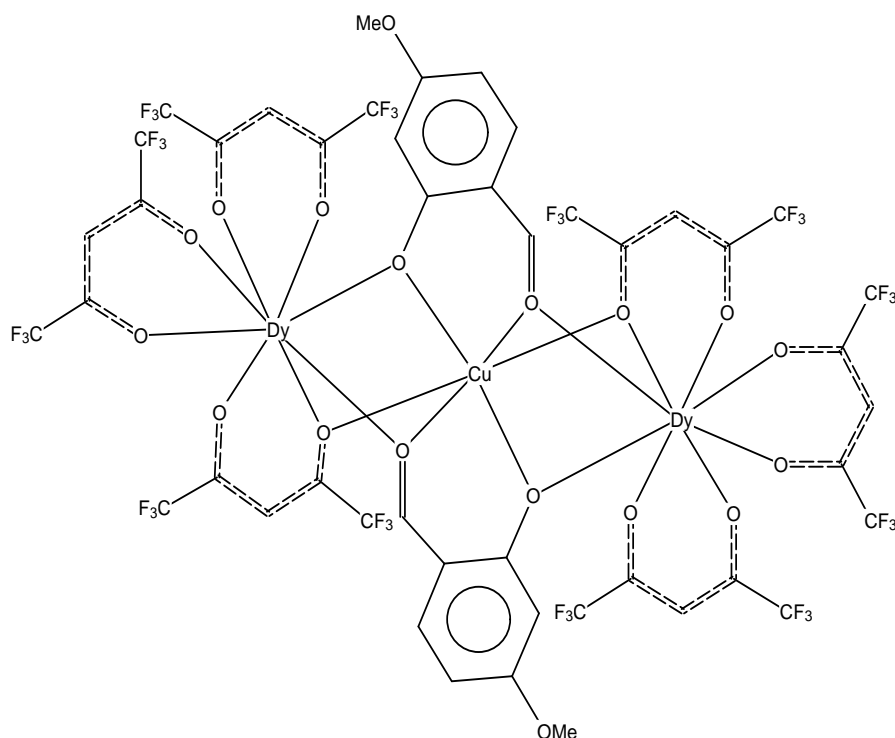
Space Group No.: 2 **(Å, °)** α 100.51(3) β 99.61(3) γ 113.18(3)

R-Factor (%): 2.65 **Temperature(K):** 113 **Density(g/cm³):** 2.098

Parameters

Fragment 1

DIST1 (D)	1.905
DIST2 (D)	1.949
DIST3 (D)	1.905
DIST4 (D)	1.949
DIST5 (D)	2.494
DIST6 (D)	2.494



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 134

ORIWES

Reference: A.Fonari, E.S.Leonova, M.Yu.Antipin (2011) *Polyhedron*, **30**,1710

Formula: C₁₈ H₂₂ Cu₁ N₄ O₁₆ S₂

Compound Name: diaqua-bis(dimethyl sulfoxide)-bis(3,5-dinitrobenzoato-O)-copper(ii)

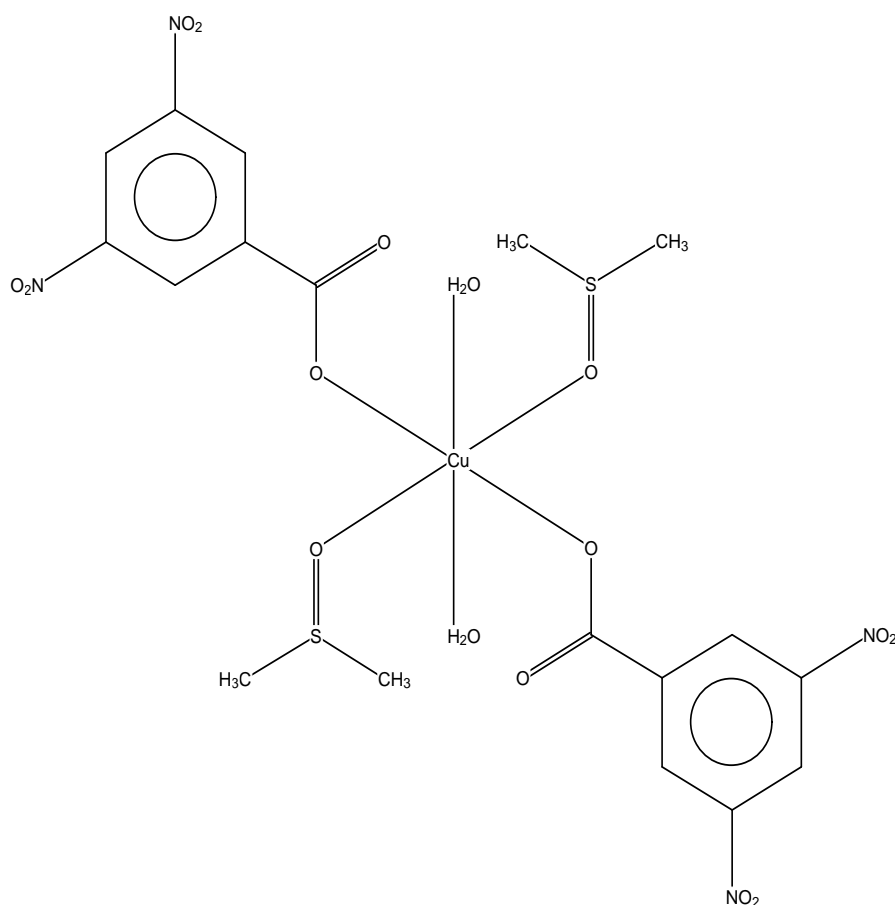
Space Group: P21/n **Cell:** **a** 10.624(1) **b** 5.282(0) **c** 22.573(3)
Space Group No.: 14 **(Å, °)** α 90.00 β 91.93(0) γ 90.00

R-Factor (%): 2.52 **Temperature(K):** 100 **Density(g/cm³):** 1.779

Parameters

Fragment 1

DIST1 (D)	1.971
DIST2 (D)	1.968
DIST3 (D)	1.968
DIST4 (D)	1.971
DIST5 (D)	2.371
DIST6 (D)	2.371



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 135

PAGKAK

Reference: V.T.Yilmaz, E.Senel, C.Kazak (2004)
Solid State Sciences ,6,859

Formula: C₁₀ H₂₀ Cu₁ N₂ O₁₀

Compound Name: trans-bis(2-Ammonioethanol)-bis(malonato)-copper(ii)

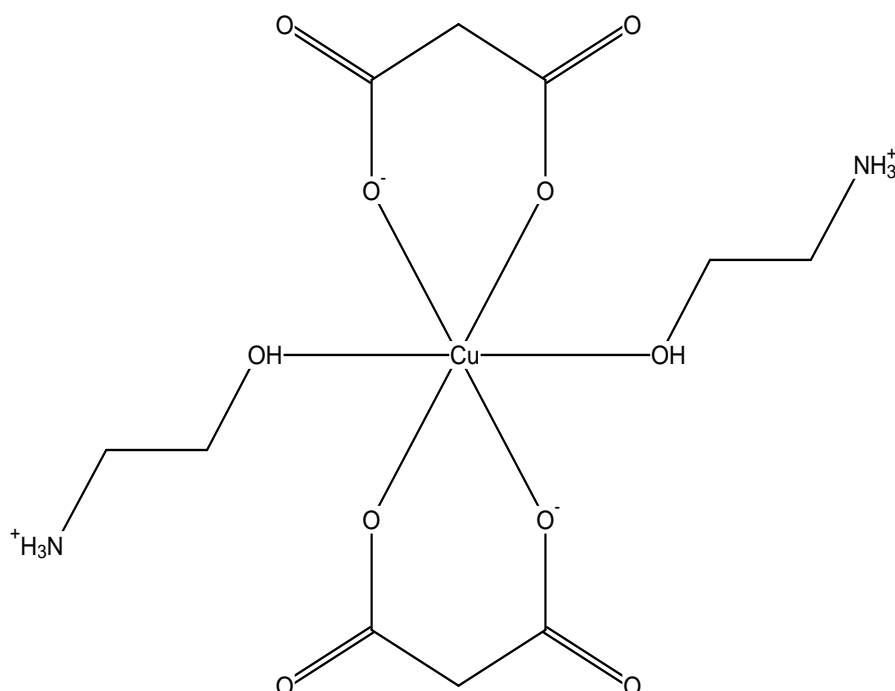
Space Group: P21/n **Cell:** **a** 8.663(0) **b** 7.512(0) **c** 11.439(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 95.53(0) γ 90.00

R-Factor (%): 2.80 **Temperature(K):** 293 **Density(g/cm³):** 1.756

Parameters

Fragment 1

DIST1 (D)	1.955
DIST2 (D)	1.933
DIST3 (D)	1.955
DIST4 (D)	1.933
DIST5 (D)	2.465
DIST6 (D)	2.465



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 136

PAKLAO

Reference: A.Bouayad, C.Brouca-Cabarrecq, J.-C.Trombe, A.Gleizes
(1992) *Inorg.Chim.Acta* ,195,193

Formula: $(C_{16}H_{32}Cu_1La_2O_{32})_n \cdot 2n(H_2O)_1$

Compound Name: catena-(tetrakis(μ_2 -Squarato-O,O')-hexadeca-aqua-di-lanthanum(iii)-copper(ii) dihydrate)

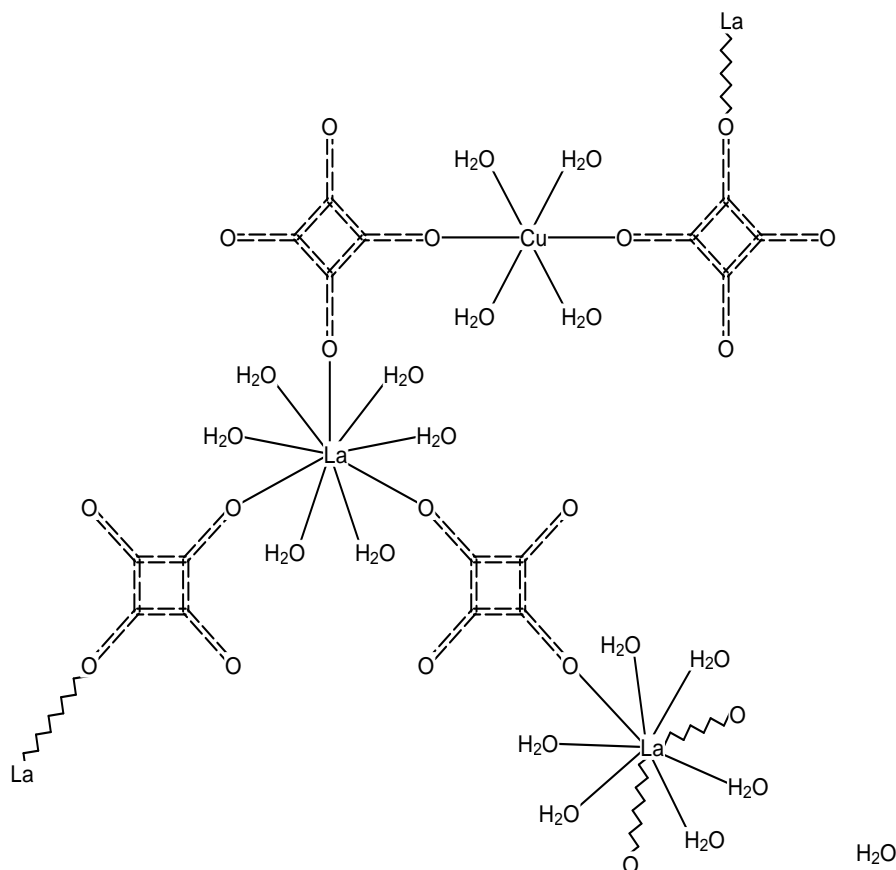
Space Group: P21/c **Cell:** **a** 6.780(2) **b** 32.311(4) **c** 8.162(2)
Space Group No.: 14 **(Å, °)** α 90.00 β 111.55(2) γ 90.00

R-Factor (%): 1.80 **Temperature(K):** 295 **Density(g/cm³):** 2.224

Parameters

Fragment 1

DIST1 (D)	1.977
DIST2 (D)	1.963
DIST3 (D)	1.963
DIST4 (D)	1.977
DIST5 (D)	2.426
DIST6 (D)	2.426



PAKLES

Reference: A.Bouayad, C.Brouca-Cabarrecq, J.-C.Trombe, A.Gleizes (1992) *Inorg.Chim.Acta* ,195,193

Formula: $(C_{16} H_{24} Cu_1 Gd_2 O_{28})_n \cdot 2n(H_2 O_1)$

Compound Name: catena-(bis(μ_3 -Squarato-O,O',O'')-bis(μ_2 -squarato-O,O')-dodeca-aqua-di-gadolinium(iii)-copper(ii) dihydrate)

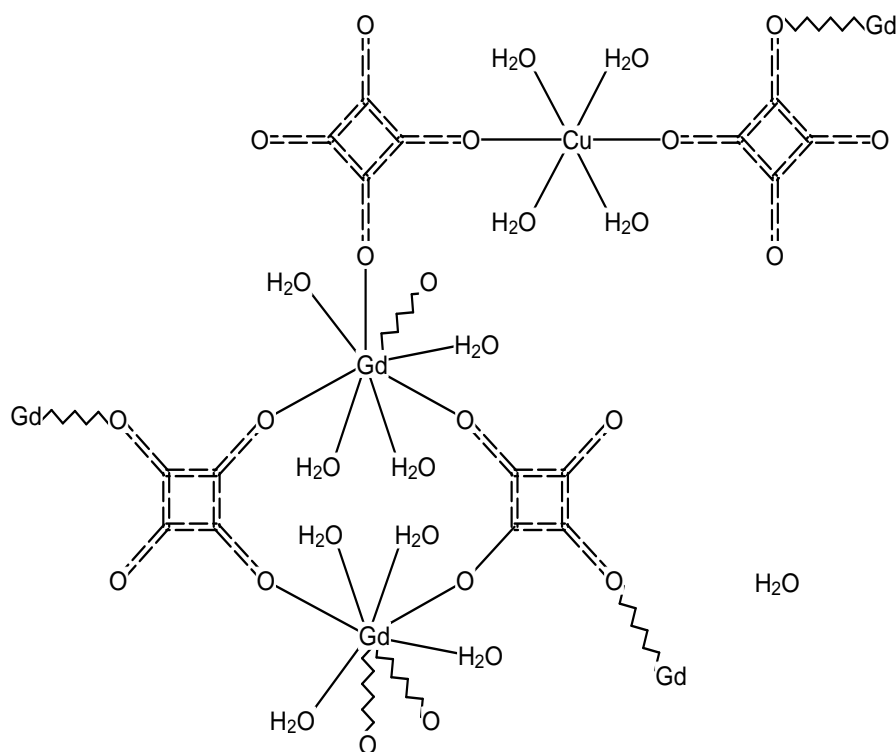
Space Group: C2/c **Cell:** **a** 13.784(1) **b** 8.219(1) **c** 26.268(2)
Space Group No.: 15 **(Å, °)** α 90.00 β 94.20(7) γ 90.00

R-Factor (%): 2.40 **Temperature(K):** 295 **Density(g/cm³):** 2.413

Parameters

Fragment 1

DIST1 (D) 1.965
DIST2 (D) 1.962
DIST3 (D) 1.962
DIST4 (D) 1.965
DIST5 (D) 2.377
DIST6 (D) 2.377



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 138

PAMSEB

Reference: H.Paulus, H.Fuess, P.Baran, D.Valigura (1992)
Z.Kristallogr. ,**202**,140

Formula: C₁₀ H₁₀ Cu₁ N₄ O₉

Compound Name: Aqua-(2,2'-bipyridine-N,N'-dioxide-O,O')-(nitrate-O,O')-(nitrate-O)-copper(ii)

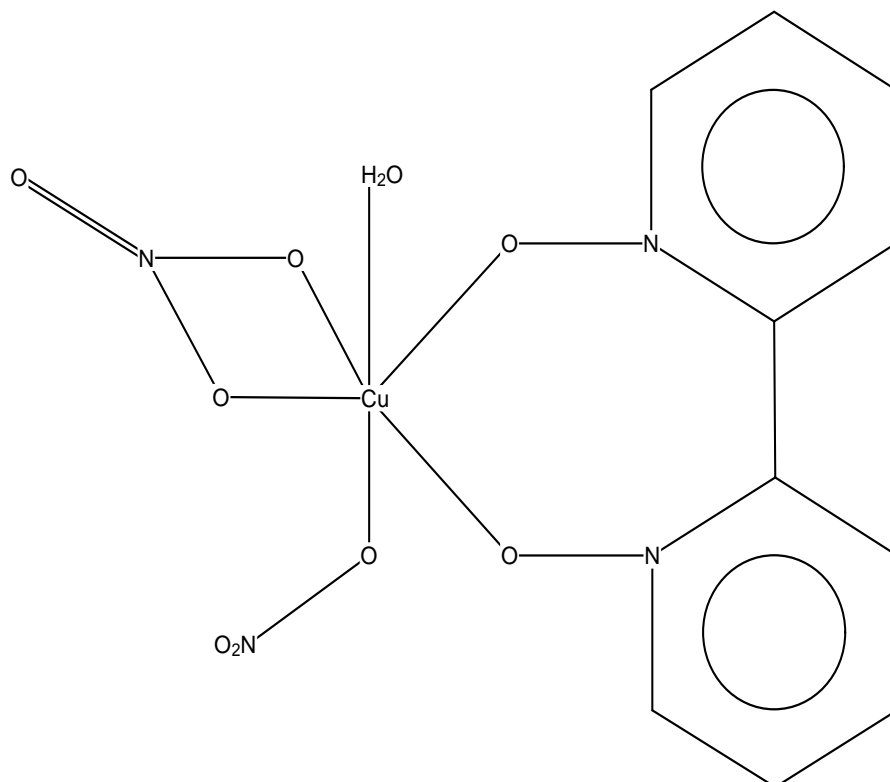
Space Group: P21/c **Cell:** **a** 6.635(2) **b** 7.188(2) **c** 29.038(3)
Space Group No.: 14 **(Å, °)** α 90.00 β 95.54(1) γ 90.00

R-Factor (%): 2.60 **Temperature(K):** 295 **Density(g/cm³):** 1.897

Parameters

Fragment 1

DIST1 (D)	1.990
DIST2 (D)	1.947
DIST3 (D)	1.944
DIST4 (D)	1.948
DIST5 (D)	2.529
DIST6 (D)	2.371



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 139

PASNEE

Reference: Feifei Xing, Yueling Bai, Xiang He, Juan Jia, Dong Zhou, Min Shao, Shourong Zhu (2012) *CrystEngComm*, **14**,4312

Formula: $(C_{24}H_{34}Cu_5O_{34})_n \cdot 4n(H_2O)_1$

Compound Name: catena(-bis(μ_5 -6-Carboxyl-benzene-1,2,3,4,5-pentacarboxylato)-deca-aqua-penta-copper tetrahydrate)

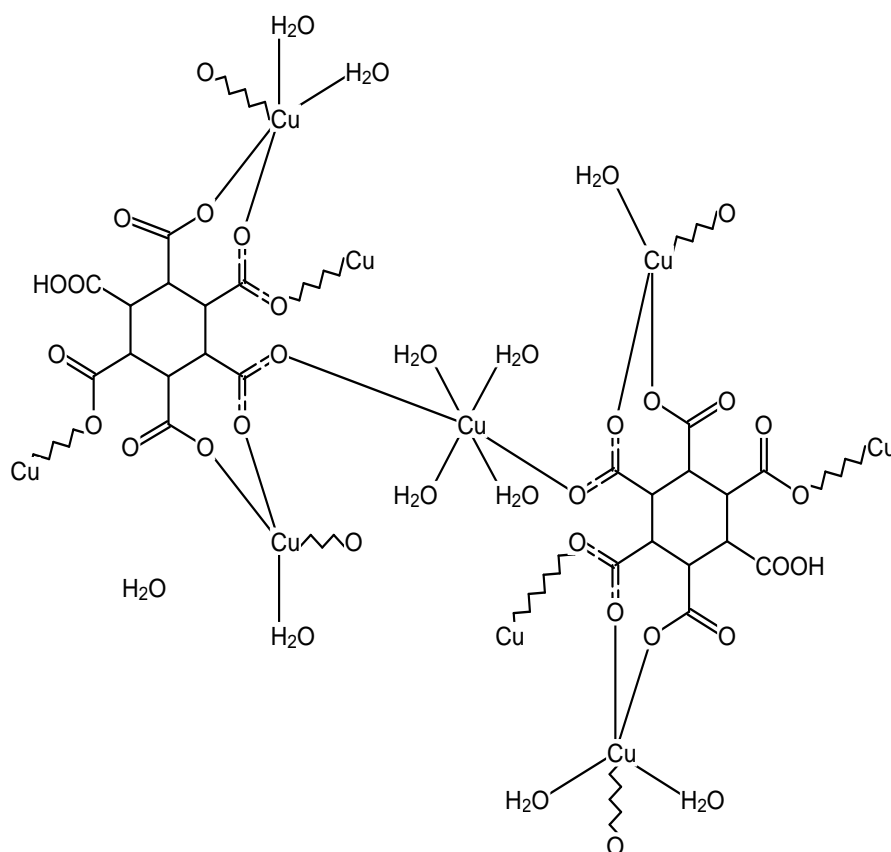
Space Group: C2/c **Cell:** **a** 17.098(1) **b** 8.386(0) **c** 27.613(3)
Space Group No.: 15 **(Å, °)** α 90.00 β 104.65(0) γ 90.00

R-Factor (%): 2.54 **Temperature(K):** 296 **Density(g/cm³):** 2.178

Parameters

Fragment 1

DIST1 (D)	1.956
DIST2 (D)	1.945
DIST3 (D)	1.945
DIST4 (D)	1.937
DIST5 (D)	2.404
DIST6 (D)	2.404



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 140

PASZAL

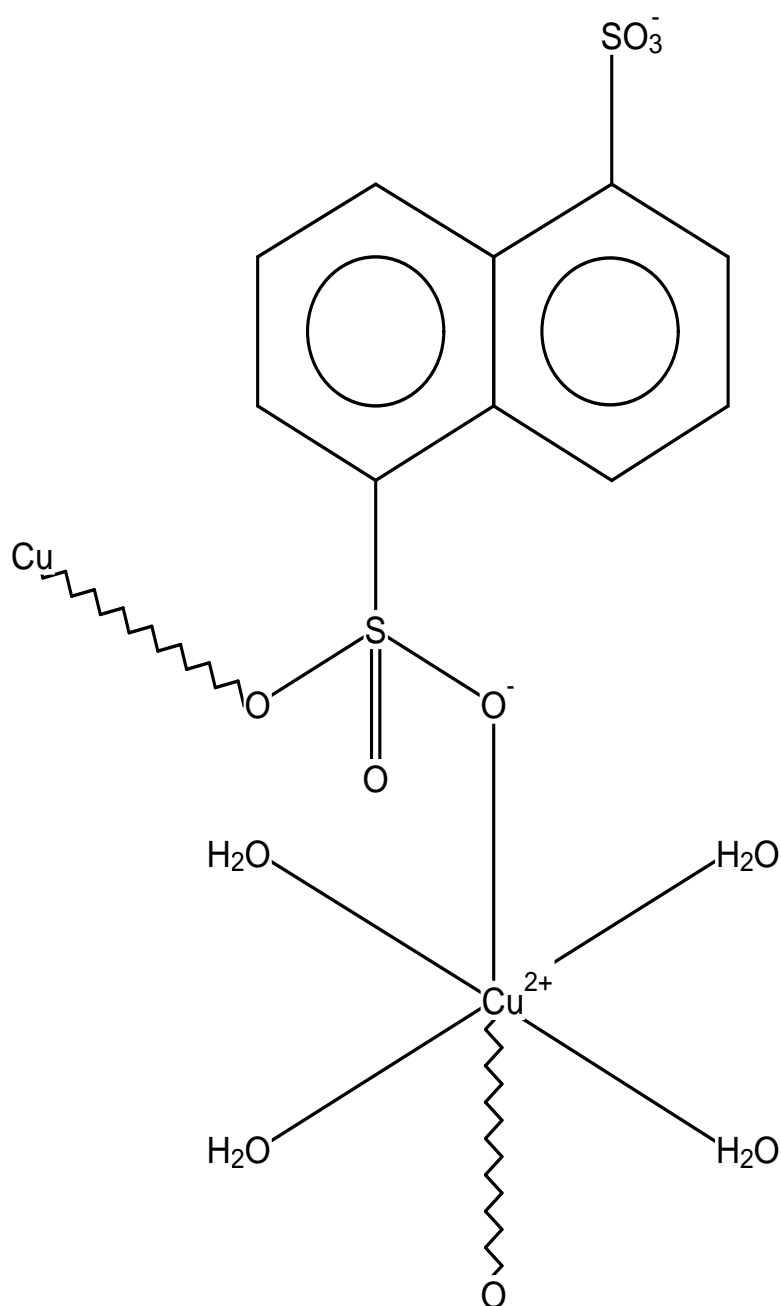
Reference: Li Wang, Xiao-Lan Yu, Jiwen Cai, Jin-Wang Huang (2005)
J.Chem.Cryst. ,**35**,481

Formula: (C₁₀ H₁₄ Cu₁ O₁₀ S₂)_n

Compound Name: catena-((μ₂-1,5-Naphthalenedisulfonato-O,O')-tetra-aqua-copper(ii))

Space Group: Pbc_a **Cell:** **a** 12.956(1) **b** 9.885(1) **c** 22.797(3)
Space Group No.: 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.57 **Temperature(K):** 293 **Density(g/cm³):** 1.920



Parameters

Fragment 1

DIST1 (D)	1.955
DIST2 (D)	1.954
DIST3 (D)	1.953
DIST4 (D)	1.979
DIST5 (D)	2.337
DIST6 (D)	2.449

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 141

PAXTUE01

Reference: B.Kozlevcar, M.Humar, P.Strauch, I.Leban (2005)
Z.Naturforsch.,B:Chem.Sci. ,**60**,1273

Formula: C₁₆ H₁₈ Cu₁ O₈,2(H₂ O₁)

Compound Name: trans-Diaqua-bis(vanillinato)-copper(ii) dihydrate

Synonym: trans-Diaqua-bis(4-formyl-2-methoxyphenolato)-copper(ii) dihydrate

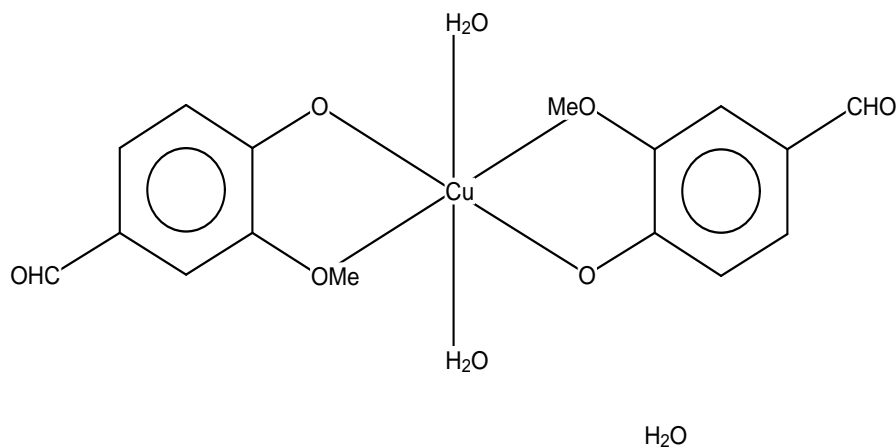
Space Group: P21/a **Cell:** **a** 6.696(0) **b** 12.825(0) **c** 10.953(1)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 100.45(0) **γ** 90.00

R-Factor (%): 2.87 **Temperature(K):** 293 **Density(g/cm³):** 1.572

Parameters

Fragment 1

DIST1 (D)	1.994
DIST2 (D)	1.950
DIST3 (D)	1.950
DIST4 (D)	1.994
DIST5 (D)	2.334
DIST6 (D)	2.334



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 142

PAXTUE02

Reference: B.Kozlevcar, M.Humar, P.Strauch, I.Leban (2005)
Z.Naturforsch.,B:Chem.Sci. ,**60**,1273

Formula: C₁₆ H₁₈ Cu₁ O₈,2(H₂ O₁)

Compound Name: trans-Diaqua-bis(vanillinato)-copper(ii) dihydrate

Synonym: trans-Diaqua-bis(4-formyl-2-methoxyphenolato)-copper(ii) dihydrate

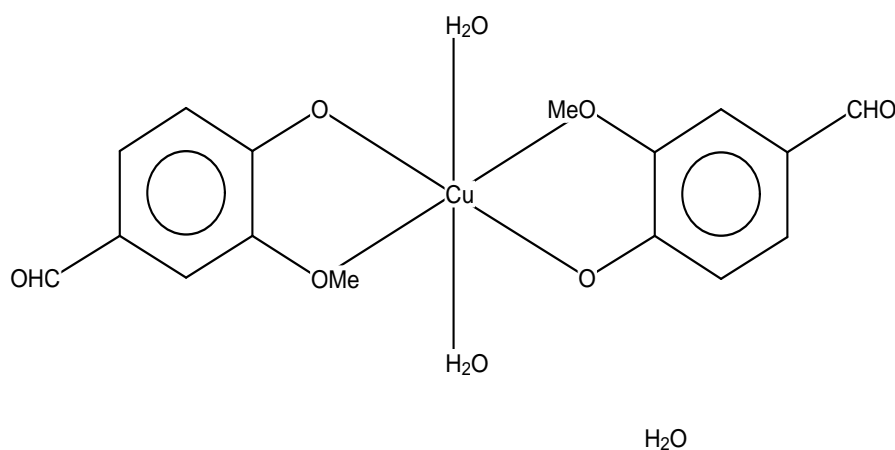
Space Group: P21/a **Cell:** **a** 6.543(0) **b** 12.885(0) **c** 10.885(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 98.61(0) γ 90.00

R-Factor (%): 2.39 **Temperature(K):** 150 **Density(g/cm³):** 1.603

Parameters

Fragment 1

DIST1 (D)	1.983
DIST2 (D)	1.959
DIST3 (D)	1.959
DIST4 (D)	1.983
DIST5 (D)	2.327
DIST6 (D)	2.327



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 143

PEWDUS

Reference: J.Olchowka, C.Falaise, C.Volkringer, N.Henry, T.Loiseau
(2013) *Chem.-Eur.J.* ,**19**,2012

Formula: (C₈ H₈ Cu₁ O₁₃ U₂)_n,n(H₂ O₁)

Compound Name: catena-[(μ_3 - Isophthalato)-bis(μ_3 -oxo)-tris(μ_2 -oxo)-diaqua-dioxo-copper-di-uranium monohydrate]

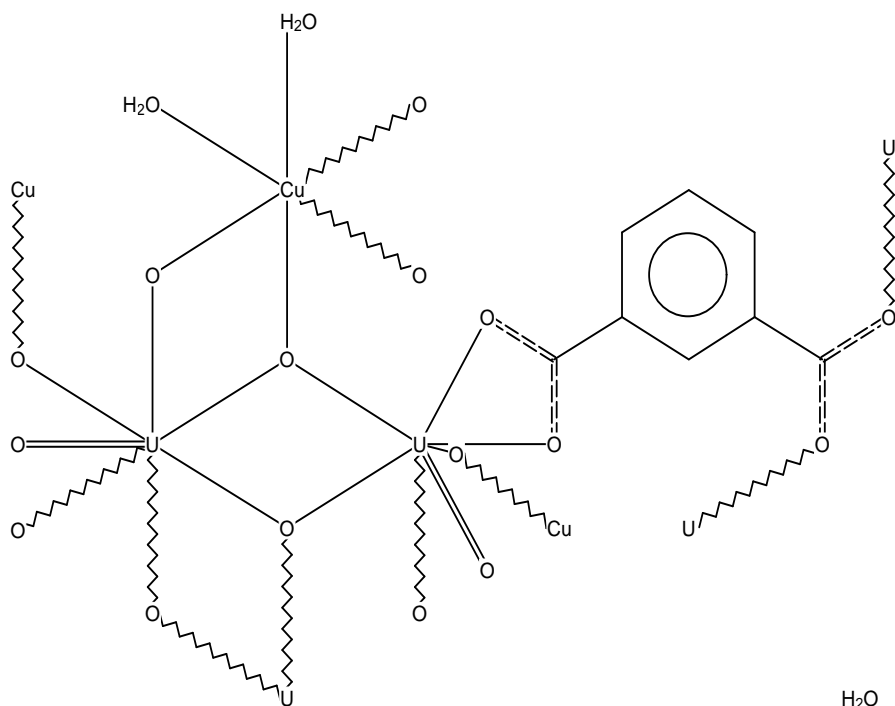
Space Group: P-1 **Cell:** **a** 8.564(0) **b** 8.750(0) **c** 12.423(0)
Space Group No.: 2 (**Å, °**) α 84.92(0) β 77.17(0) γ 61.93(0)

R-Factor (%): 2.39 **Temperature(K):** 293 **Density(g/cm³):** 3.607

Parameters

Fragment 1

DIST1 (D)	2.001
DIST2 (D)	1.912
DIST3 (D)	1.977
DIST4 (D)	1.991
DIST5 (D)	2.350
DIST6 (D)	2.692



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 144

PEWFAA

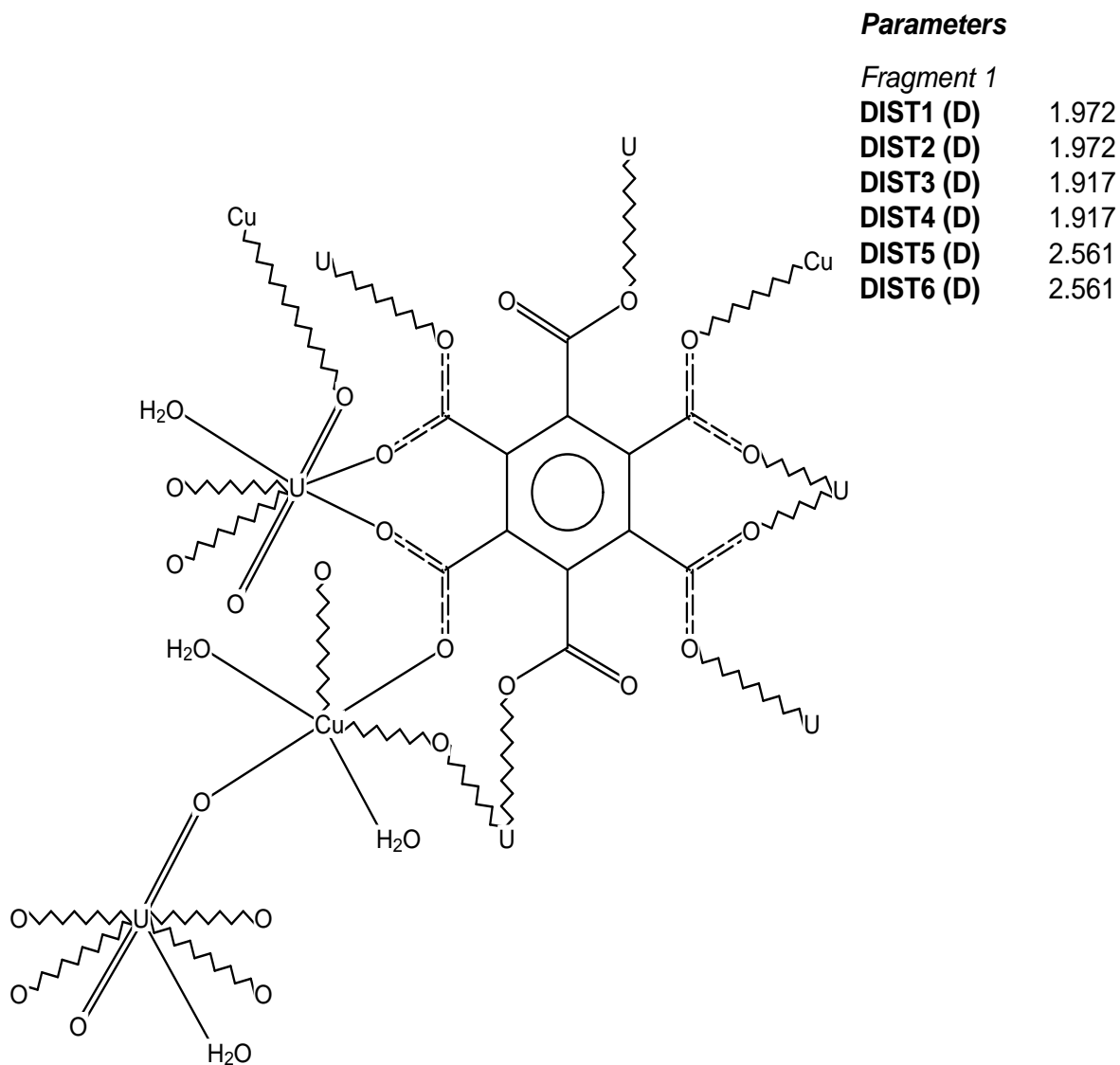
Reference: J.Olchowka, C.Falaise, C.Volkringer, N.Henry, T.Loiseau
(2013) *Chem.-Eur.J.* ,**19**,2012

Formula: (C₁₂ H₈ Cu₁ O₂₀ U₂)_n

Compound Name: catena-[(μ_8 -Benzene-1,2,3,4,5,6-hexacarboxylato)-bis(μ_2 -oxo)-tetra-aqua-dioxo-copper-di-uranium]

Space Group: P21/c **Cell:** **a** 7.984(0) **b** 11.546(0) **c** 10.972(0)
Space Group No.: 14 (**Å**, °) α 90.00 β 105.35(0) γ 90.00

R-Factor (%): 1.85 **Temperature(K):** 293 **Density(g/cm³):** 3.445



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 145

PEWFEE

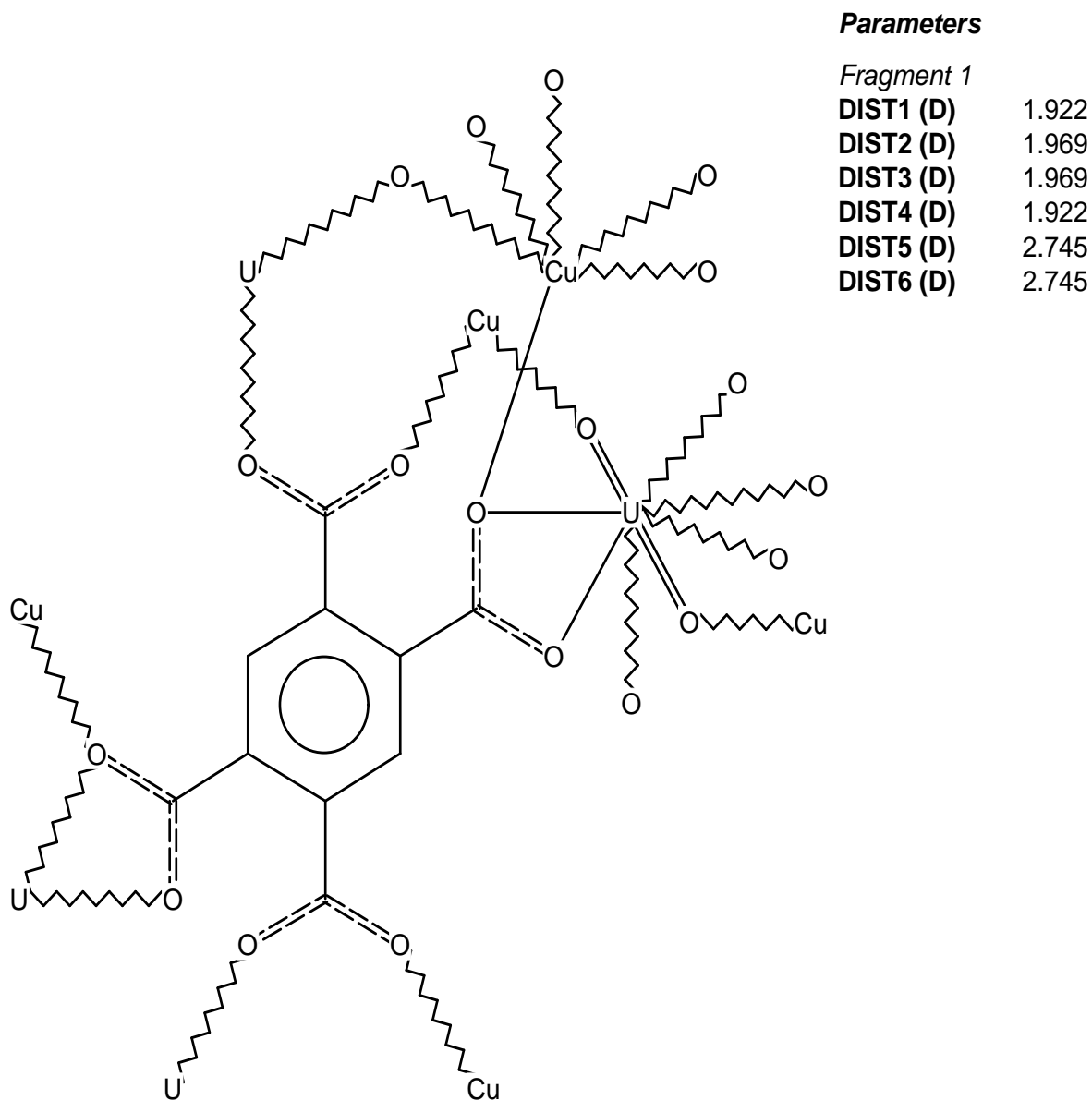
Reference: J.Olchowka, C.Falaise, C.Volkringer, N.Henry, T.Loiseau
(2013) *Chem.-Eur.J.* ,19,2012

Formula: (C₁₀ H₂ Cu₁ O₁₀ U₁)_n

Compound Name: catena-[(μ₈-Benzene-1,2,4,5-tetracarboxylato)-bis(μ₂-oxo)-copper-uranium]

Space Group: P-1 **Cell:** **a** 4.996(0) **b** 6.971(0) **c** 8.514(0)
Space Group No.: 2 **(Å, °)** **α** 97.31(0) **β** 106.42(0) **γ** 91.96(0)

R-Factor (%): 2.67 **Temperature(K):** 293 **Density(g/cm³):** 3.439



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 146

PEWFII

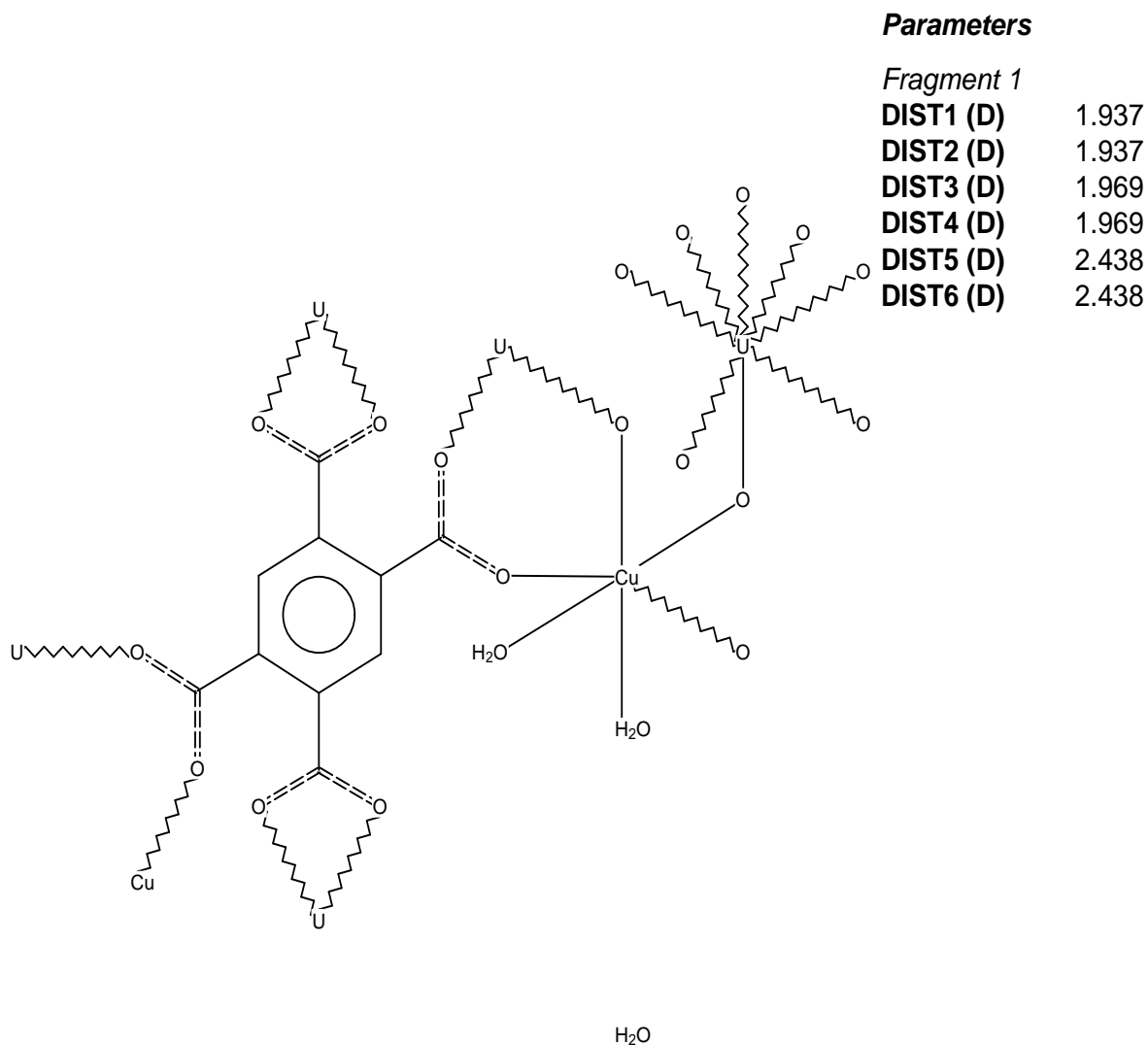
Reference: J.Olchowka, C.Falaise, C.Volkringer, N.Henry, T.Loiseau
(2013) *Chem.-Eur.J.* ,**19**,2012

Formula: $(C_{10} H_6 Cu_1 O_{12} U_1)_n, 4n(H_2 O_1)$

Compound Name: catena-((μ_6 -Benzene-1,2,4,5-tetracarboxylato)-bis(μ_2 -oxo)-diaqua-copper-uranium tetrahydrate)

Space Group: P-1 **Cell:** **a** 7.107(0) **b** 7.223(0) **c** 9.205(0)
Space Group No.: 2 (**Å, °**) α 95.38(0) β 91.26(0) γ 114.89(0)

R-Factor (%): 1.76 **Temperature(K):** 293 **Density(g/cm³):** 2.698



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 147

PEWFII01

Reference: Qing Lin Guan, Xue Gao, Jing Liu, Wen Juan Wei,
Yong Heng Xing, Feng Ying Bai (2016) *J.Coord.Chem.* ,69,1026

Formula: $(C_{10} H_6 Cu_1 O_{12} U_1)_n \cdot 4(H_2 O)_1$

Compound Name: catena-[(μ -benzene-1,2,4,5-tetracarboxylato)-bis(μ -oxo)-diaqua-copper-uranium tetrahydrate]

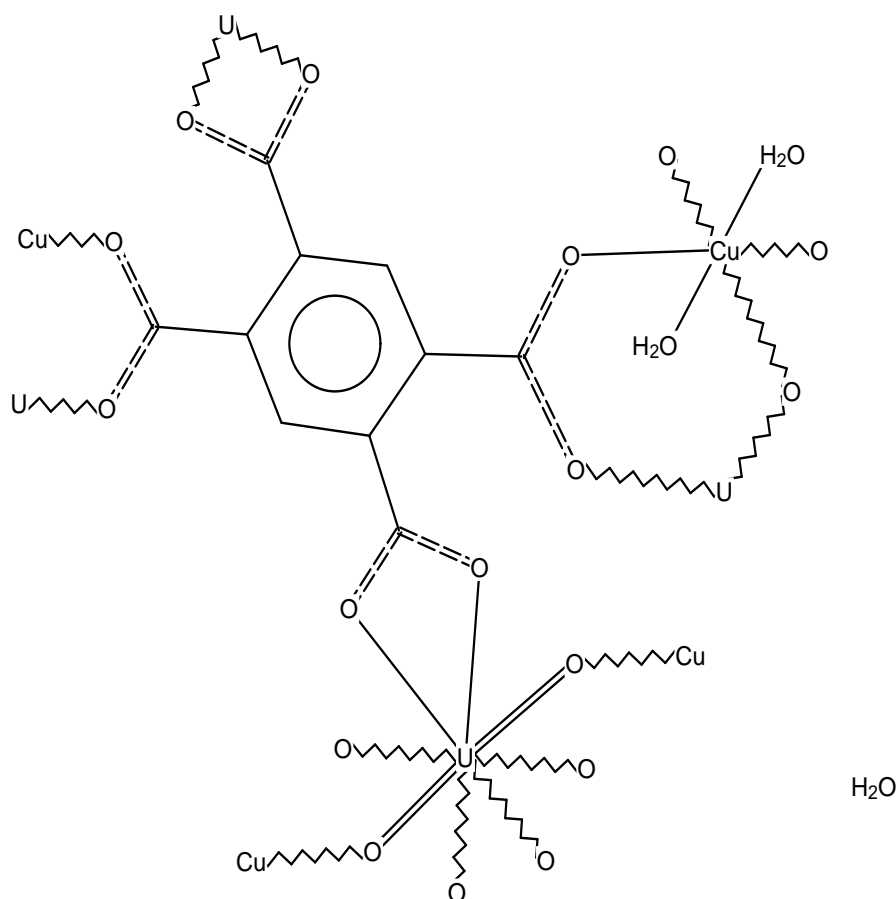
Space Group: P-1 **Cell:** **a** 7.116(0) **b** 7.235(0) **c** 9.214(0)
Space Group No.: 2 (**Å, °**) α 95.36(0) β 91.22(0) γ 114.93(0)

R-Factor (%): 2.33 **Temperature(K):** 296 **Density(g/cm³):** 2.688

Parameters

Fragment 1

DIST1 (D)	1.940
DIST2 (D)	1.972
DIST3 (D)	1.940
DIST4 (D)	1.972
DIST5 (D)	2.439
DIST6 (D)	2.439



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 148

PEWFOO

Reference: J.Olchowka, C.Falaise, C.Volkringer, N.Henry, T.Loiseau
(2013) *Chem.-Eur.J.* ,**19**,2012

Formula: (C₁₆ H₁₂ Cu₁ O₁₂ U₁)_n

Compound Name: catena-(bis(μ_3 -Phthalato)-bis(μ_2 -oxo)-diaqua-copper-uranium)

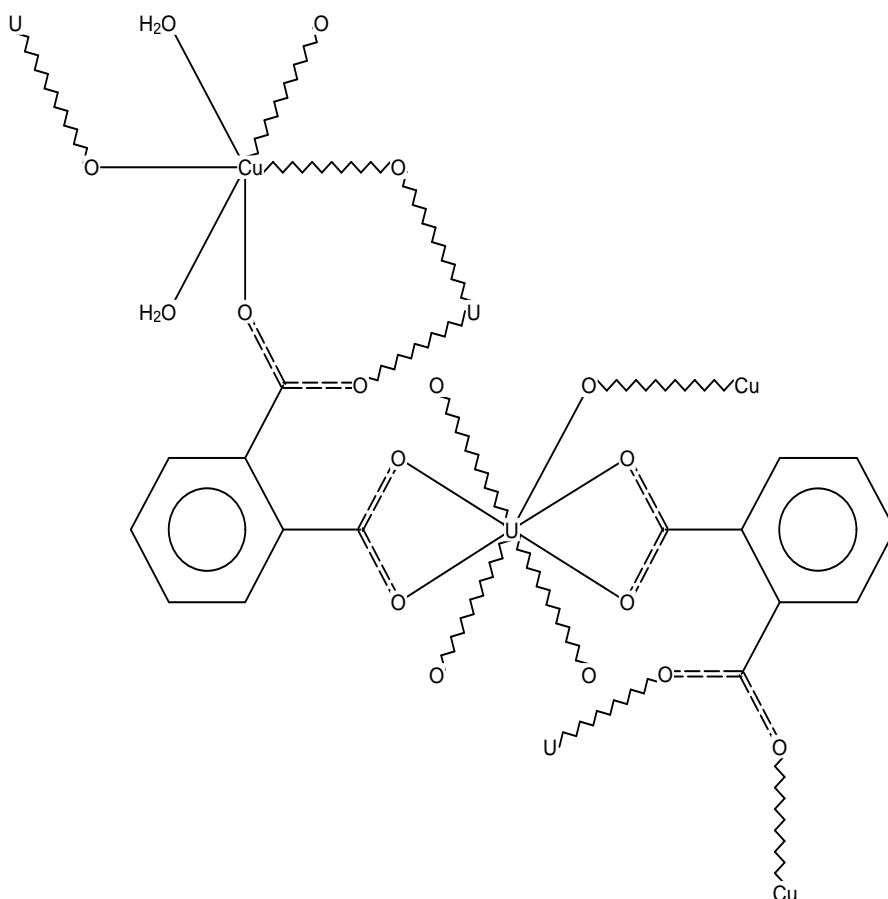
Space Group: P-1 **Cell:** **a** 6.990(0) **b** 7.091(0) **c** 10.071(1)
Space Group No.: 2 **(Å, °)** α 100.54(0) β 96.43(0) γ 114.22(0)

R-Factor (%): 2.78 **Temperature(K):** 293 **Density(g/cm³):** 2.658

Parameters

Fragment 1

DIST1 (D)	1.973
DIST2 (D)	1.973
DIST3 (D)	1.923
DIST4 (D)	1.923
DIST5 (D)	2.517
DIST6 (D)	2.517



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 149

PEWLEI

Reference: R.Kaplonek, G.Fechtcl, U.Baumeister, H.Hartung (1993)
Z.Anorg.Allg.Chem., **619**,1616

Formula: $(C_8 H_{12} Cu_1 O_9)_n, 2n(H_2 O_1)$

Compound Name: catena((Diaqua-5-exo,6-cis-dihydroxy-7-oxabicyclo(2.2.1)heptane-2,3-dicarboxylato-O,O',O'')-copper dihydrate)

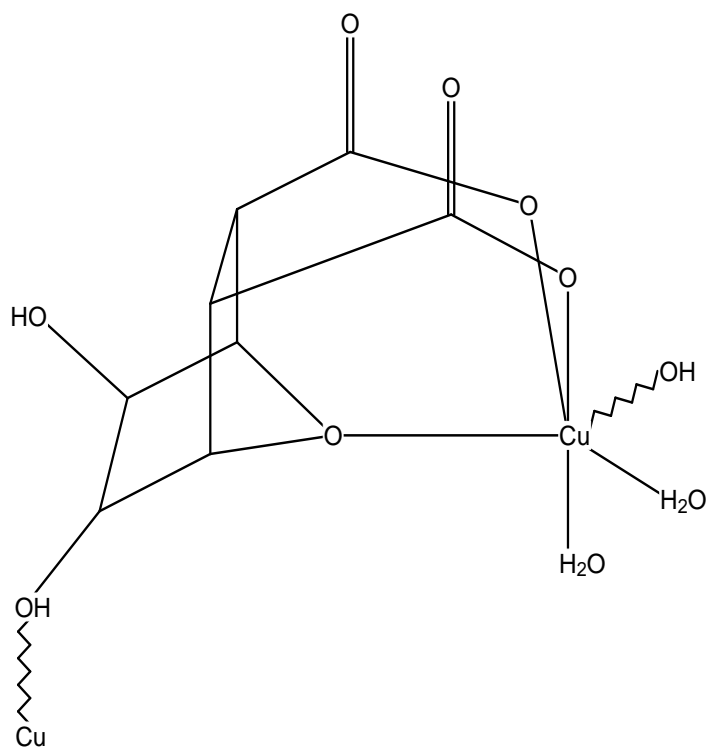
Space Group: P-1 **Cell:** **a** 7.273(2) **b** 7.457(2) **c** 12.135(3)
Space Group No.: 2 (**Å, °**) α 74.22(1) β 79.93(1) γ 70.11(1)

R-Factor (%): 2.70 **Temperature(K):** 295 **Density(g/cm³):** 1.970

Parameters

Fragment 1

DIST1 (D)	2.006
DIST2 (D)	1.946
DIST3 (D)	2.006
DIST4 (D)	1.958
DIST5 (D)	2.316
DIST6 (D)	2.384



H₂O

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 150

PHXCUA01

Reference: Yong-hong Zhou (2010)
Huaxue Yanjiu(Chin.)(Chem.Res.) ,21,1-1

Formula: C₁₆ H₁₆ Cl₂ Cu₁ O₈

Compound Name: Diaqua-bis(((4-chlorophenyl)oxy)acetato)-copper(ii)

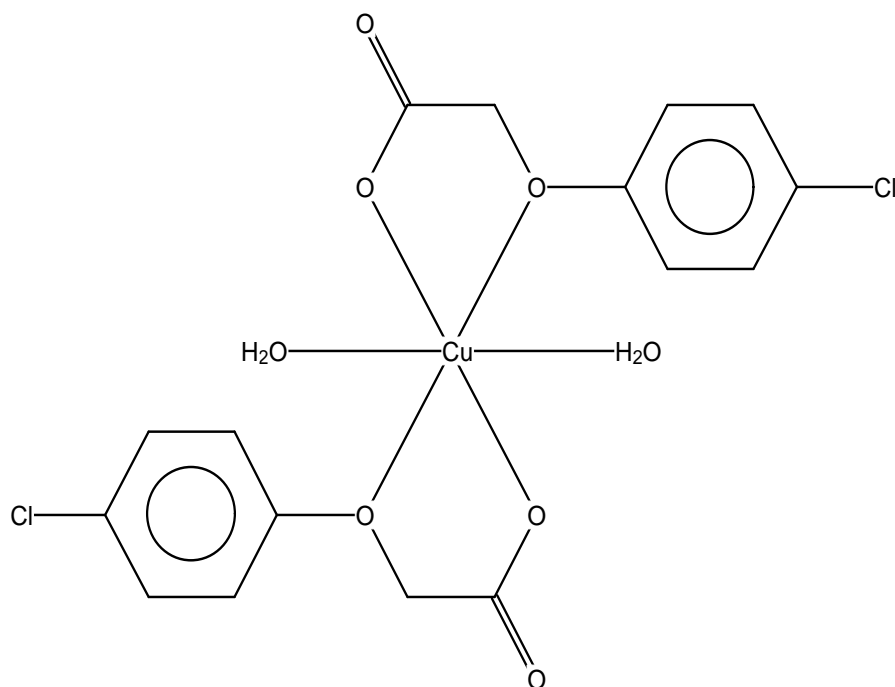
Space Group: P-1 **Cell:** **a** 5.115(0) **b** 7.064(0) **c** 13.264(0)
Space Group No.: 2 **(Å, °)** α 81.78(0) β 86.36(0) γ 76.40(0)

R-Factor (%): 2.64 **Temperature(K):** 298 **Density(g/cm³):** 1.696

Parameters

Fragment 1

DIST1 (D) 1.949
DIST2 (D) 1.951
DIST3 (D) 1.951
DIST4 (D) 1.949
DIST5 (D) 2.402
DIST6 (D) 2.402



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 151

PIDWUV

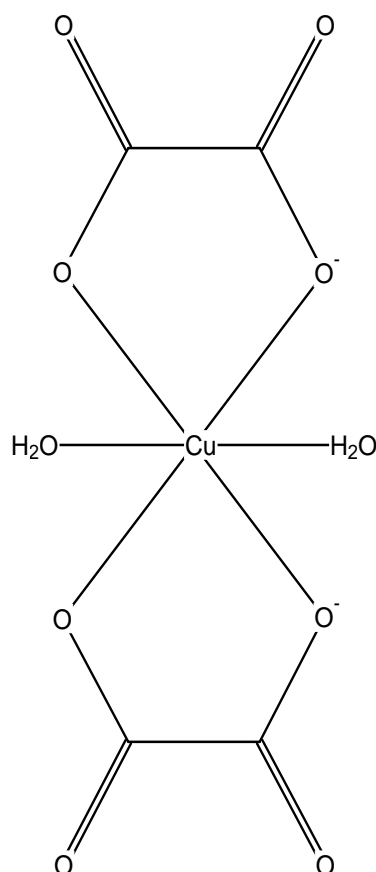
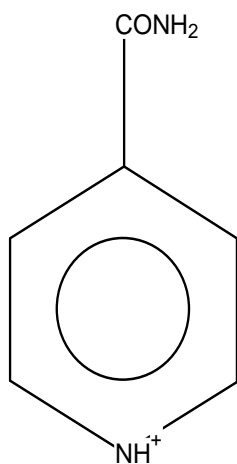
Reference: Chuan-Bi Li, Ying-Chun Gao (2007)
Acta Crystallogr., Sect. E: Struct. Rep. Online, **63**, m1337

Formula: $2(\text{C}_6\text{H}_7\text{N}_2\text{O}_1^{1+}), \text{C}_4\text{H}_4\text{Cu}_1\text{O}_{10}^{2-}$

Compound Name: bis(4-Carboxamidopyridinium) diaqua-dioxalato-copper(ii)

Space Group: P-1 **Cell:** **a** 6.788(2) **b** 6.957(2) **c** 10.849(3)
Space Group No.: 2 **(Å, °)** α 76.13(0) β 75.20(0) γ 79.48(0)

R-Factor (%): 2.50 **Temperature(K):** 295 **Density(g/cm³):** 1.817



Parameters

Fragment 1

DIST1 (D)	1.943
DIST2 (D)	1.987
DIST3 (D)	1.943
DIST4 (D)	1.987
DIST5 (D)	2.488
DIST6 (D)	2.488

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 152

PIJSIL

Reference: Jiang-Bo She, Guo-Fang Zhang, Feng-Qi Zhao, Zhong-Li Lei, Xue-Zhong Fan (2007) *Struct. Chem.*, **18**,373

Formula: C₁₀ H₁₂ Cu₁ N₆ O₁₆

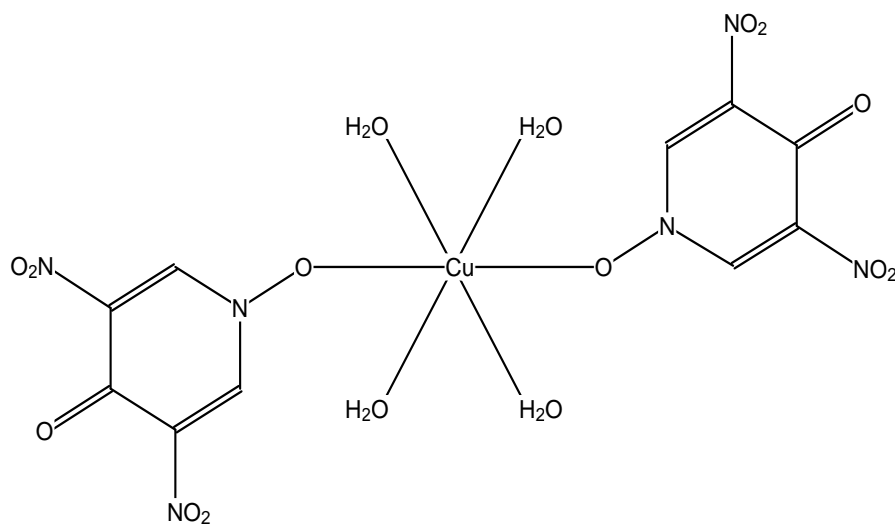
Compound Name: tetra-aqua-(3,5-dinitro-4-pyridone-N-hydroxylate)-copper(ii)

Space Group: P21/n **Cell:** **a** 8.370(1) **b** 9.931(1) **c** 10.577(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 98.02(0) γ 90.00

R-Factor (%): 2.76 **Temperature(K):** 273 **Density(g/cm³):** 2.044

Parameters

Fragment 1	
DIST1 (D)	2.088
DIST2 (D)	1.942
DIST3 (D)	1.942
DIST4 (D)	2.088
DIST5 (D)	2.233
DIST6 (D)	2.233



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 153

QEKFUI01

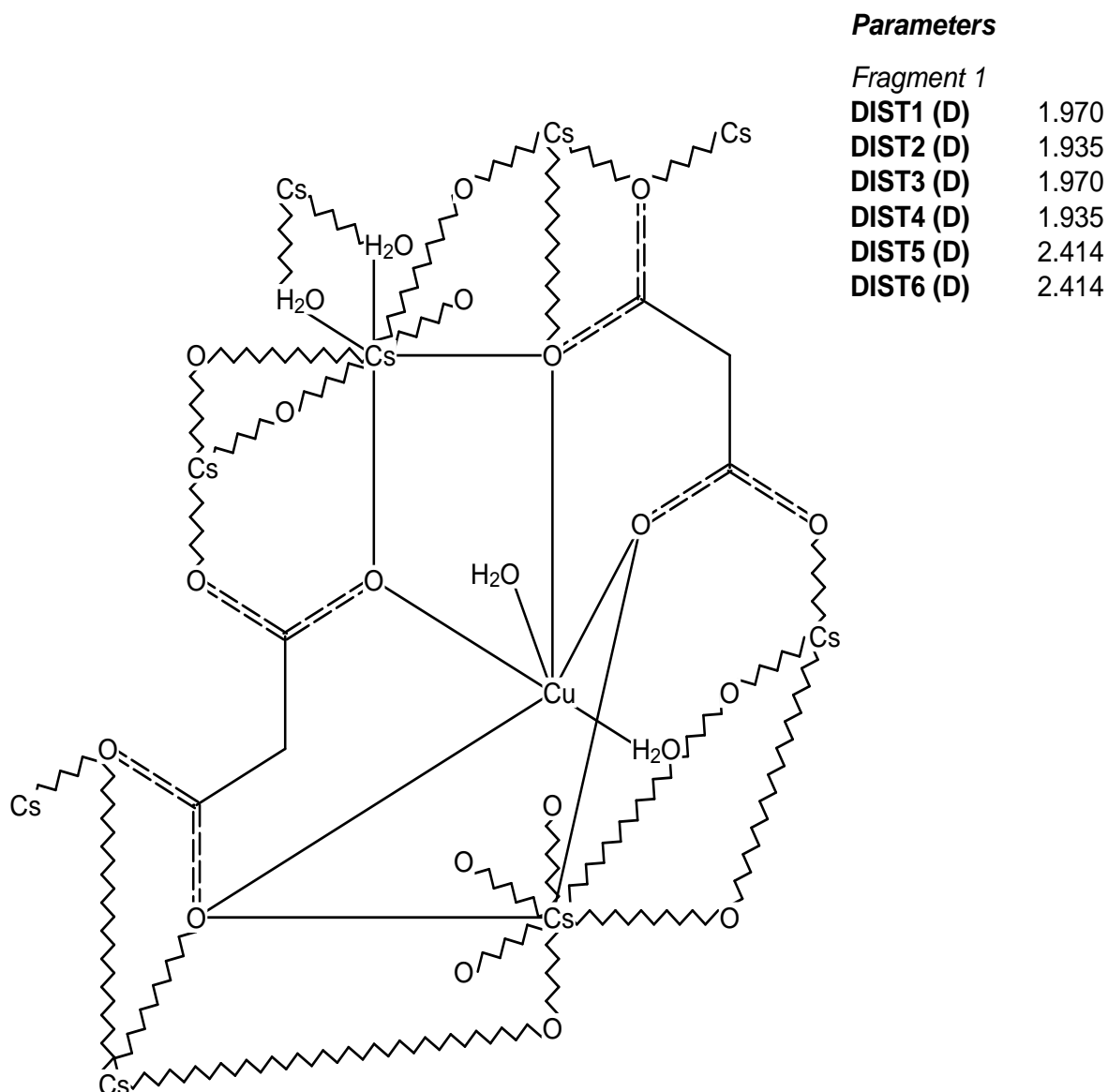
Reference: F.S.Delgado, C.Ruiz-Perez, J.Sanchiz, F.Lloret, M.Julve
(2006) *CrystEngComm*, **8**,507

Formula: $(C_6 H_{12} Cs_2 Cu_1 O_{12})_n$

Compound Name: catena-(bis((μ_6 -Malonato)-(μ_2 -aqua)-(aqua))-copper(ii)-di-cesium)

Space Group: P-1 **Cell:** **a** 7.117(0) **b** 7.132(0) **c** 7.521(0)
Space Group No.: 2 (**Å, °**) α 87.33(0) β 79.43(0) γ 86.70(0)

R-Factor (%): 2.87 **Temperature(K):** 293 **Density(g/cm³):** 2.686



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 154

QIGFER

Reference: D.V.Baxter, K.G.Caulton, Wen-Chung Chiang, M.H.Chisholm, V.F.DiStasi, S.G.Dutremez, J.D.Martin, W.E.Streib (2001) *New J.Chem.* ,**25**,400

Formula: (C₁₄ H₁₈ Cu₁ O₁₂)_n

Compound Name: catena-(bis(μ_2 -tris(Methoxycarbonyl)methanato-O,O',O'')-copper(ii))

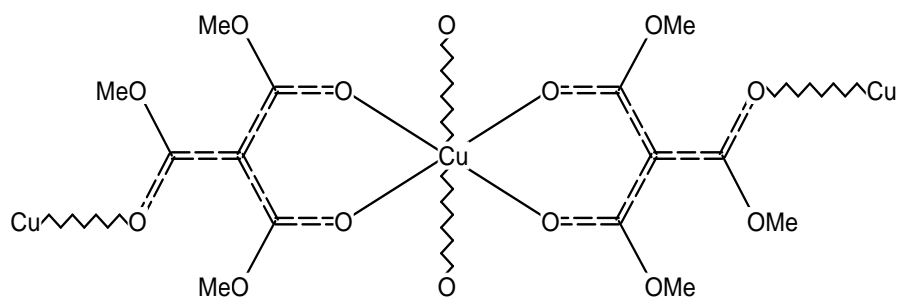
Space Group: P21/n **Cell:** **a** 6.622(0) **b** 10.554(0) **c** 13.220(1)
Space Group No.: 14 (**Å, °**) α 90.00 β 102.72(0) γ 90.00

R-Factor (%): 2.72 **Temperature(K):** 151 **Density(g/cm³):** 1.628

Parameters

Fragment 1

DIST1 (D) 1.912
DIST2 (D) 1.925
DIST3 (D) 1.912
DIST4 (D) 1.925
DIST5 (D) 2.584
DIST6 (D) 2.584



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 155

QIXNUI

Reference: Zhi-Kun Qu, Kai Yu, Zhi-Feng Zhao, Zhan-hua Su, Jing-Quan Sha, Chun-Mei Wang, Bai-Bin Zhou (2014) *Dalton Trans.* , 43,6744

Formula: (C₈₄ H₄₈ Cu₈ Mo₁₂ N₁₂ O₆₂)_n

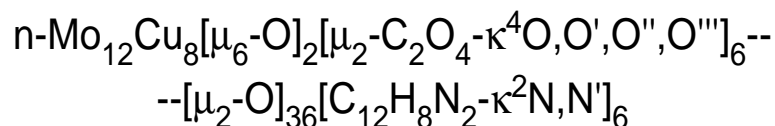
Compound Name: catena-[bis(μ₆-oxido)-hexakis(μ₂-oxalato)-hexatricontakis(μ₂-oxido)-hexakis(1,10-phenanthroline)-octa-copper-dodeca-molybdenum]

Space Group:	R-3c	Cell:	a 14.972(0)	b 14.972(0)	c 80.713(3)
Space Group No.:	167	(Å, °)	α 90.00	β 90.00	γ 120.00
R-Factor (%):	2.87	Temperature(K):	293	Density(g/cm³):	2.465

Parameters

Fragment 1

DIST1 (D)	2.080
DIST2 (D)	2.080
DIST3 (D)	2.080
DIST4 (D)	2.080
DIST5 (D)	2.080
DIST6 (D)	2.080



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 156

QQQEXG01

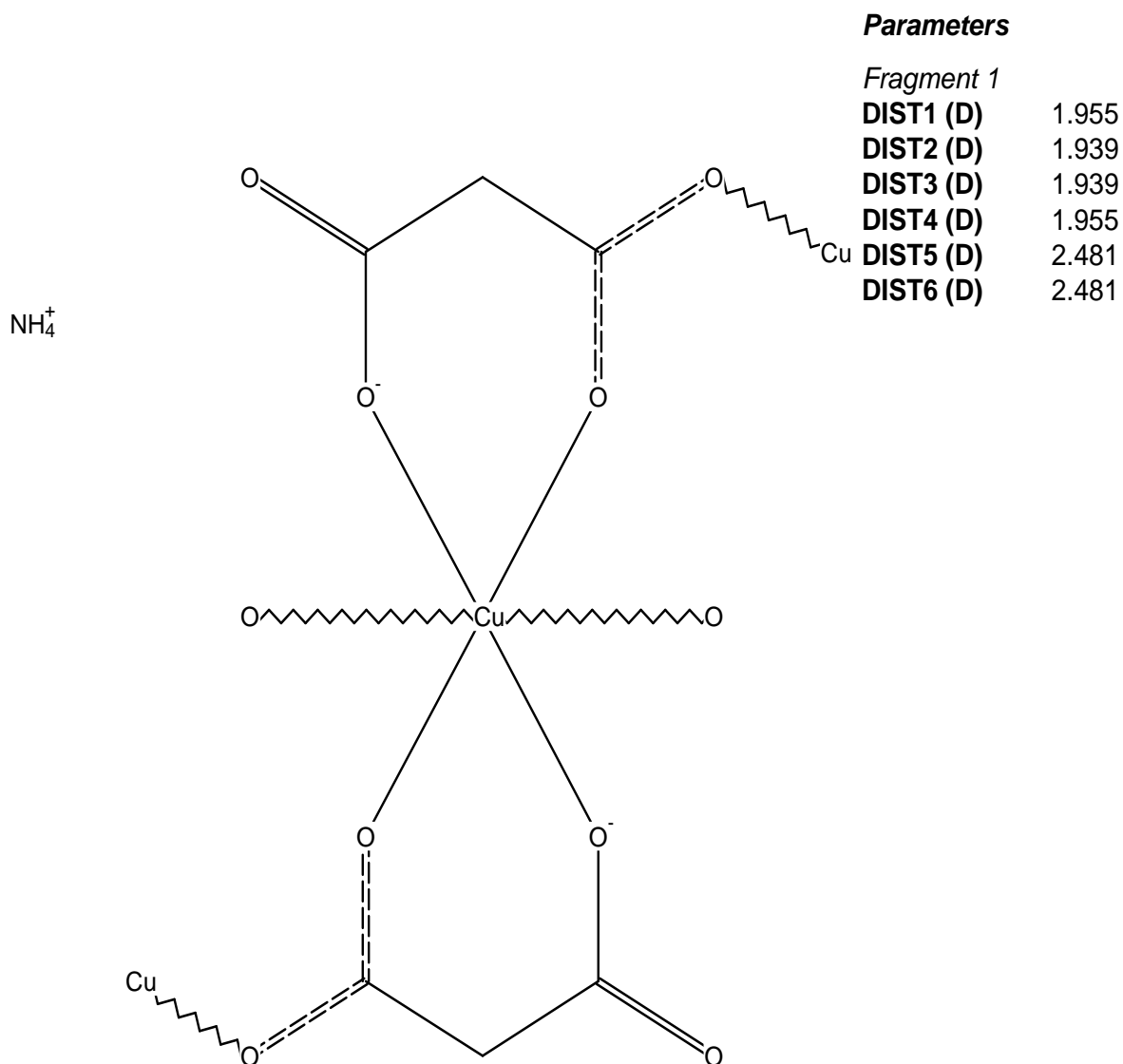
Reference: F.S.Delgado, C.Ruiz-Perez, J.Sanchiz, F.Lloret, M.Julve (2006) *CrystEngComm*, **8**,530

Formula: $(\text{H}_4 \text{N}_1^{1+})_2 \text{n}, \text{n}(\text{C}_6 \text{H}_4 \text{Cu}_1 \text{O}_8^{2-})$

Compound Name: catena-(Diammonium bis(μ_2 -malonato)-copper(ii))

Space Group: Fdd2 **Cell:** **a** 13.848(0) **b** 16.454(0) **c** 9.107(0)
Space Group No.: 43 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 1.97 **Temperature(K):** 293 **Density(g/cm³):** 1.944



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 157

QQQEXG02

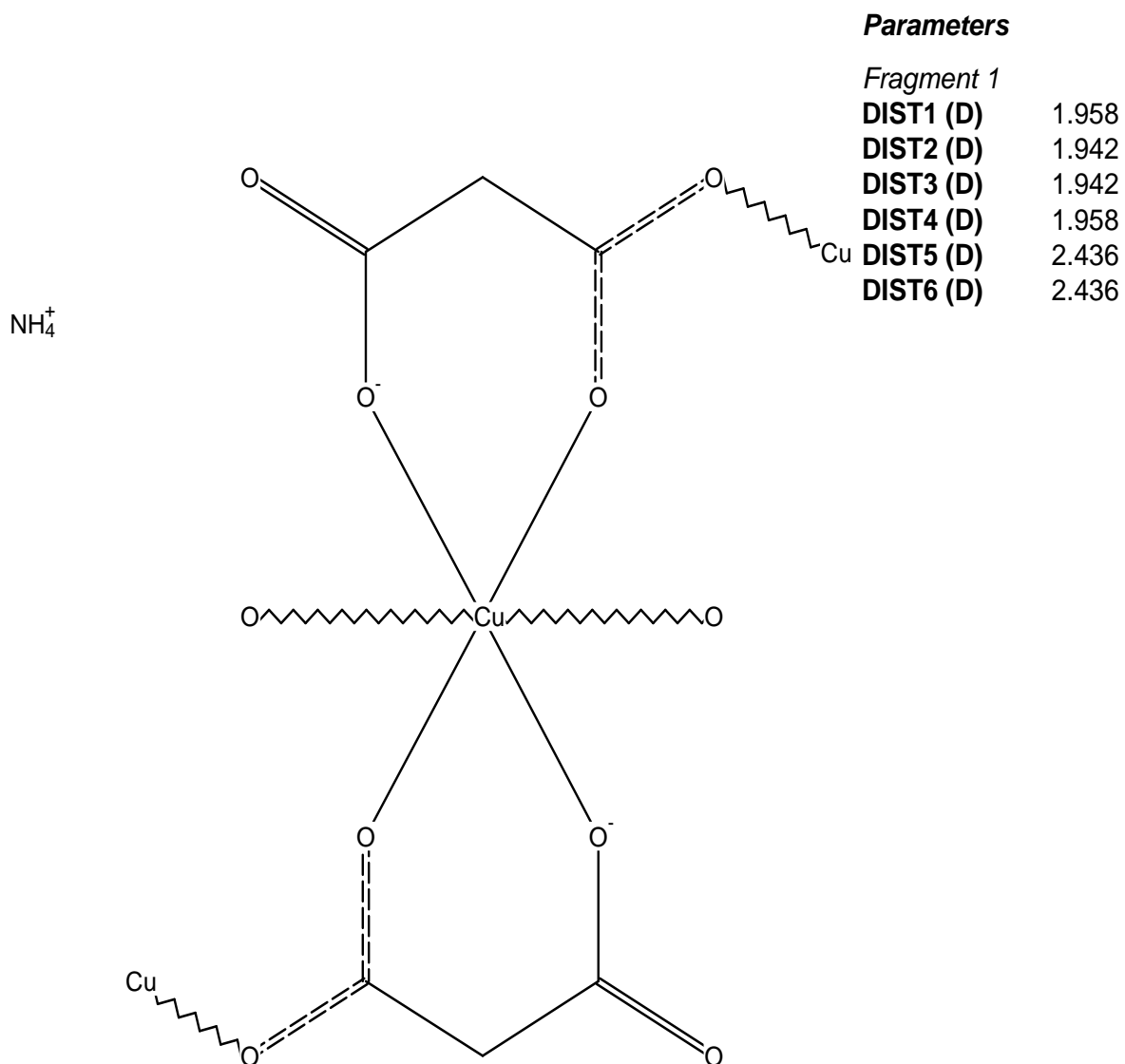
Reference: F.S.Delgado, C.Ruiz-Perez, J.Sanchiz, F.Lloret, M.Julve (2006) *CrystEngComm*, **8**,530

Formula: $(\text{H}_4 \text{N}_1^{1+})_2 \text{n}, \text{n}(\text{C}_6 \text{H}_4 \text{Cu}_1 \text{O}_8^{2-})$

Compound Name: catena-(Diammonium bis(μ_2 -malonato)-copper(ii))

Space Group: Fdd2 **Cell:** **a** 13.656(1) **b** 16.444(0) **c** 9.088(0)
Space Group No.: 43 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.26 **Temperature(K):** 100 **Density(g/cm³):** 1.977



QUTQAZ

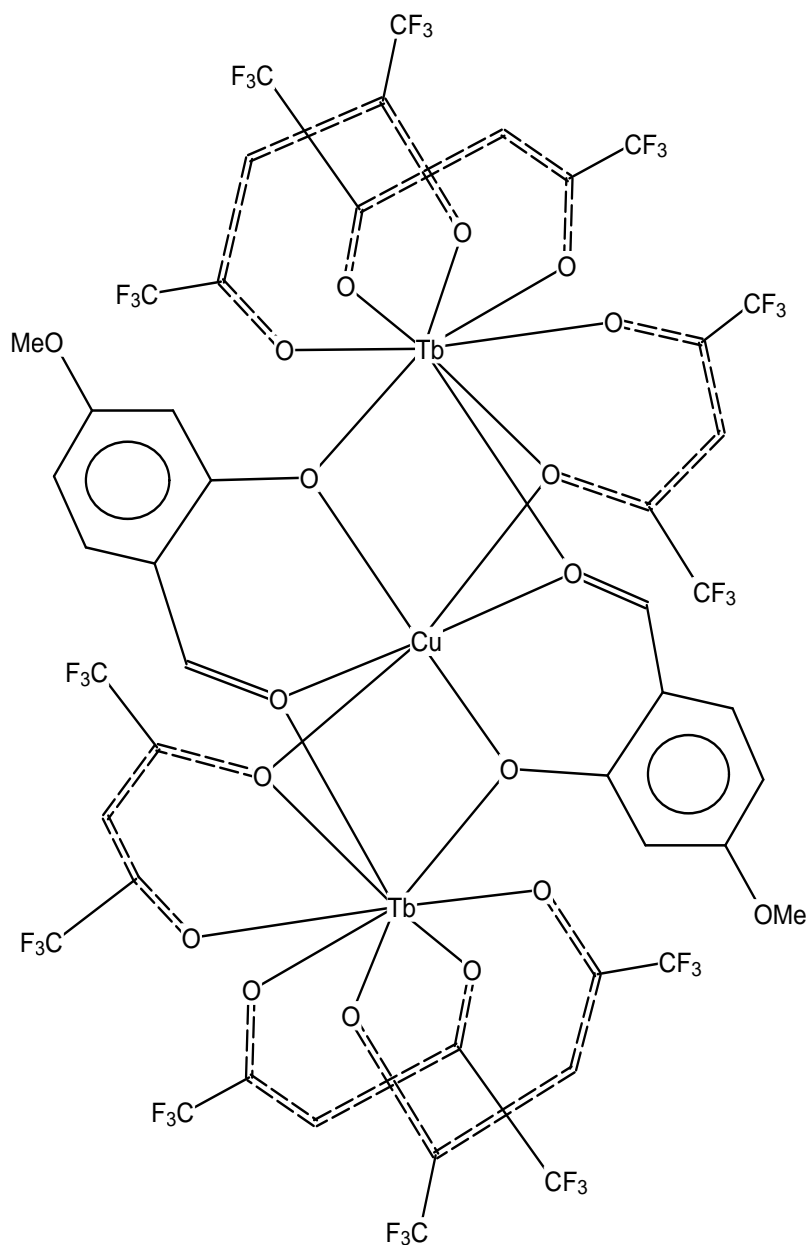
Reference: Junqing Zhang, Cun Li, Juanjuan Wang, Mei Zhu, Licun Li (2016) *Eur.J.Inorg.Chem.* ,1383

Formula: C₄₆ H₂₀ Cu₁ F₃₆ O₁₈ Tb₂

Compound Name: bis(μ₃-2-Oxy-4-methoxybenzaldehyde)-bis(μ₂-hexafluoroacetylacetonato-O,O')-tetrakis(hexafluoroacetylacetonato)-copper-di-terbium

Space Group: P-1 **Cell:** **a** 9.881(2) **b** 11.136(2) **c** 15.946(3)
Space Group No.: 2 **(Å, °)** α 100.44(3) β 99.11(3) γ 113.24(3)

R-Factor (%): 2.67 **Temperature(K):** 113 **Density(g/cm³):** 2.086



Parameters

Fragment 1	
DIST1 (D)	1.912
DIST2 (D)	1.946
DIST3 (D)	1.912
DIST4 (D)	1.946
DIST5 (D)	2.487
DIST6 (D)	2.487

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 159

QUTQED

Reference: Junqing Zhang, Cun Li, Juanjuan Wang, Mei Zhu, Licun Li (2016) *Eur.J.Inorg.Chem.* ,1383

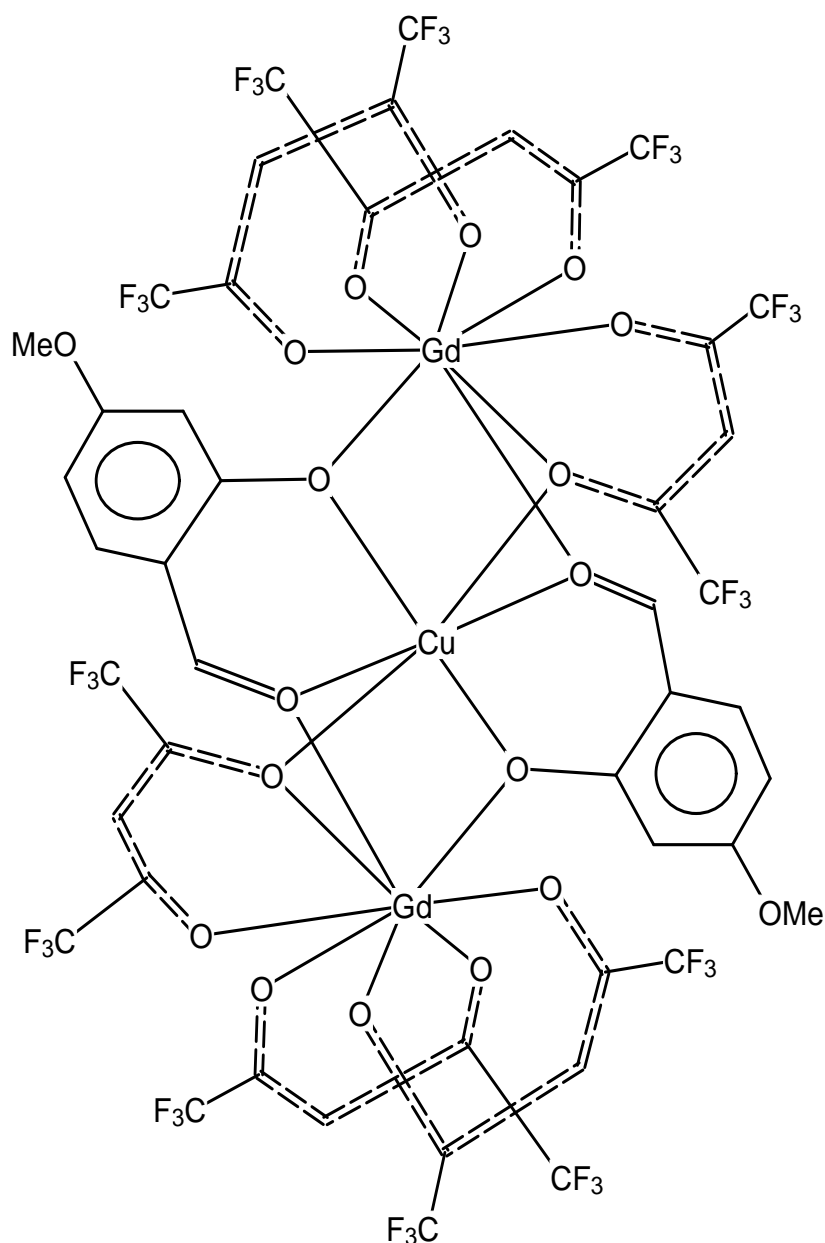
Formula: C₄₆ H₂₀ Cu₁ F₃₆ Gd₂ O₁₈

Compound Name: bis(μ_3 -2-Oxy-4-methoxybenzaldehyde)-bis(μ_2 -hexafluoroacetylacetonato-O,O')-tetrakis(hexafluoroacetylacetonato)-copper-di-gadolinium

Space Group: P-1 **Cell:** **a** 9.879(2) **b** 11.137(3) **c** 15.918(4)

Space Group No.: 2 **(Å, °)** α 100.33(0) β 98.88(0) γ 113.42(0)

R-Factor (%): 2.20 **Temperature(K):** 113 **Density(g/cm³):** 2.086



Parameters

Fragment 1

DIST1 (D)	1.906
DIST2 (D)	1.945
DIST3 (D)	1.906
DIST4 (D)	1.945
DIST5 (D)	2.482
DIST6 (D)	2.482

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 160

QUXKUQ

Reference: M.T.M.Al-Dajani, H.H.Abdallah, N.Mohamed,
M.Hemamalini, H.-K.Fun (2010)
Acta Crystallogr., Sect.E: Struct.Rep.Online ,**66**,m774

Formula: C₈ H₁₄ Cu₁ O₁₄·2(H₂ O₁)

Compound Name: Diaqua-bis(hydrogen tartrato)-copper(ii) dihydrate

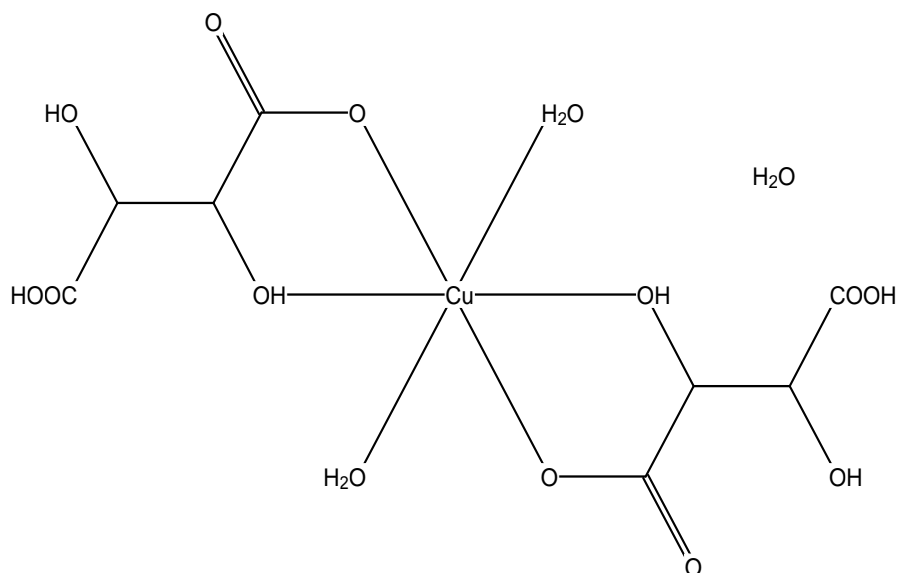
Space Group: P21/c **Cell:** **a** 7.158(0) **b** 14.099(1) **c** 7.891(0)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 109.14(0) **γ** 90.00

R-Factor (%): 2.31 **Temperature(K):** 100 **Density(g/cm³):** 1.915

Parameters

Fragment 1

DIST1 (D)	1.933
DIST2 (D)	1.964
DIST3 (D)	1.964
DIST4 (D)	1.933
DIST5 (D)	2.465
DIST6 (D)	2.465



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 161

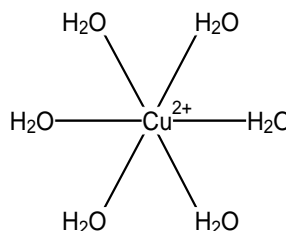
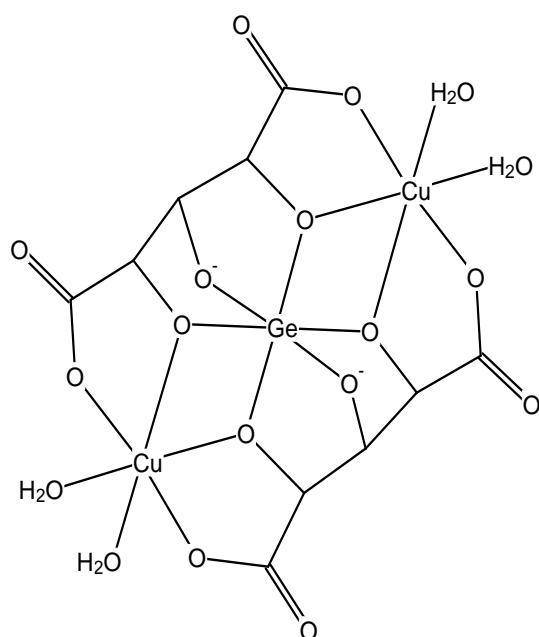
RAGXAA

Reference: E.E.Martsinko, A.G.Pesaroglo, L.Kh.Minacheva, I.I.Seifullina, V.S.Sergienko, A.V.Churakov (2011) *Zh.Neorg.Khim.(Russ.)(Russ.J.Inorg.Chem.)*, **56**,228

Formula: $H_{12} Cu_1 O_6^{2+}, C_{10} H_{14} Cu_2 Ge_1 O_{18}^{2-}, 4(H_2 O_1)$

Compound Name: Hexa-aqua-copper(ii) bis(μ_3 -triolatoglutarato)-tetra-aqua-di-copper(ii)-germanium(iv) tetrahydrate

Space Group: P21/n **Cell:** **a** 10.216(2) **b** 12.272(3) **c** 10.679(2)
Space Group No.: 14 **(Å, °)** α 90.00 β 93.13(3) γ 90.00
R-Factor (%): 2.61 **Temperature(K):** 100 **Density(g/cm³):** 2.150



H₂O

Parameters

Fragment 1

DIST1 (D) 1.948
DIST2 (D) 1.938
DIST3 (D) 1.948
DIST4 (D) 1.938
DIST5 (D) 2.515
DIST6 (D) 2.515

Fragment 2

DIST1 (D) 1.984
DIST2 (D) 1.950
DIST3 (D) 2.004
DIST4 (D) 1.976
DIST5 (D) 2.481
DIST6 (D) 2.364

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 162

RELCUG01

Reference: J.Bebendorf, H.-B.Burgi, E.Gamp, M.A.Hitchman, A.Murphy, D.Reinen, M.J.Riley, H.Stratemeier (1996) *Inorg.Chem.* ,**35**, 7419

Formula: C₁₂ H₂₄ Cu₁ O₆²⁺, 2(C₇ H₇ O₃ S₁¹⁻)

Compound Name: bis(1,3,5-Trihydroxycyclohexane)-copper(ii) ditosylate

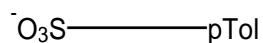
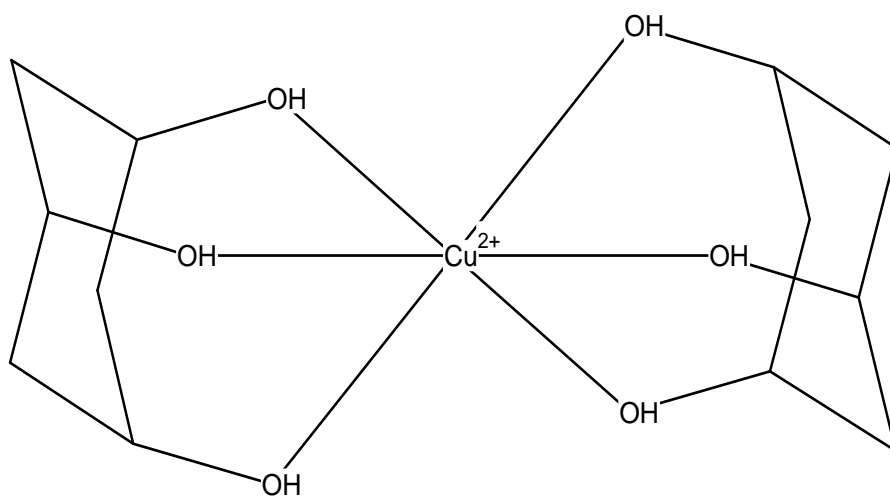
Space Group: P-1 **Cell:** **a** 6.385(4) **b** 9.401(7) **c** 12.410(9)
Space Group No.: 2 (**Å, °**) **α** 76.82(6) **β** 87.68(5) **γ** 77.06(6)

R-Factor (%): 2.60 **Temperature(K):** 93 **Density(g/cm³):** 1.575

Parameters

Fragment 1

DIST1 (D)	1.968
DIST2 (D)	2.022
DIST3 (D)	1.968
DIST4 (D)	2.022
DIST5 (D)	2.223
DIST6 (D)	2.223



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 163

ROLCEC

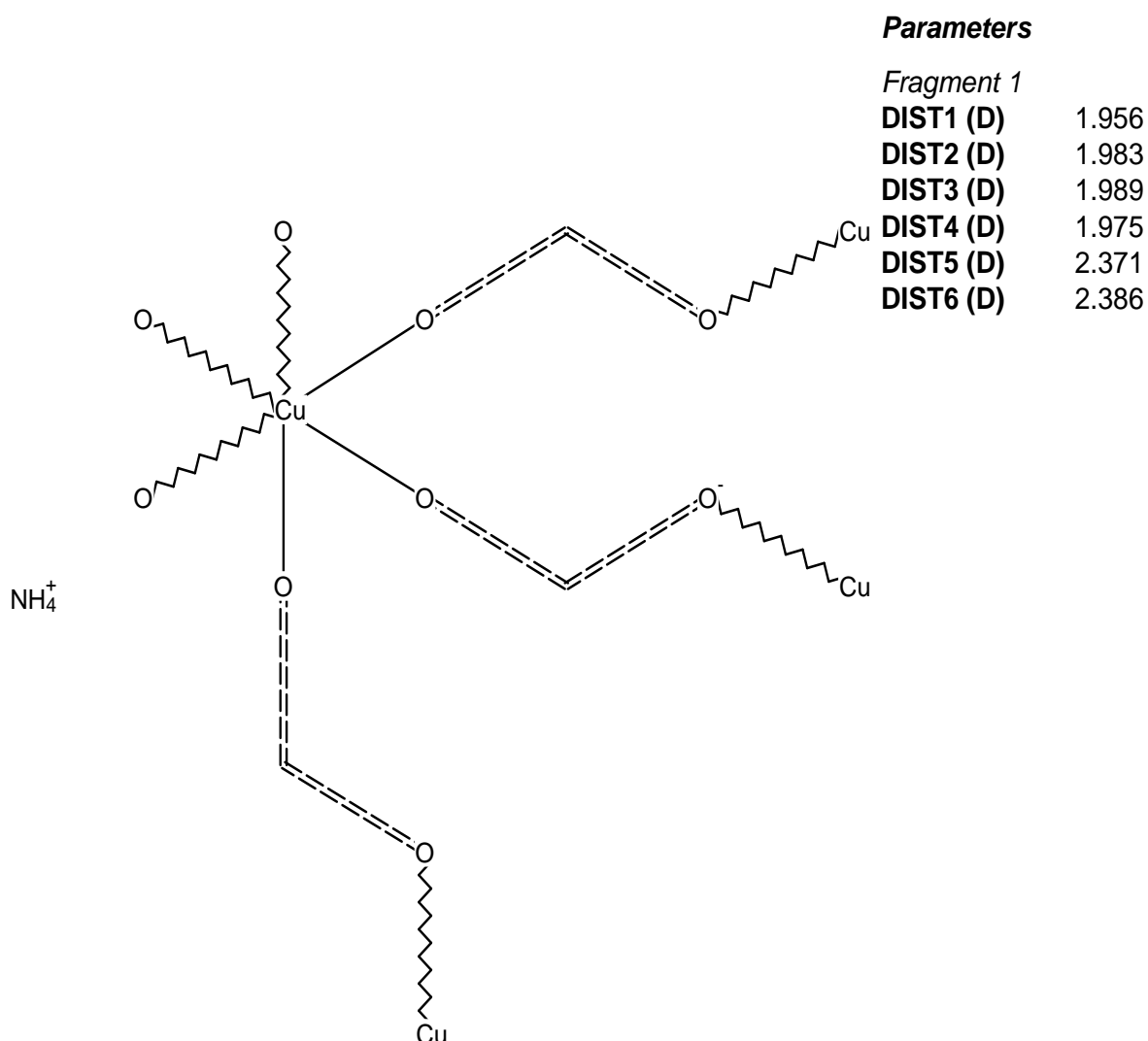
Reference: Ran Shang, Sa Chen, Zhe-Ming Wang, Song Gao (2014)
Chem.-Eur.J., **20**,15872

Formula: $(C_3 H_3 Cu_1 O_6^{1-})_n, H_4 N_1^{1+}$

Compound Name: catena-(Ammonium tris(μ -formato)-copper)

Space Group: P212121 **Cell:** **a** 7.020(0) **b** 13.369(0) **c** 8.068(0)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.59 **Temperature(K):** 94 **Density(g/cm³):** 1.900



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 164

ROLCEC01

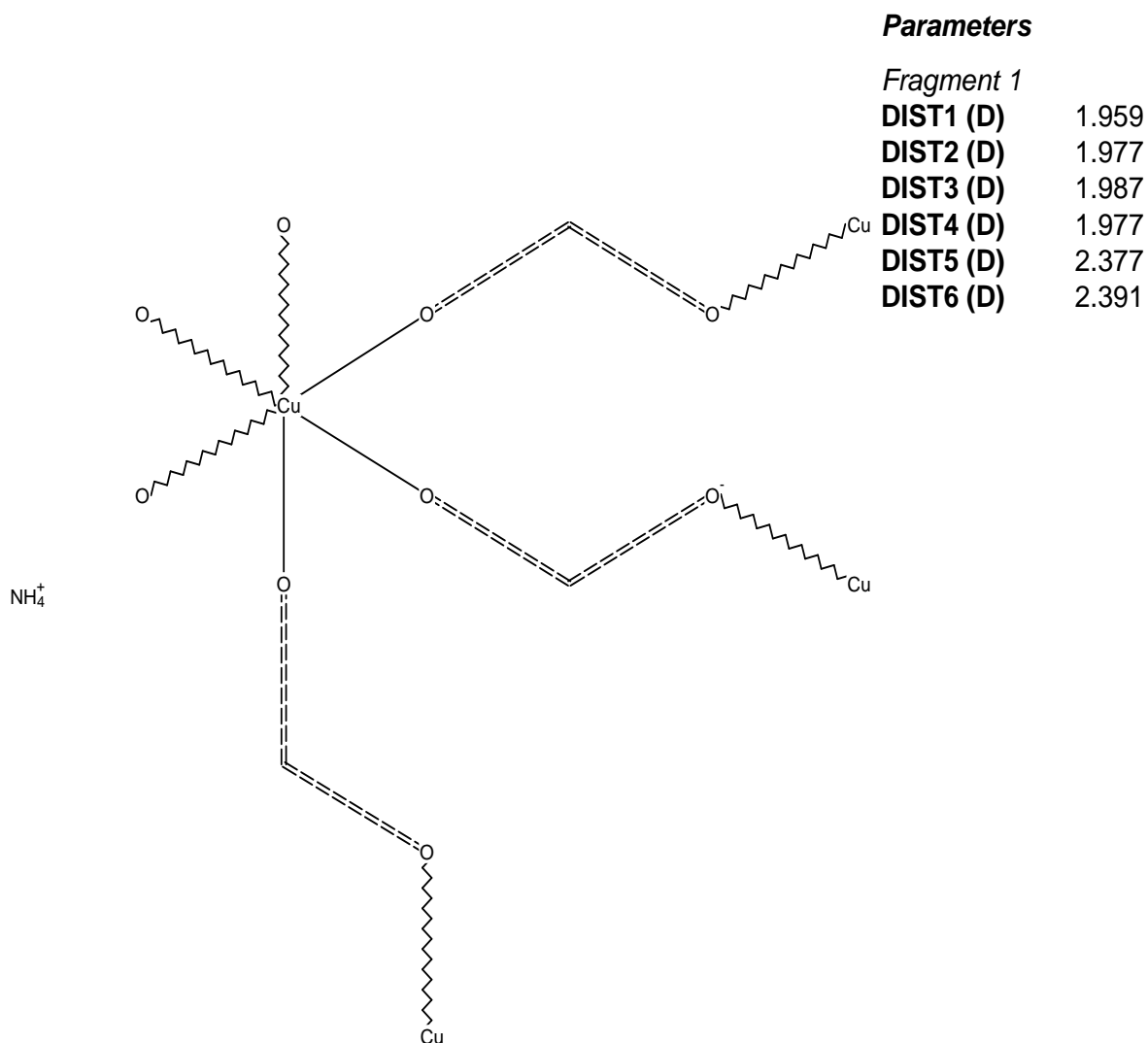
Reference: Ran Shang, Sa Chen, Zhe-Ming Wang, Song Gao (2014)
Chem.-Eur.J., **20**,15872

Formula: $(C_3 H_3 Cu_1 O_6^{1-})_n, H_4 N_1^{1+}$

Compound Name: catena-(Ammonium tris(μ -formato)-copper)

Space Group: P212121 **Cell:** **a** 7.030(0) **b** 13.349(0) **c** 8.077(0)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.46 **Temperature(K):** 140 **Density(g/cm³):** 1.898



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 165

ROLCEC02

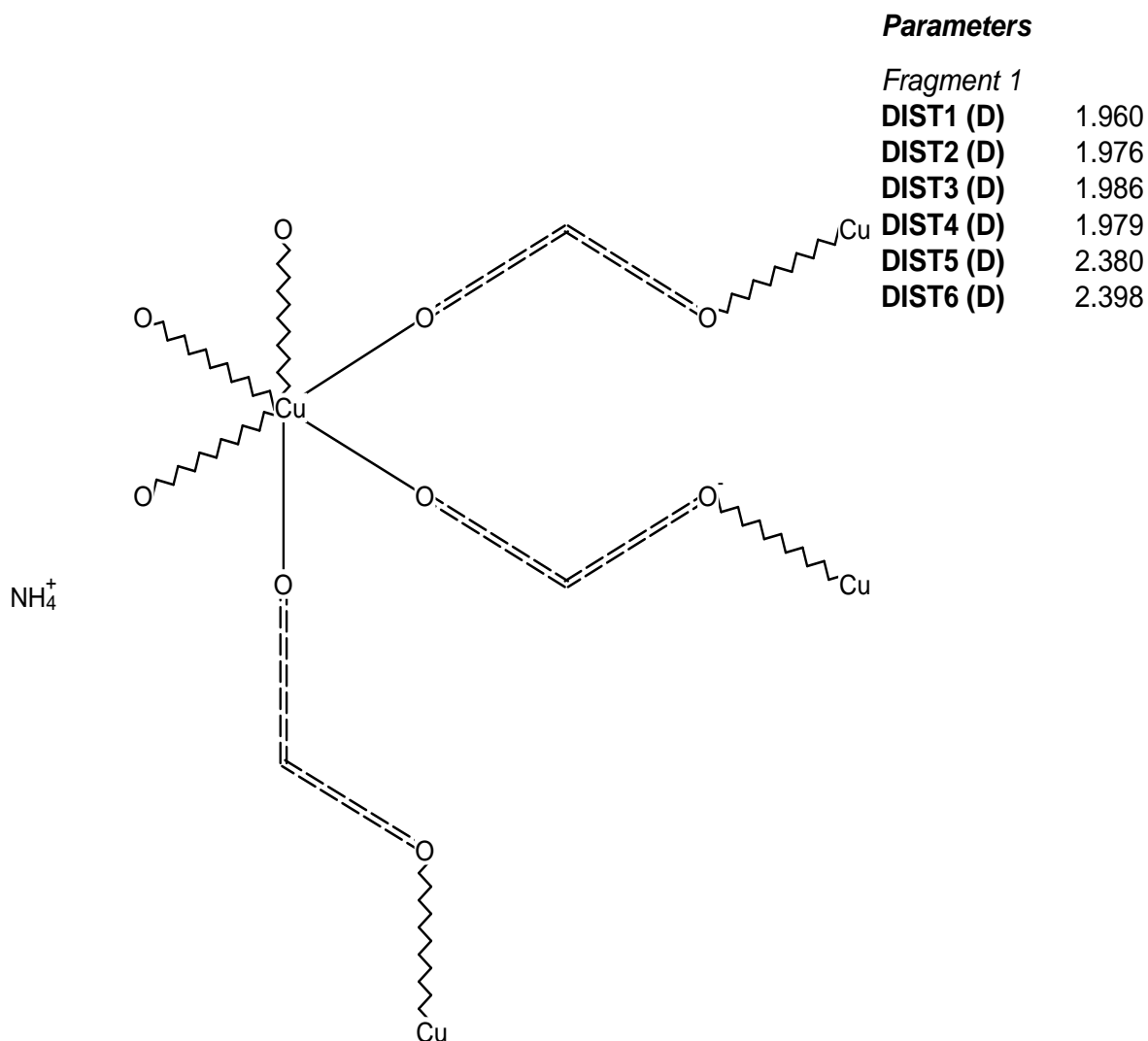
Reference: Ran Shang, Sa Chen, Zhe-Ming Wang, Song Gao (2014)
Chem.-Eur.J., **20**,15872

Formula: $(C_3 H_3 Cu_1 O_6^{1-})_n, H_4 N_1^{1+}$

Compound Name: catena-(Ammonium tris(μ -formato)-copper)

Space Group: P212121 **Cell:** **a** 7.046(0) **b** 13.301(0) **c** 8.085(0)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.74 **Temperature(K):** 180 **Density(g/cm³):** 1.899



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 166

ROLCEC03

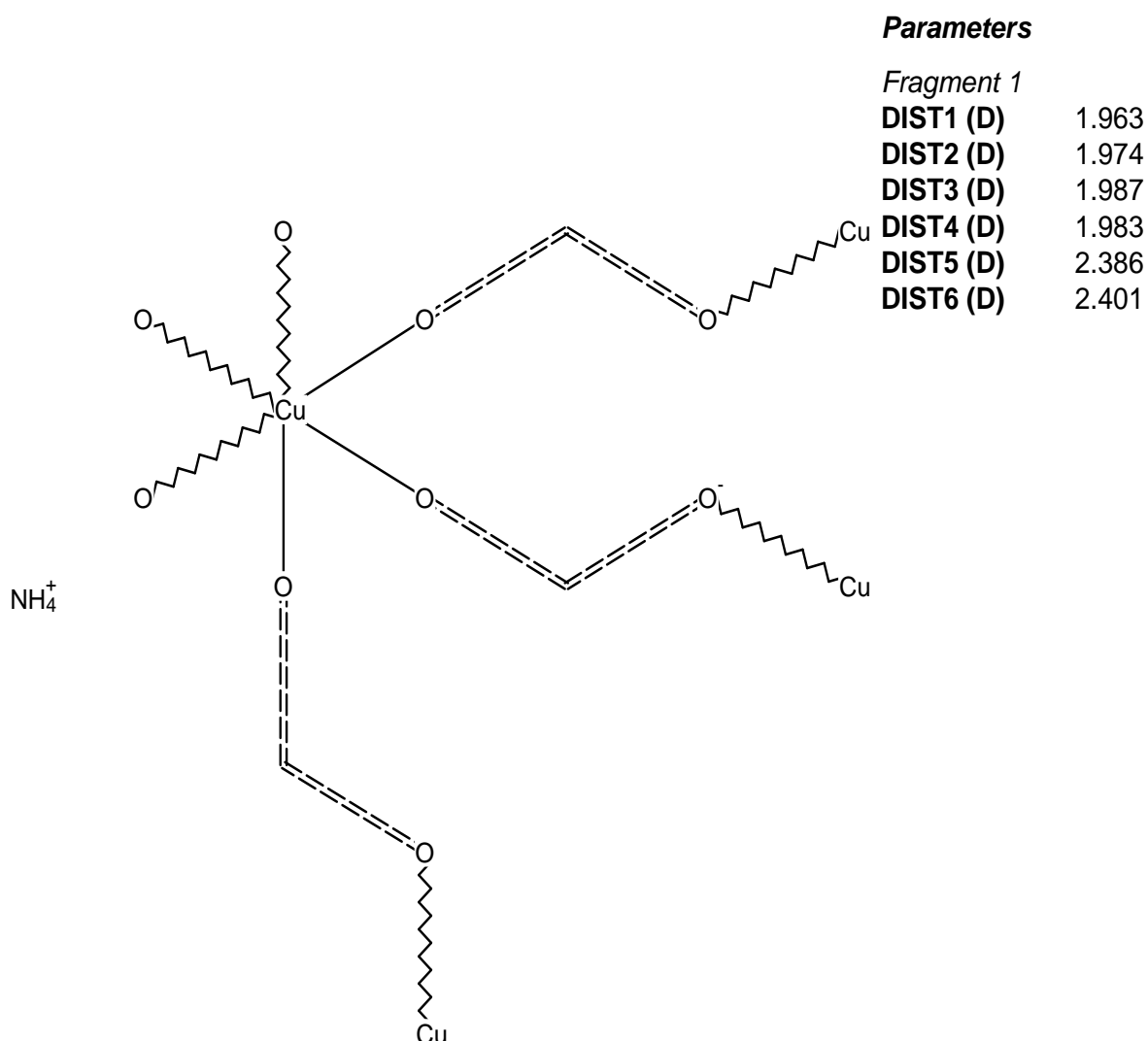
Reference: Ran Shang, Sa Chen, Zhe-Ming Wang, Song Gao (2014)
Chem.-Eur.J., **20**,15872

Formula: $(C_3 H_3 Cu_1 O_6^{1-})_n, H_4 N_1^{1+}$

Compound Name: catena-(Ammonium tris(μ -formato)-copper)

Space Group: P212121 **Cell:** **a** 7.065(0) **b** 13.247(0) **c** 8.103(0)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.59 **Temperature(K):** 200 **Density(g/cm³):** 1.897



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 167

ROLCEC04

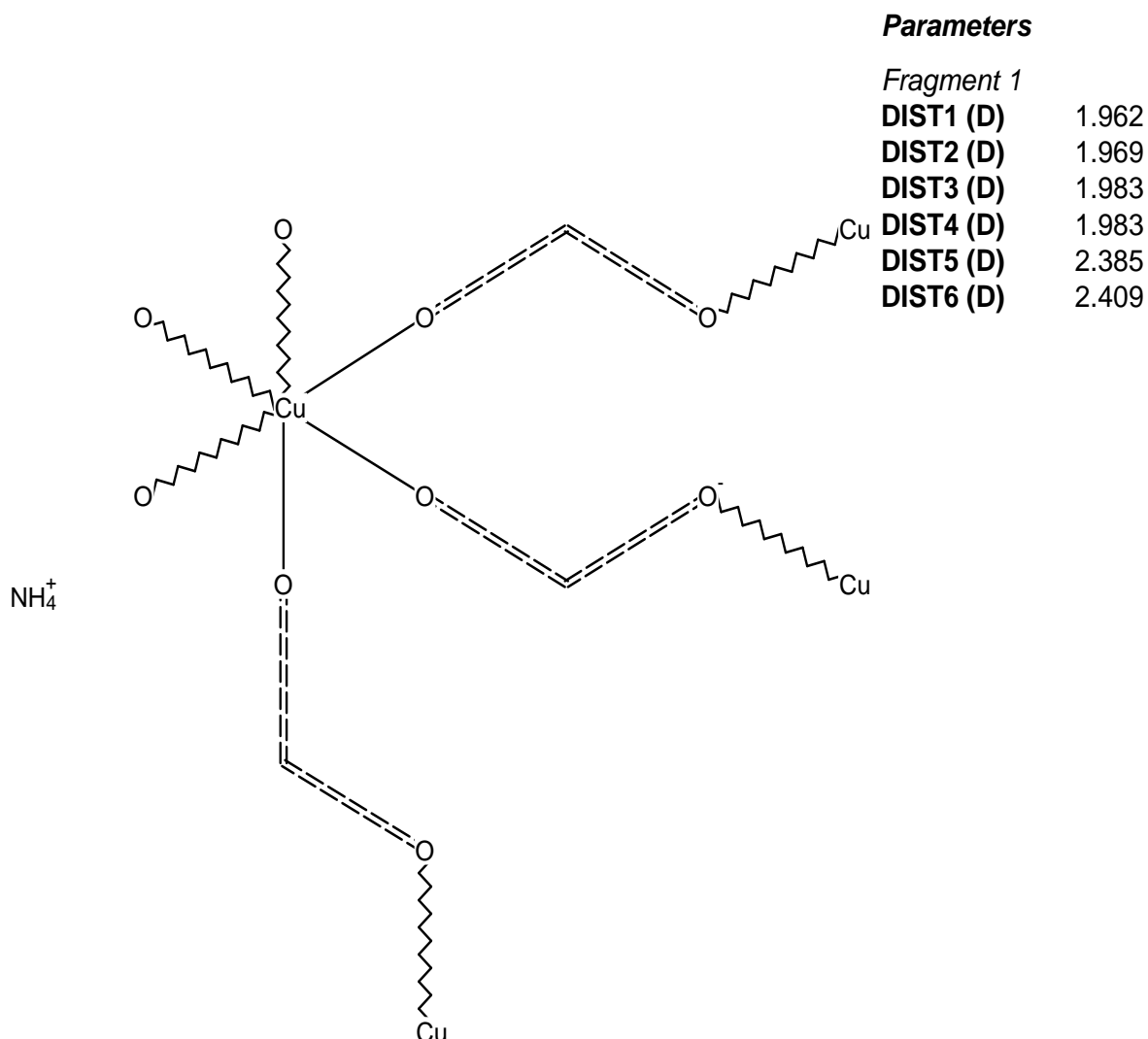
Reference: Ran Shang, Sa Chen, Zhe-Ming Wang, Song Gao (2014)
Chem.-Eur.J., **20**,15872

Formula: $(C_3 H_3 Cu_1 O_6^{1-})_n, H_4 N_1^{1+}$

Compound Name: catena-(Ammonium tris(μ -formato)-copper)

Space Group: P212121 **Cell:** **a** 7.095(0) **b** 13.148(0) **c** 8.123(0)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.64 **Temperature(K):** 220 **Density(g/cm³):** 1.899



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 168

ROLCEC05

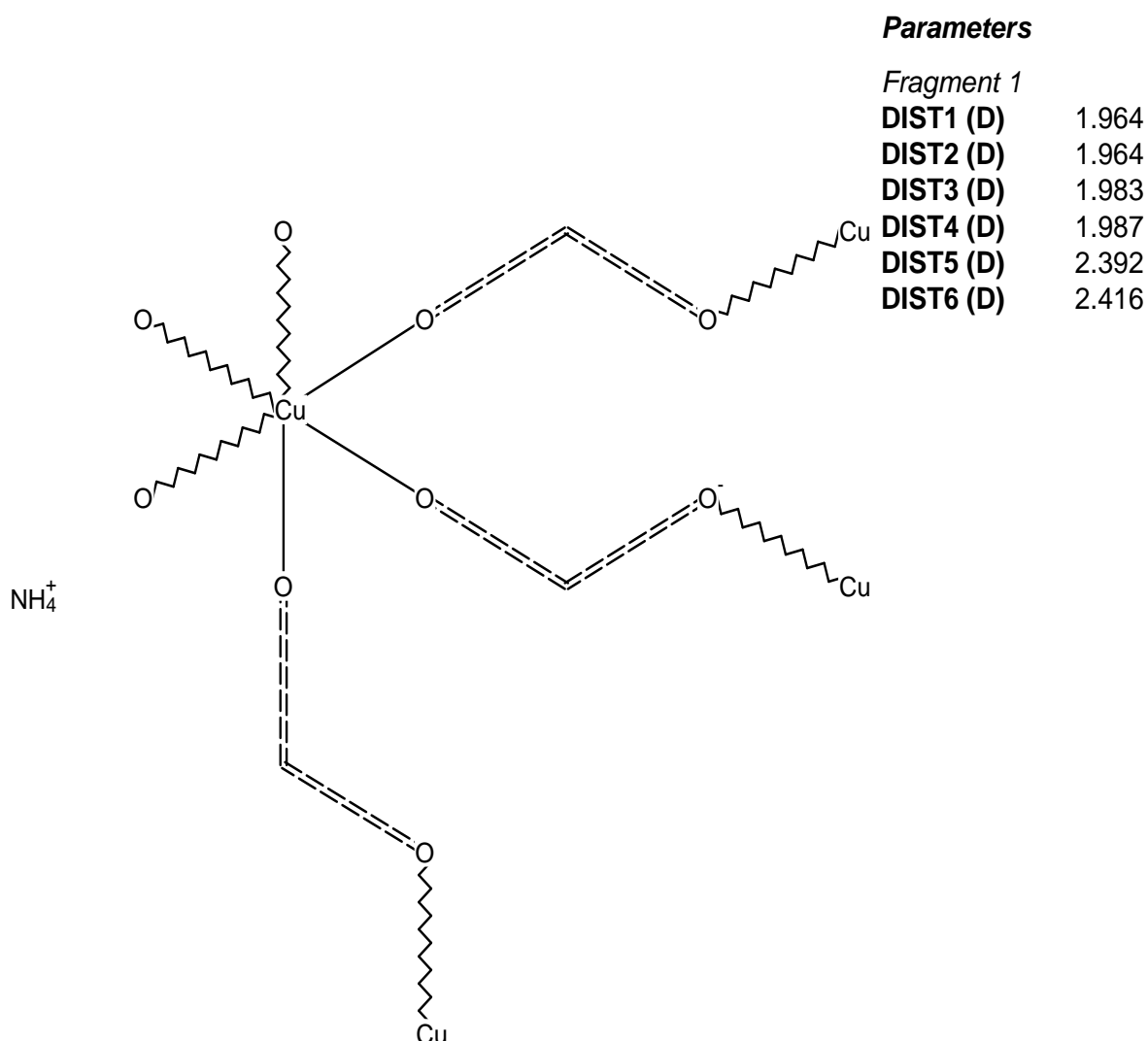
Reference: Ran Shang, Sa Chen, Zhe-Ming Wang, Song Gao (2014)
Chem.-Eur.J., **20**,15872

Formula: $(C_3 H_3 Cu_1 O_6^{1-})_n, H_4 N_1^{1+}$

Compound Name: catena-(Ammonium tris(μ -formato)-copper)

Space Group: P212121 **Cell:** **a** 7.128(0) **b** 13.050(0) **c** 8.141(0)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.70 **Temperature(K):** 240 **Density(g/cm³):** 1.900



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 169

ROLCEC06

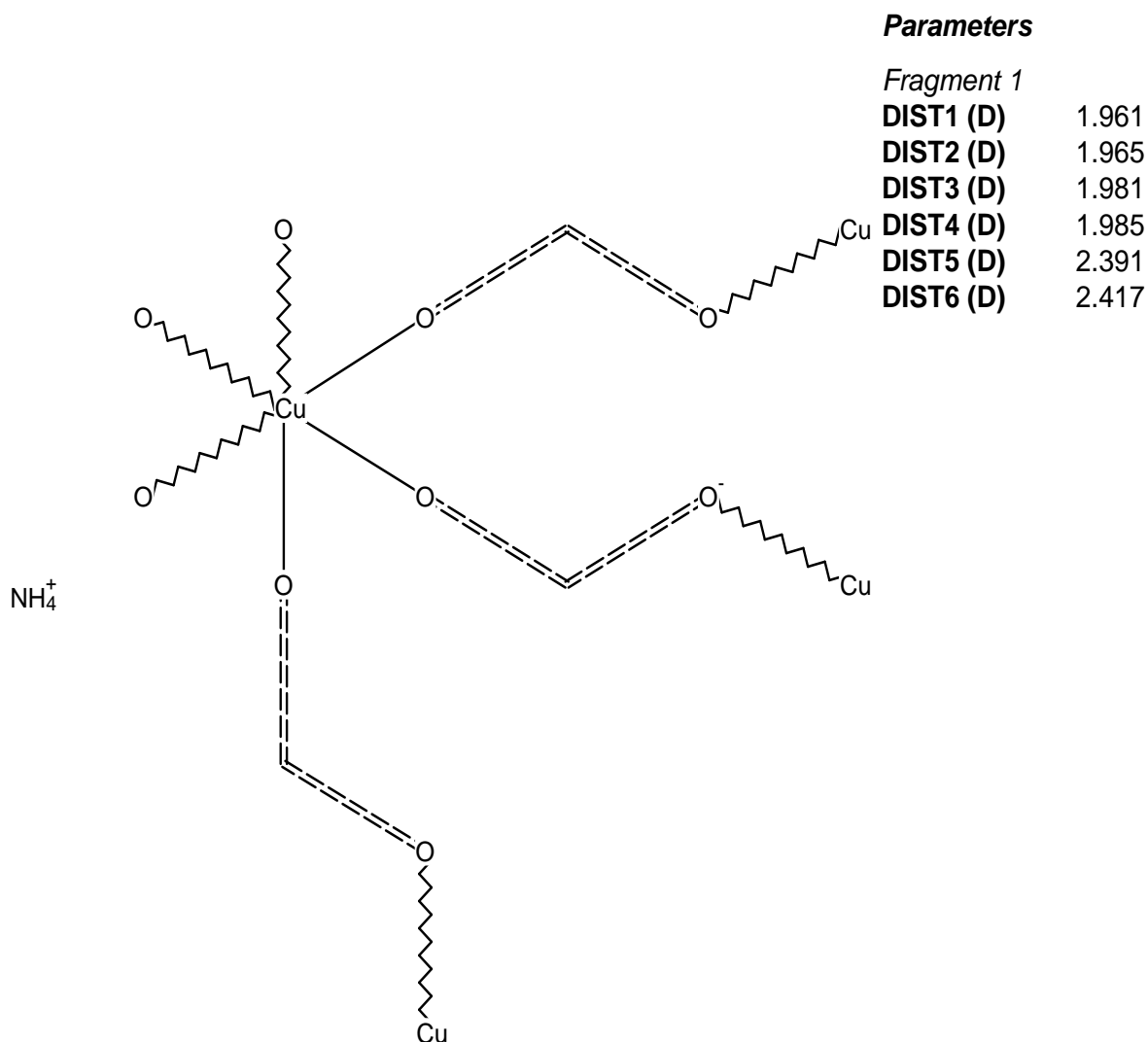
Reference: Ran Shang, Sa Chen, Zhe-Ming Wang, Song Gao (2014)
Chem.-Eur.J., **20**,15872

Formula: $(C_3 H_3 Cu_1 O_6^{1-})_n, H_4 N_1^{1+}$

Compound Name: catena-(Ammonium tris(μ -formato)-copper)

Space Group: P212121 **Cell:** **a** 7.151(0) **b** 13.000(0) **c** 8.145(0)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.81 **Temperature(K):** 260 **Density(g/cm³):** 1.901



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 170

ROLCEC07

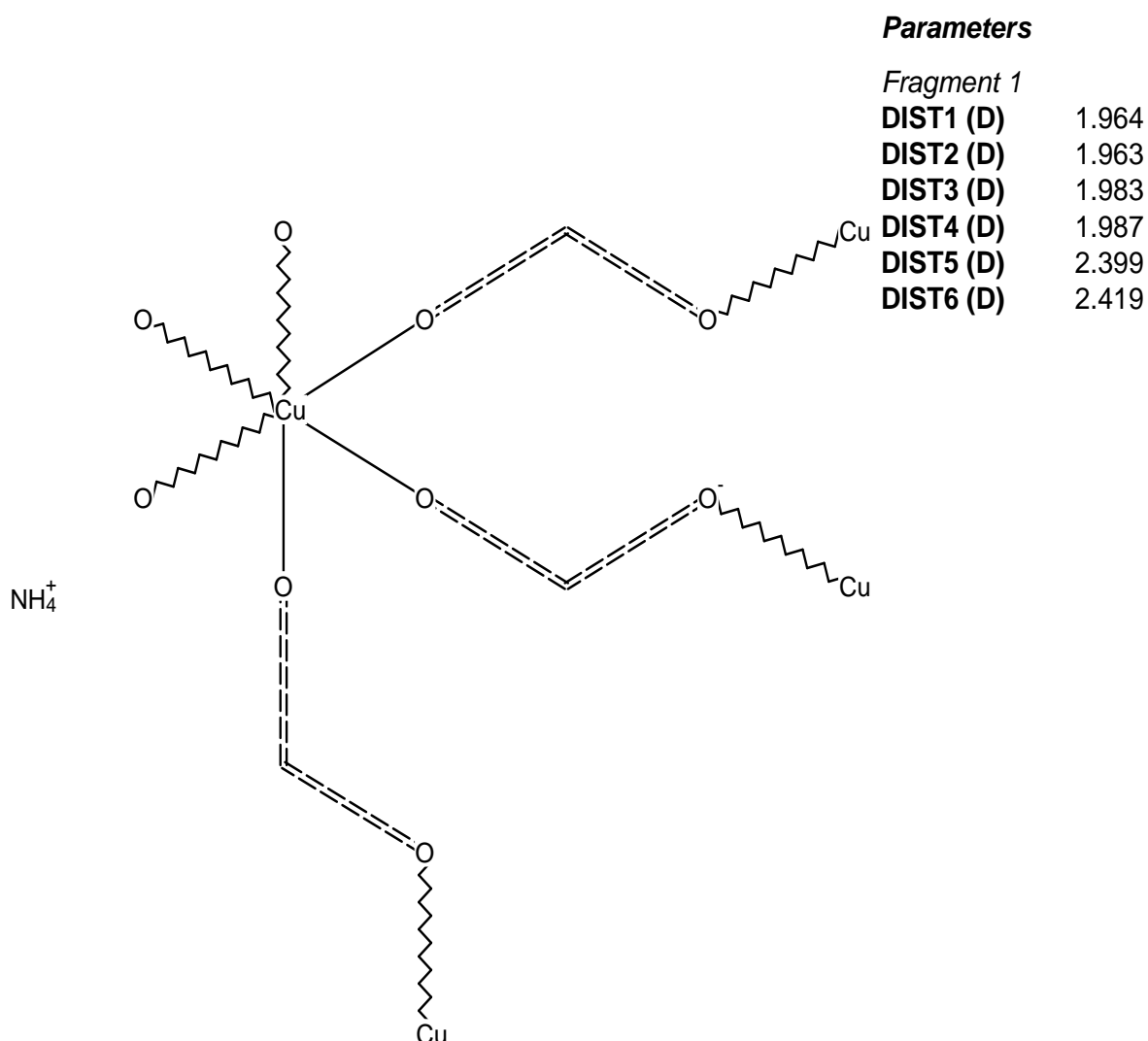
Reference: Ran Shang, Sa Chen, Zhe-Ming Wang, Song Gao (2014)
Chem.-Eur.J., **20**,15872

Formula: $(C_3 H_3 Cu_1 O_6^{1-})_n, H_4 N_1^{1+}$

Compound Name: catena-(Ammonium tris(μ -formato)-copper)

Space Group: P212121 **Cell:** **a** 7.171(0) **b** 12.964(0) **c** 8.143(0)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.83 **Temperature(K):** 290 **Density(g/cm³):** 1.901



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 171

ROLSAN

Reference: Zhiqin Ji, Shaopeng Wei, Wenjun Wu (2009)
Acta Crystallogr., Sect. E: Struct. Rep. Online ,65,m182

Formula: C₁₆ H₂₈ Cu₁ N₂ O₁₀

Compound Name: bis(4-Ammonio-4-methylpentan-2-one)-bis(oxalato-O,O')-copper(ii)

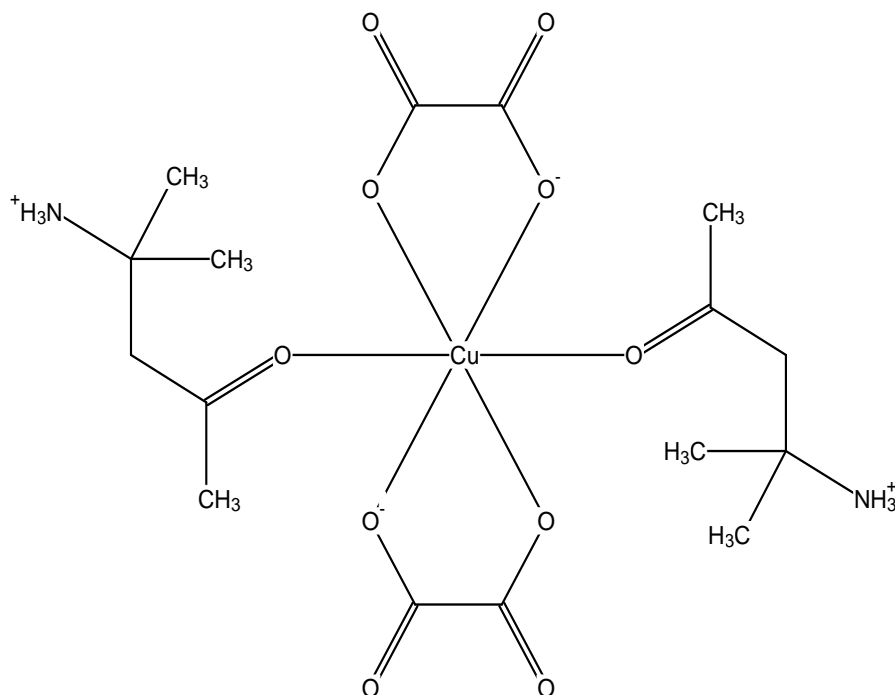
Space Group: C2/m **Cell:** **a** 13.639(3) **b** 7.975(1) **c** 10.958(2)
Space Group No.: 12 **(Å, °)** **α** 90.00 **β** 113.27(3) **γ** 90.00

R-Factor (%): 2.62 **Temperature(K):** 113 **Density(g/cm³):** 1.431

Parameters

Fragment 1

DIST1 (D)	1.938
DIST2 (D)	1.938
DIST3 (D)	1.938
DIST4 (D)	1.938
DIST5 (D)	2.663
DIST6 (D)	2.663



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 172

RUSPEB

Reference: Xiao-Hua Xie, Bai-Mu Wang, S.W.Ng (2010)
Acta Crystallogr., Sect. E: Struct. Rep. Online ,**66**,m271

Formula: C₁₂ H₃₂ Cu₂ N₂ O₂₇ Ti₂·7(H₂ O₁)

Compound Name: bis(μ_2 -Nitrilotriacetato)-(μ_2 -oxo)-bis(peroxo-O,O')-deca-aqua-di-copper(ii)-di-titanium(iv) heptahydrate

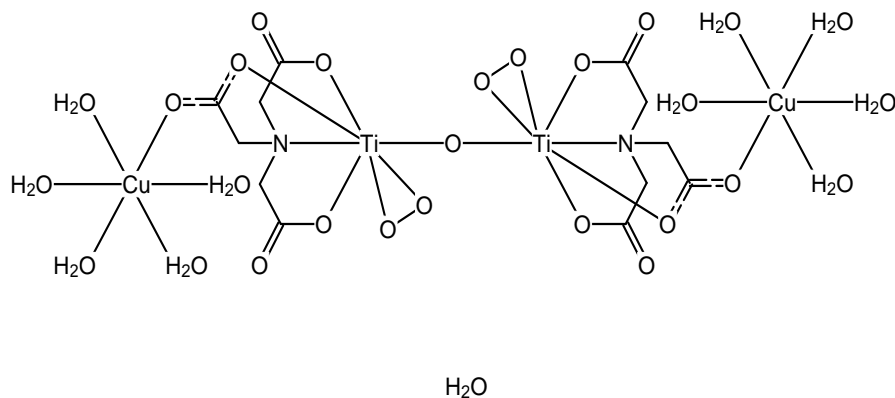
Space Group: C2/c **Cell:** **a** 14.931(1) **b** 13.289(0) **c** 17.445(1)
Space Group No.: 15 **(Å, °)** α 90.00 β 100.83(0) γ 90.00

R-Factor (%): 2.58 **Temperature(K):** 293 **Density(g/cm³):** 1.925

Parameters

Fragment 1

DIST1 (D)	1.986
DIST2 (D)	2.016
DIST3 (D)	1.964
DIST4 (D)	1.931
DIST5 (D)	2.269
DIST6 (D)	2.446



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 173

RUWMUR03

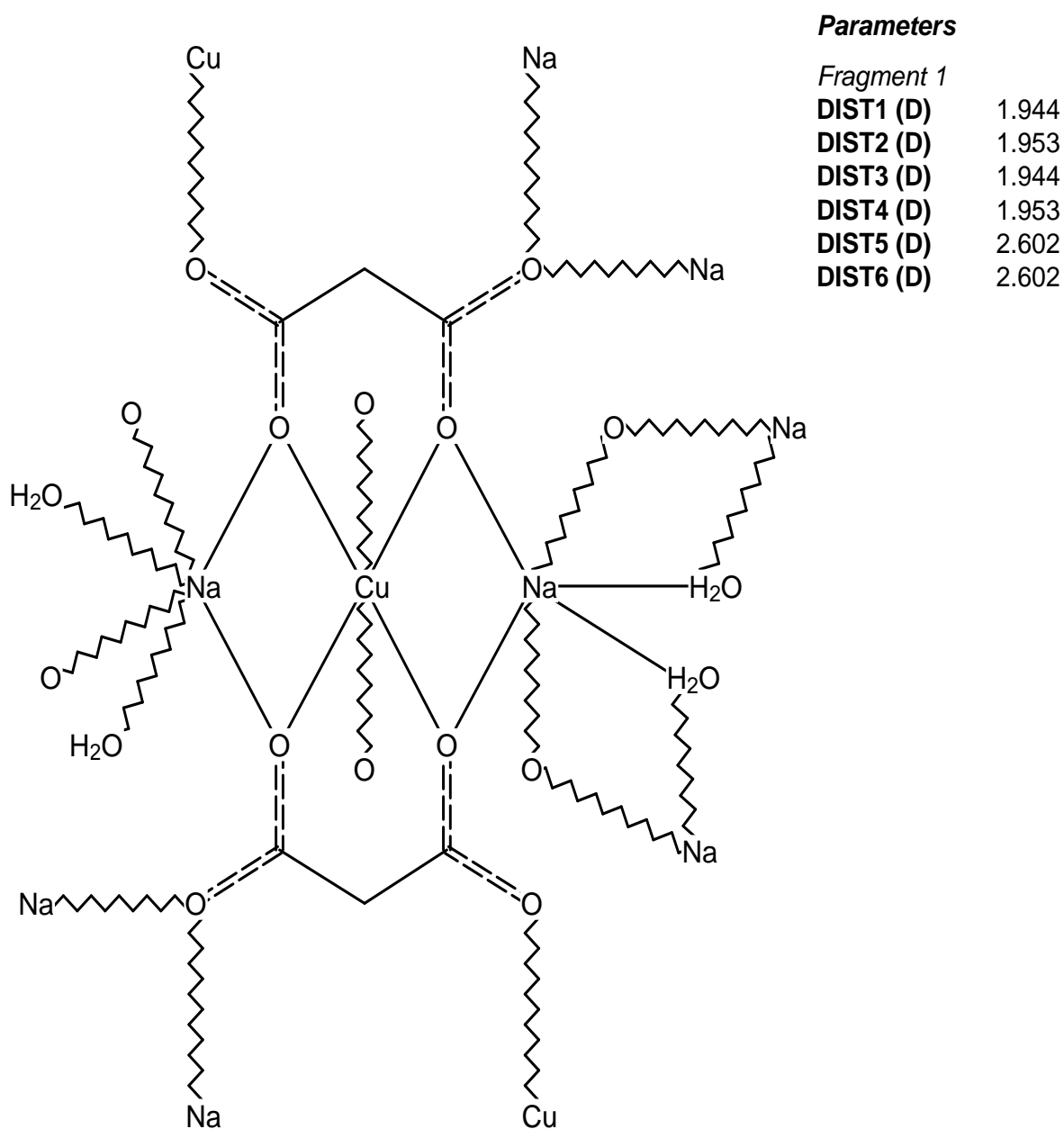
Reference: D.Ghoshal, T.K.Maji, T.Mallah, Tian-Huey Lu, G.Mostafa, N.R.Chaudhuri (2005) *Inorg.Chim.Acta* ,358,1027

Formula: $(C_6 H_8 Cu_1 Na_2 O_{10})_n$

Compound Name: catena-(bis(μ_6 -Malonato)-bis(μ_2 -aqua)-copper(ii)-di-sodium)

Space Group: Pbc_a **Cell:** **a** 6.827(0) **b** 9.512(1) **c** 16.399(2)
Space Group No.: 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.28 **Temperature(K):** 296 **Density(g/cm³):** 2.181



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 174

SANMAX

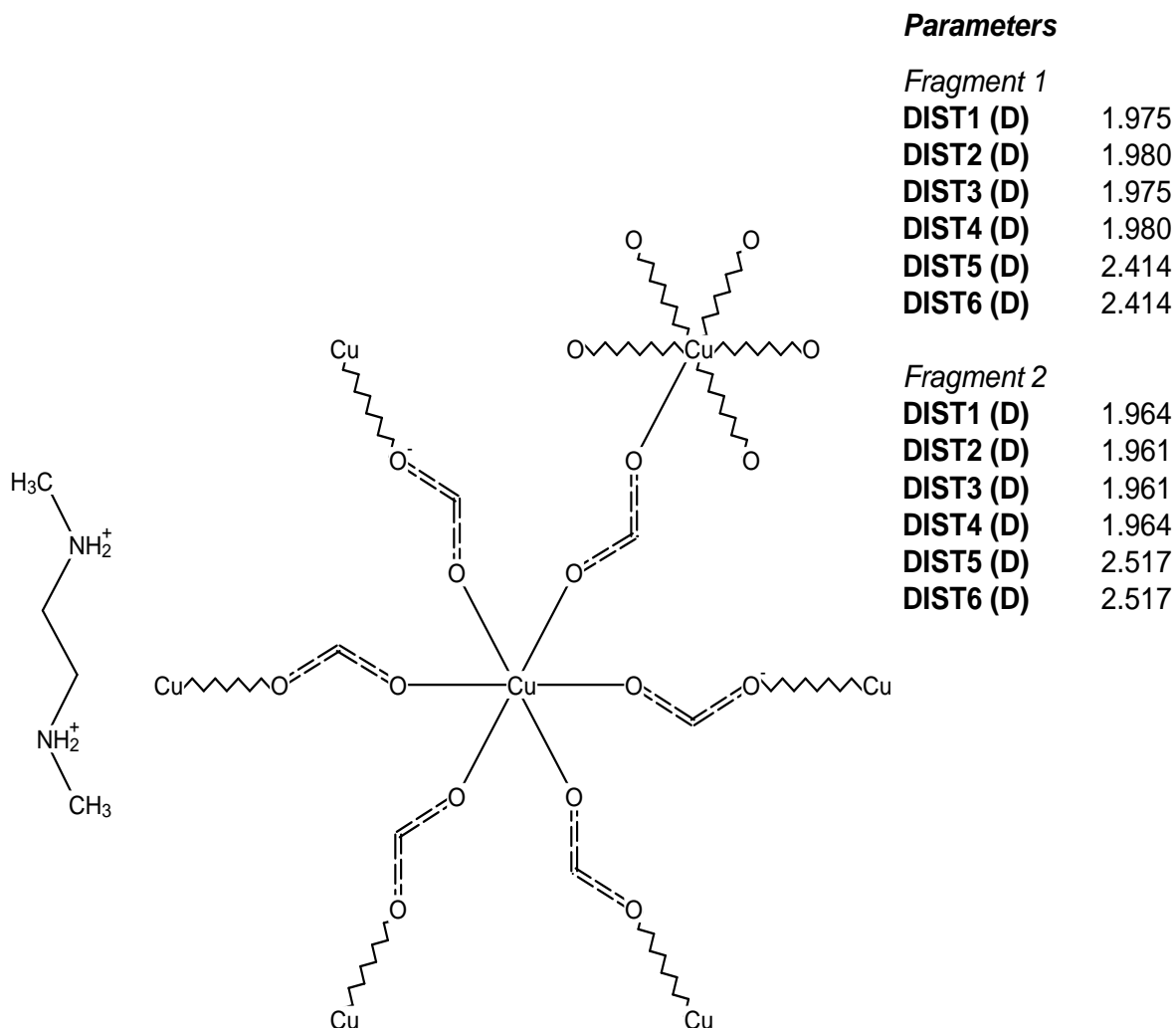
Reference: Meng-Yuan Li, M.Kurmoo, Zhe-Ming Wang, Song Gao
(2011) *Chem.Asian J.* ,6,3084

Formula: $(C_4 H_{14} N_2^{2+})_n, n(C_6 H_6 Cu_2 O_{12}^{2-})$

Compound Name: catena-[1,2-bis(Methylammonio)ethane hexakis(μ_2 -formate-O,O')-copper(ii)]

Space Group: C2/c **Cell:** **a** 8.661(0) **b** 13.640(0) **c** 14.583(0)
Space Group No.: 15 **(Å, °)** α 90.00 β 90.88(0) γ 90.00

R-Factor (%): 2.70 **Temperature(K):** 293 **Density(g/cm³):** 1.879



SAVTEP

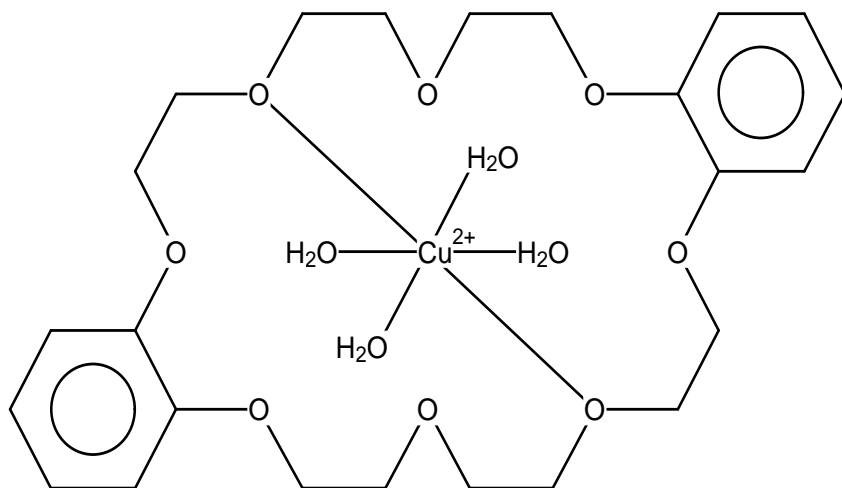
Reference: V.Shivaiah, S.K.Das (2005) *Inorg.Chem.* ,**44**,7313

Formula: $C_{24} H_{40} Cu_1 O_{12}^{2+}, Mo_6 O_{19}^{2-}$

Compound Name: (Dibenzo-24-crown-8)-tetraaqua-copper(ii) (μ_6 -oxo)-dodecakis(μ_2 -oxo)-hexaoxo-hexa-molybdenum(vi)

Space Group: P-1 **Cell:** **a** 9.329(0) **b** 10.878(0) **c** 12.249(0)
Space Group No.: 2 **(Å, °)** α 101.63(0) β 107.70(0) γ 111.91(0)

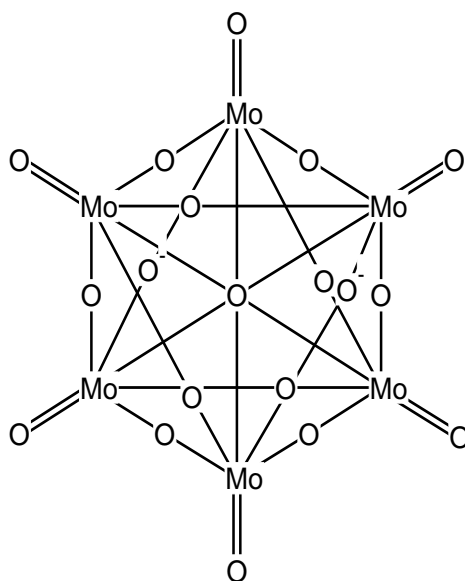
R-Factor (%): 2.41 **Temperature(K):** 298 **Density(g/cm³):** 2.368



Parameters

Fragment 1

DIST1 (D)	1.940
DIST2 (D)	1.973
DIST3 (D)	1.940
DIST4 (D)	1.973
DIST5 (D)	2.383
DIST6 (D)	2.383



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 176

SOHTUF

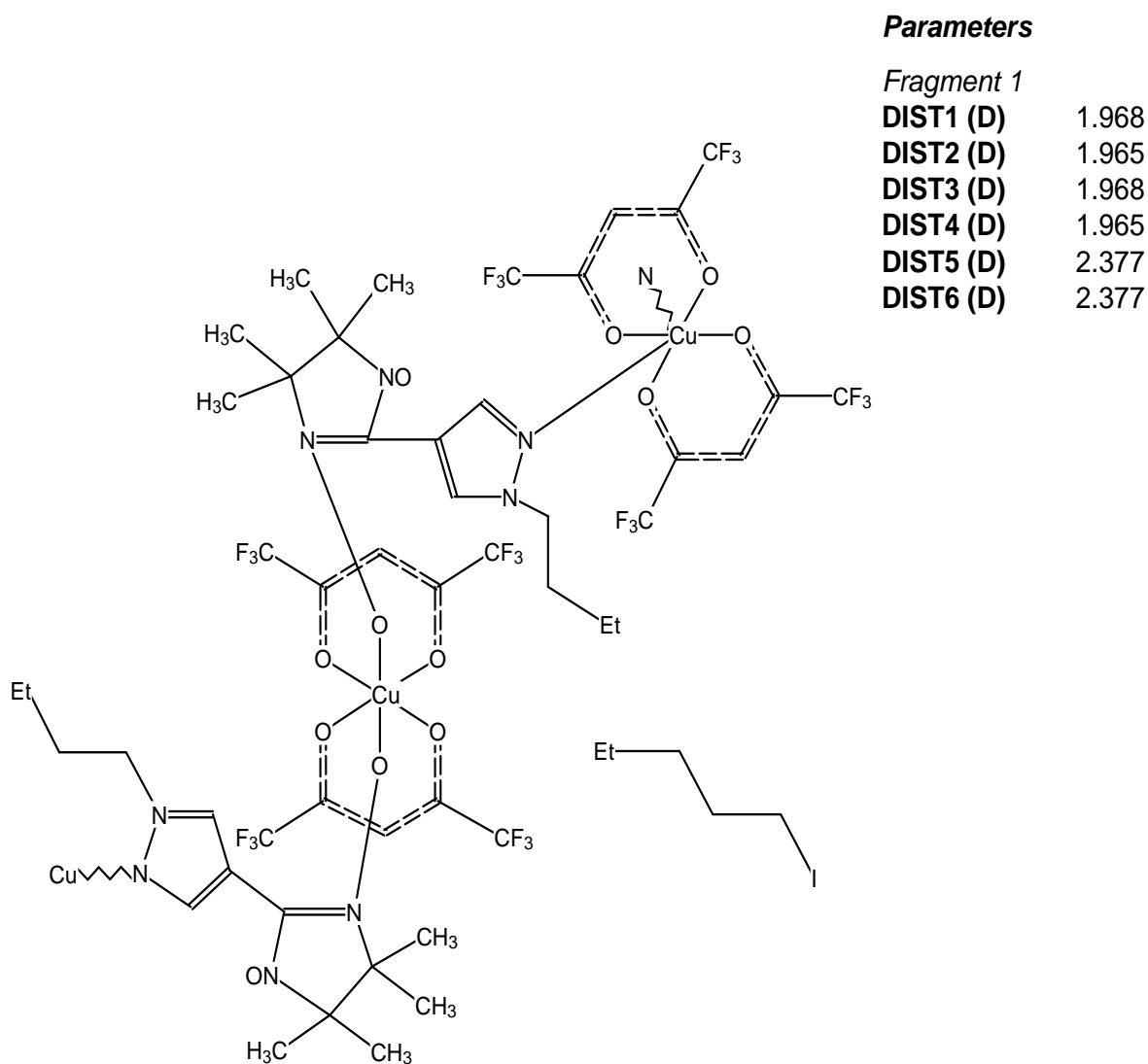
Reference: V.I.Ovcharenko, G.V.Romanenko, K.Yu.Maryunina, A.S.Bogomyakov, E.V.Gorelik (2008) *Inorg.Chem.* ,**47**,9537

Formula: (C₄₈ H₅₀ Cu₂ F₂₄ N₈ O₁₂)_n,n(C₅ H₁₁ I₁)

Compound Name: catena-(bis(μ_2 -4,4,5,5-Tetramethyl-2-(1-butylpyrazole-4-yl)-4,5-dihydro-1H-imidazol-3-oxide-1-oxyl)-tetrakis(1,1,1,5,5,5-hexafluoropentan-2,4-dionato)-di-copper(ii) iodopentane solvate)

Space Group: P-1 **Cell:** **a** 10.632(1) **b** 13.265(1) **c** 13.309(1)
Space Group No.: 2 (**Å, °**) α 98.58(0) β 108.68(0) γ 98.25(0)

R-Factor (%): 2.71 **Temperature(K):** 100 **Density(g/cm³):** 1.652



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 177

SOLDAZ

Reference: A.Castineiras, I.Garcia-Santos, J.M.Gonzalez-Perez,
J.Niclos-Gutierrez (2008)
CSD Communication(Private Communication) ,

Formula: $(C_5 H_6 N_5^{1+})_2 n, n(C_6 H_4 Cu_1 O_8^{2-}), 2n(H_2 O_1)$

Compound Name: catena-(bis(Adeninium) bis(μ_2 -malonato)-copper dihydrate)

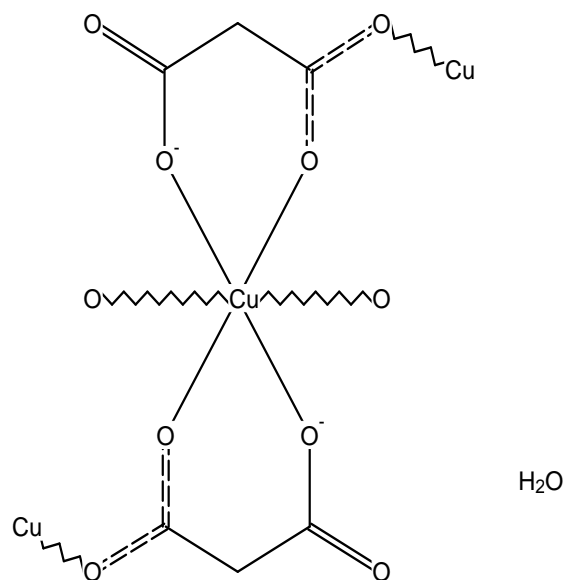
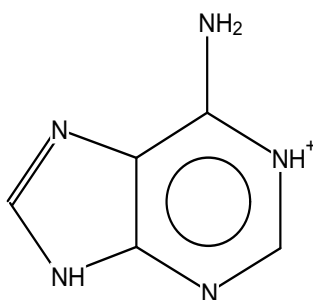
Space Group: P-1 **Cell:** **a** 5.060(0) **b** 9.337(0) **c** 11.267(0)
Space Group No.: 2 (**Å, °**) α 92.65(0) β 96.30(0) γ 95.43(0)

R-Factor (%): 2.73 **Temperature(K):** 100 **Density(g/cm³):** 1.819

Parameters

Fragment 1

DIST1 (D)	1.926
DIST2 (D)	1.938
DIST3 (D)	1.938
DIST4 (D)	1.926
DIST5 (D)	2.608
DIST6 (D)	2.608



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 178

SOPKOY

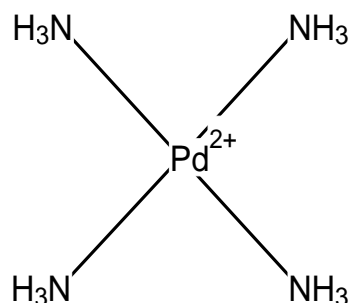
Reference: K.V.Yusenkov, E.Yu.Filatov, D.B.Vasilchenko, I.A.Baidina, A.V.Zadesenez, Yu.V.Shubin (2007) *Z.Kristallogr.*, **222**,289

Formula: $H_{12} N_4 Pd_1^{2+}, C_4 H_4 Cu_1 O_{10}^{2-}, H_2 O_1$

Compound Name: Tetraammine-palladium diaqua-bis(ethanedioato- κ^2O^1,O^2)-copper(ii) monohydrate

Space Group: I222 **Cell:** **a** 6.718(0) **b** 7.432(0) **c** 14.968(0)
Space Group No.: 23 **(Å, °)** α 90.00 β 90.00 γ 90.00

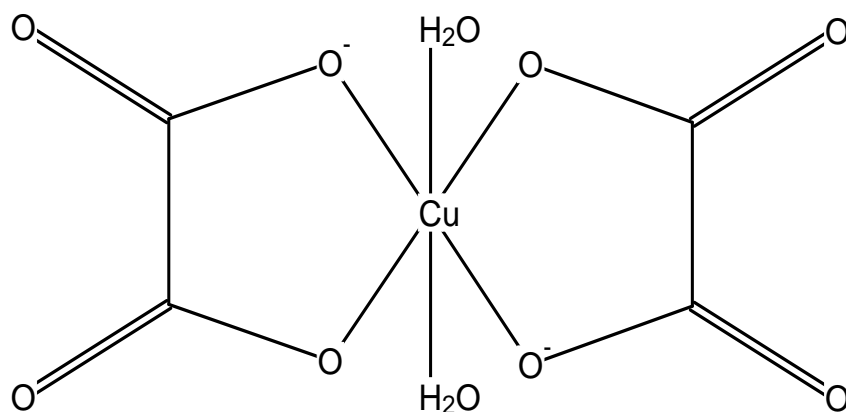
R-Factor (%): 2.00 **Temperature(K):** 293 **Density(g/cm³):** 2.081



Parameters

Fragment 1

DIST1 (D)	1.939
DIST2 (D)	1.939
DIST3 (D)	1.939
DIST4 (D)	1.939
DIST5 (D)	2.357
DIST6 (D)	2.357



H₂O

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 179

SOPKUE

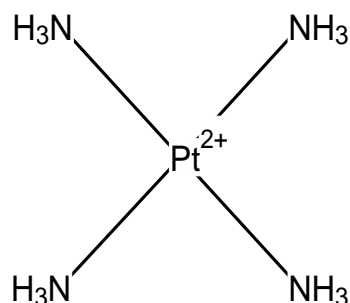
Reference: K.V.Yusenkov, E.Yu.Filatov, D.B.Vasilchenko, I.A.Baidina, A.V.Zadesenez, Yu.V.Shubin (2007) *Z.Kristallogr.*, **222**,289

Formula: $H_{12} N_4 Pt_1^{2+}, C_4 H_4 Cu_1 O_{10}^{2-}, H_2 O_1$

Compound Name: Tetraammine-platinum diaqua-bis(ethanedioato- κ^2O^1,O^2)-copper(ii) monohydrate

Space Group: I222 **Cell:** **a** 6.738(0) **b** 7.411(0) **c** 14.989(0)
Space Group No.: 23 **(Å, °)** α 90.00 β 90.00 γ 90.00

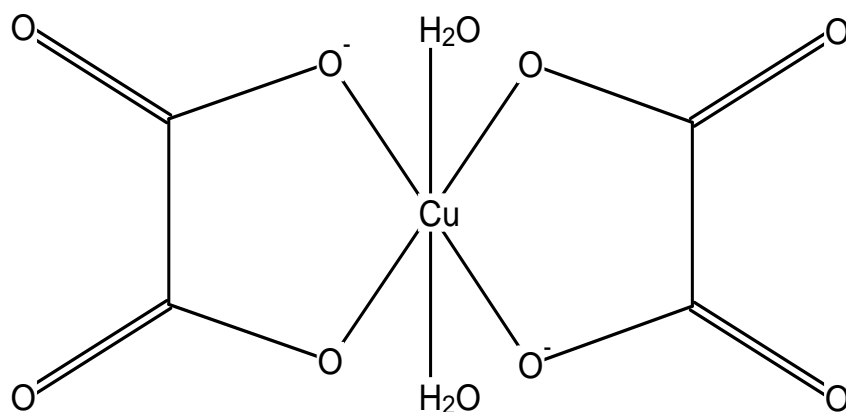
R-Factor (%): 1.81 **Temperature(K):** 293 **Density(g/cm³):** 2.471



Parameters

Fragment 1

DIST1 (D)	1.946
DIST2 (D)	1.946
DIST3 (D)	1.946
DIST4 (D)	1.946
DIST5 (D)	2.260
DIST6 (D)	2.260



H₂O

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 180

TAMSCU10

Reference: F.Charbonnier, R.Faure, H.Loiseleur (1977)
Acta Crystallogr., Sect.B:Struct. Crystallogr. Cryst. Chem. ,**33**,1845

Formula: C₂ H₁₄ Cu₁ O₁₀ S₂

Compound Name: Tetra-aqua-bis(methanesulfonato)-copper(ii)

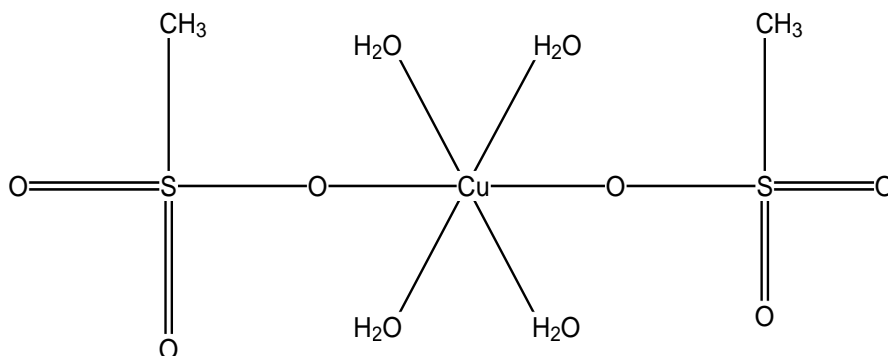
Space Group: P21/c **Cell:** **a** 9.306(0) **b** 9.632(2) **c** 7.308(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 122.18(1) γ 90.00

R-Factor (%): 2.60 **Temperature(K):** 295 **Density(g/cm³):** 1.952

Parameters

Fragment 1

DIST1 (D) 1.969
DIST2 (D) 1.947
DIST3 (D) 1.969
DIST4 (D) 1.947
DIST5 (D) 2.387
DIST6 (D) 2.387



TAYSAN

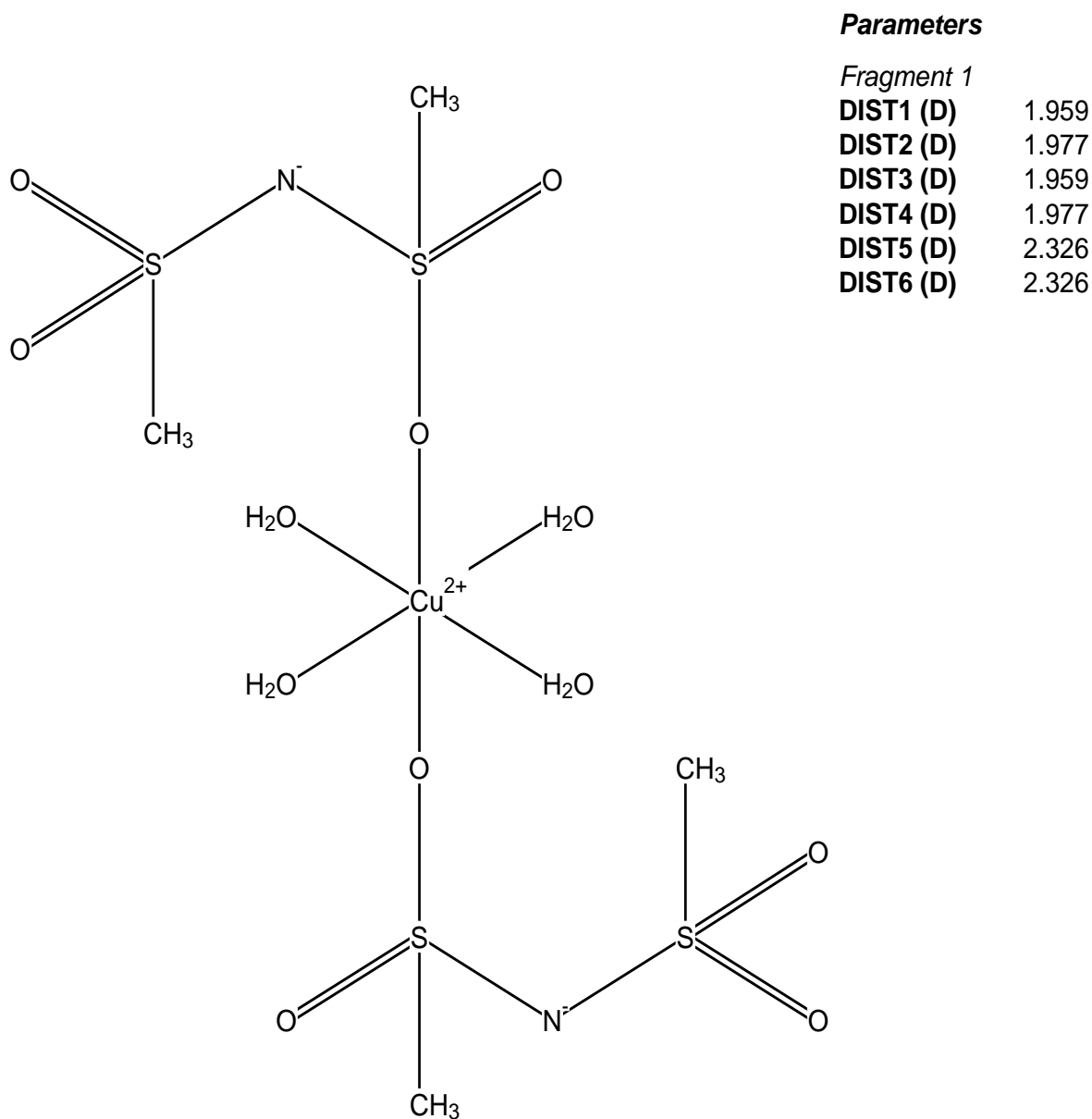
Reference: D.Henschel, K.Linoh, K.-H.Nagel, A.Blaschette, P.G.Jones (1996) *Z.Anorg.Allg.Chem.* ,**622**,1065

Formula: C₄ H₂₀ Cu₁ N₂ O₁₂ S₄

Compound Name: Tetra-aqua-bis(mesylamido)-copper(ii)

Space Group: P-1 **Cell:** **a** 7.298(4) **b** 7.913(4) **c** 8.392(3)
Space Group No.: 2 **(Å, °)** **α** 69.12(3) **β** 74.19(3) **γ** 64.96(3)

R-Factor (%): 2.20 **Temperature(K):** 143 **Density(g/cm³):** 1.963



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 182

TEHXEL

Reference: Yue-Ling Bai, Feifei Xing, Shourong Zhu, Jun Tao (2012)
Inorg.Chem.Commun. ,**20**,50

Formula: (C₁₆ H₂₈ Cu₁ O₂₆ Tb₂)_n,2n(H₂ O₁)

Compound Name: catena-[bis(μ₃-D-Malato)-bis(μ₂-D-malato)-hexa-aqua-copper(ii)-di-terbium(iii) dihydrate]

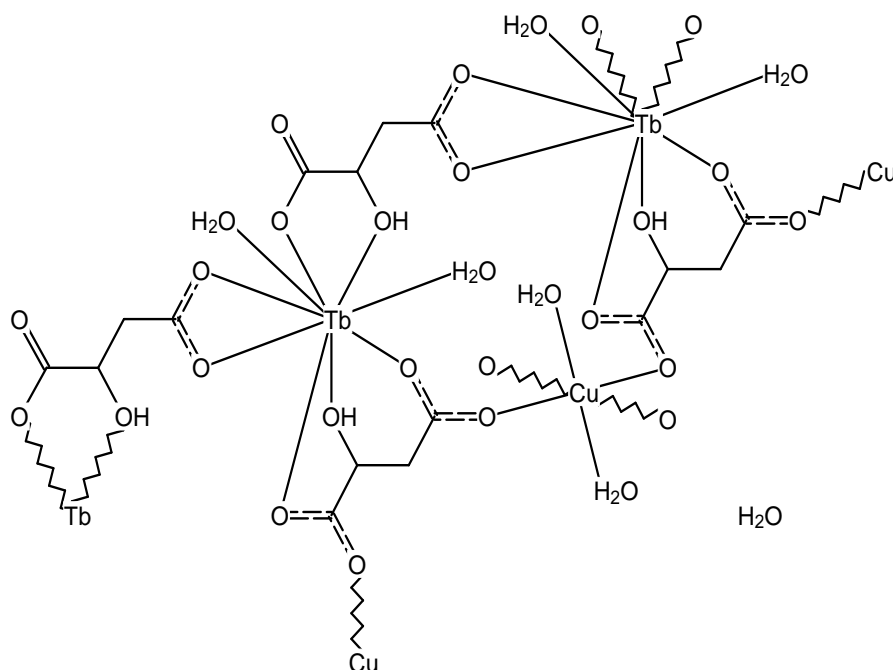
Space Group: C2 **Cell:** **a** 15.188(4) **b** 7.771(1) **c** 12.701(3)
Space Group No.: 5 **(Å, °)** α 90.00 β 113.99(0) γ 90.00

R-Factor (%): 2.51 **Temperature(K):** 298 **Density(g/cm³):** 2.555

Parameters

Fragment 1

DIST1 (D)	1.960
DIST2 (D)	1.994
DIST3 (D)	1.960
DIST4 (D)	1.994
DIST5 (D)	2.435
DIST6 (D)	2.435



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 183

TINPOV

Reference: S.Kawata, S.Kitagawa, H.Kumagai, C.Kudo, H.Kamesaki, T.Ishiyama, R.Suzuki, M.Kondo, M.Katada (1996) *Inorg.Chem.* ,**35**, 4449

Formula: $(C_{12}H_8N_2^{2+})_n, n(C_6H_4Cl_2Cu_1O_6^{2-})$

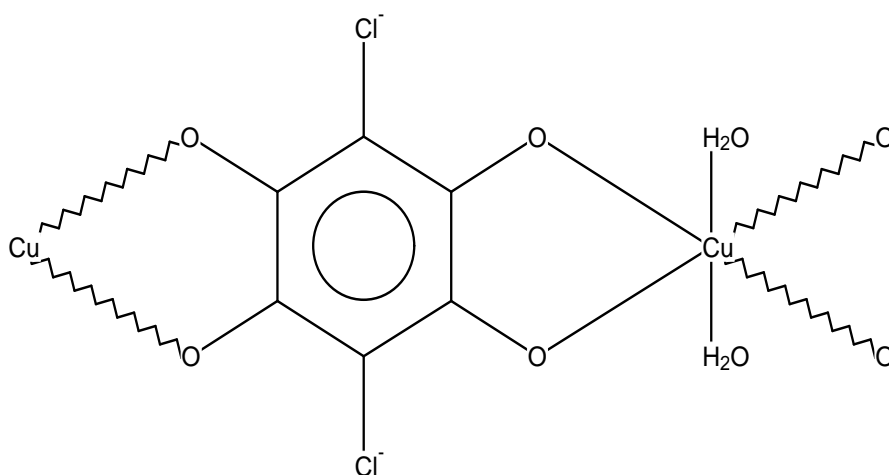
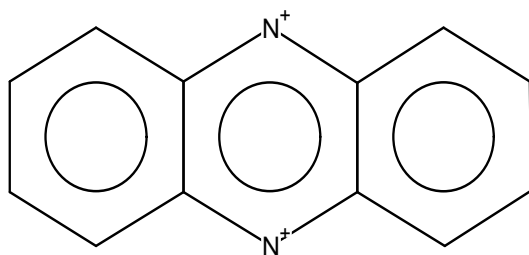
Compound Name: catena(Phenazinium (μ_2 -3,6-dichloro-1,2,4,5-tetrahydroxyphenyl)-diaqua-copper(ii))

Space Group: P-1 **Cell:** **a** 8.071(0) **b** 11.266(1) **c** 4.990(0)
Space Group No.: 2 **(Å, °)** α 97.80(1) β 99.58(1) γ 83.02(0)
R-Factor (%): 2.70 **Temperature(K):** 295 **Density(g/cm³):** 1.833

Parameters

Fragment 1

DIST1 (D) 1.963
DIST2 (D) 2.073
DIST3 (D) 2.073
DIST4 (D) 1.963
DIST5 (D) 2.228
DIST6 (D) 2.228



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 184

TIYKUJ

Reference: N.L.Nkhili, W.Rekik, T.Mhiri, K.T.Mahmudov, M.N.Kopylovich, H.Naili (2014) *Inorg.Chim.Acta* ,**412**,27

Formula: $C_4 H_{12} N_2^{2+}, H_8 Cu_1 O_{12} Se_2^{2-}, 2(H_2 O_1)$

Compound Name: Piperazinedium tetra-aqua-bis(selenato)-copper dihydrate

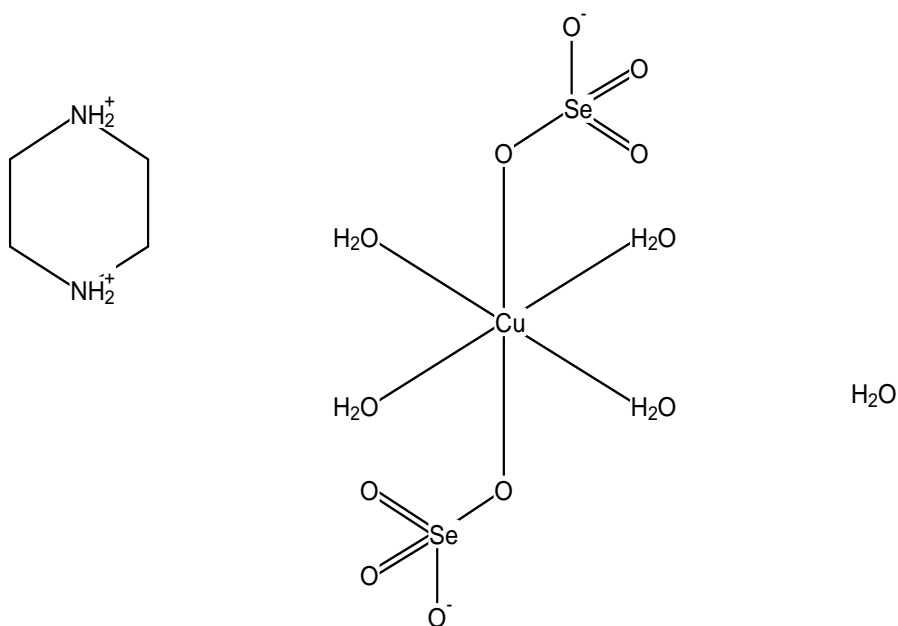
Space Group: P21/n **Cell:** **a** 7.033(1) **b** 11.687(0) **c** 10.623(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 104.13(1) γ 90.00

R-Factor (%): 2.01 **Temperature(K):** 293 **Density(g/cm³):** 2.140

Parameters

Fragment 1

DIST1 (D) 1.992
DIST2 (D) 1.962
DIST3 (D) 1.992
DIST4 (D) 1.962
DIST5 (D) 2.290
DIST6 (D) 2.290



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 185

TIZZOS

Reference: A.N.Chekhlov (2007)
Zh.Neorg.Khim.(Russ.)(Russ.J.Inorg.Chem.), **52**,768

Formula: C₁₈ H₃₈ N₂ O₆²⁺, Cu₁ N₄ O₁₂²⁻

Compound Name: 4,7,13,16,21,24-Hexaoxa-1,10-diazoniabicyclo(8.8.8)-hexacosane bis(nitrato-O,O)-dinitrato-copper(ii)

Synonym: dihydrogen (2,2,2-cryptand) bis(nitrato-O,O)-dinitrato-copper(ii)

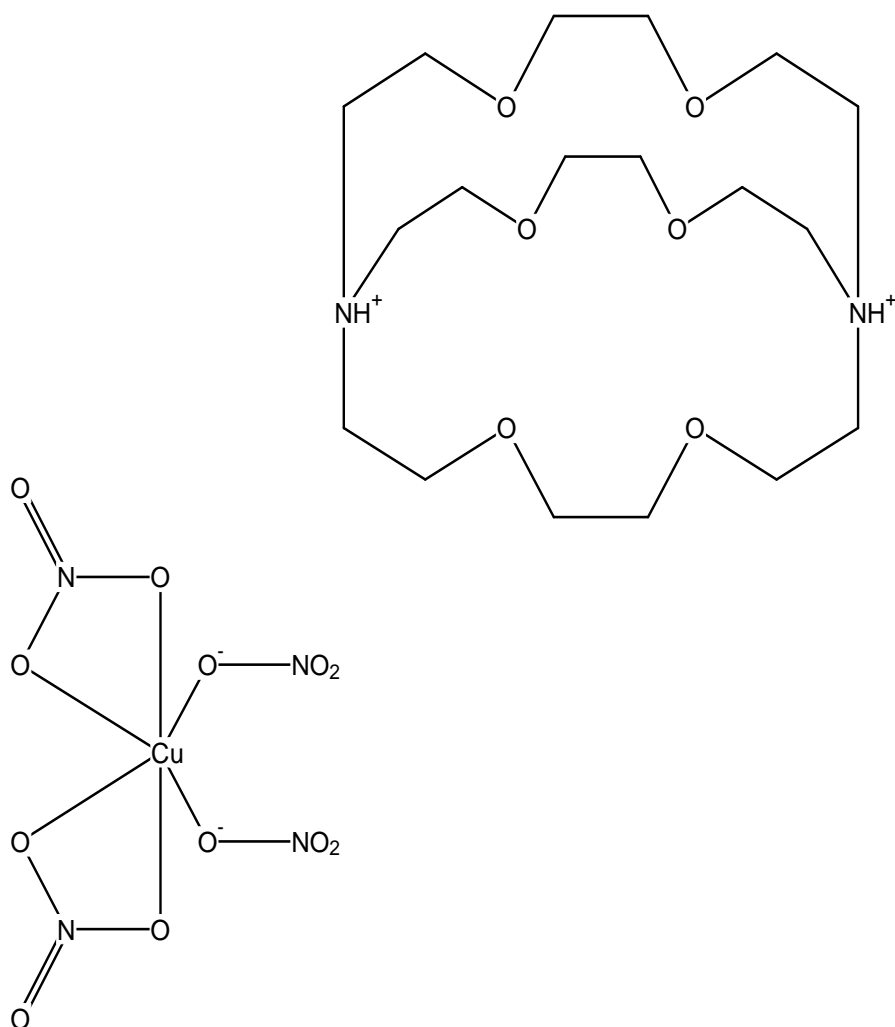
Space Group: P21/c **Cell:** **a** 10.264(2) **b** 14.798(2) **c** 19.516(3)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 100.20(2) **γ** 90.00

R-Factor (%): 2.50 **Temperature(K):** 295 **Density(g/cm³):** 1.571

Parameters

Fragment 1

DIST1 (D)	1.965
DIST2 (D)	1.965
DIST3 (D)	1.977
DIST4 (D)	1.965
DIST5 (D)	2.563
DIST6 (D)	2.599



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 186

UNIXEW

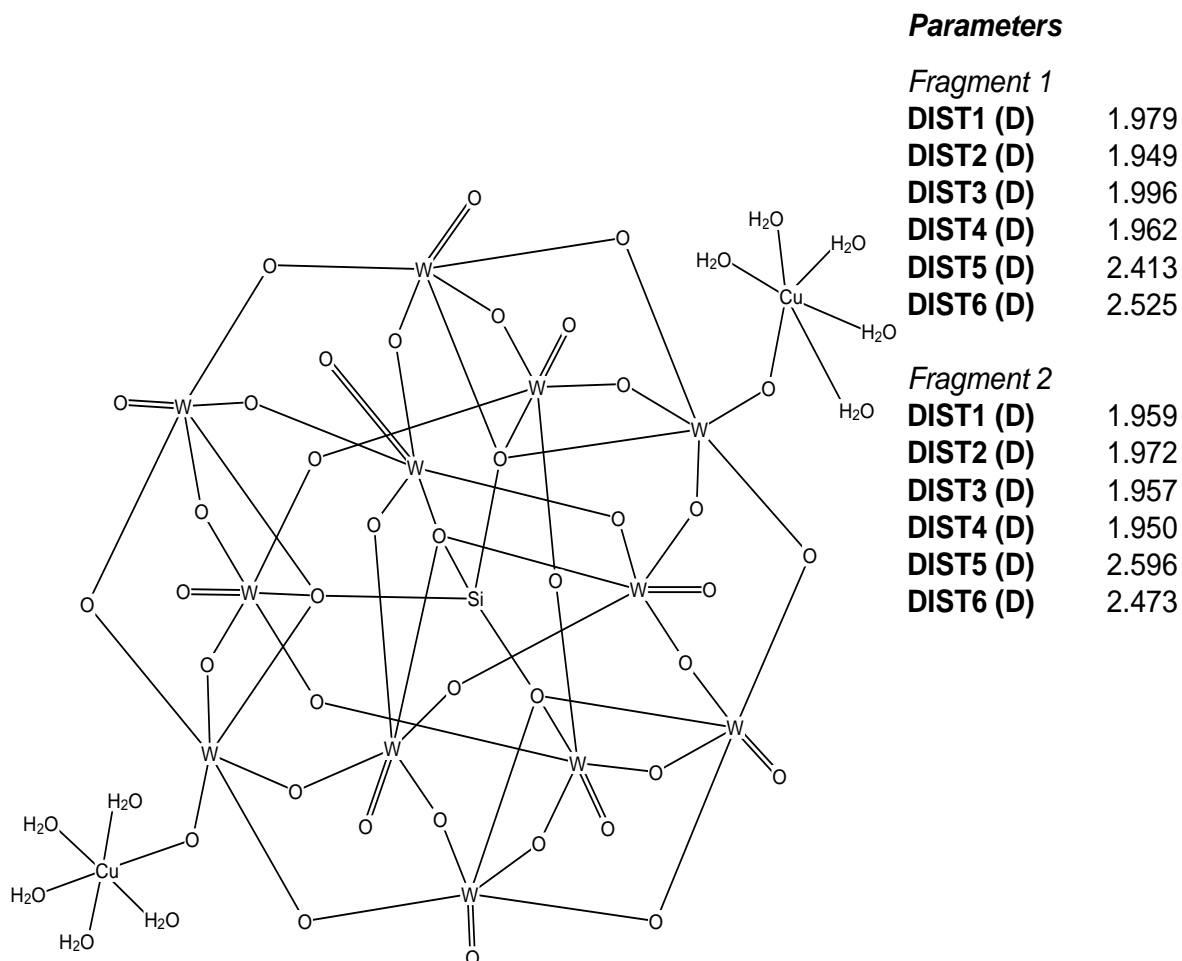
Reference: S.R.Bajpe, S.Henke, Jung-Hoon Lee, P.D.Bristowe, A.K.Cheetham (2016) *CrystEngComm*, **18**,5327

Formula: $H_{20} Cu_2 O_{50} Si_1 W_{12}, 6(H_2 O_1)$

Compound Name: (μ -silicato)-hexacosakis(μ -oxo)-deca-aqua-decaoxo-di-copper-dodecatungsten hexahydrate

Space Group: P-1 **Cell:** **a** 12.890(0) **b** 14.007(0) **c** 15.338(0)
Space Group No.: 2 (**Å, °**) α 63.17(0) β 71.08(0) γ 63.83(0)

R-Factor (%): 2.66 **Temperature(K):** 125 **Density(g/cm³):** 4.987



H₂O

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 187

UNIXIA01

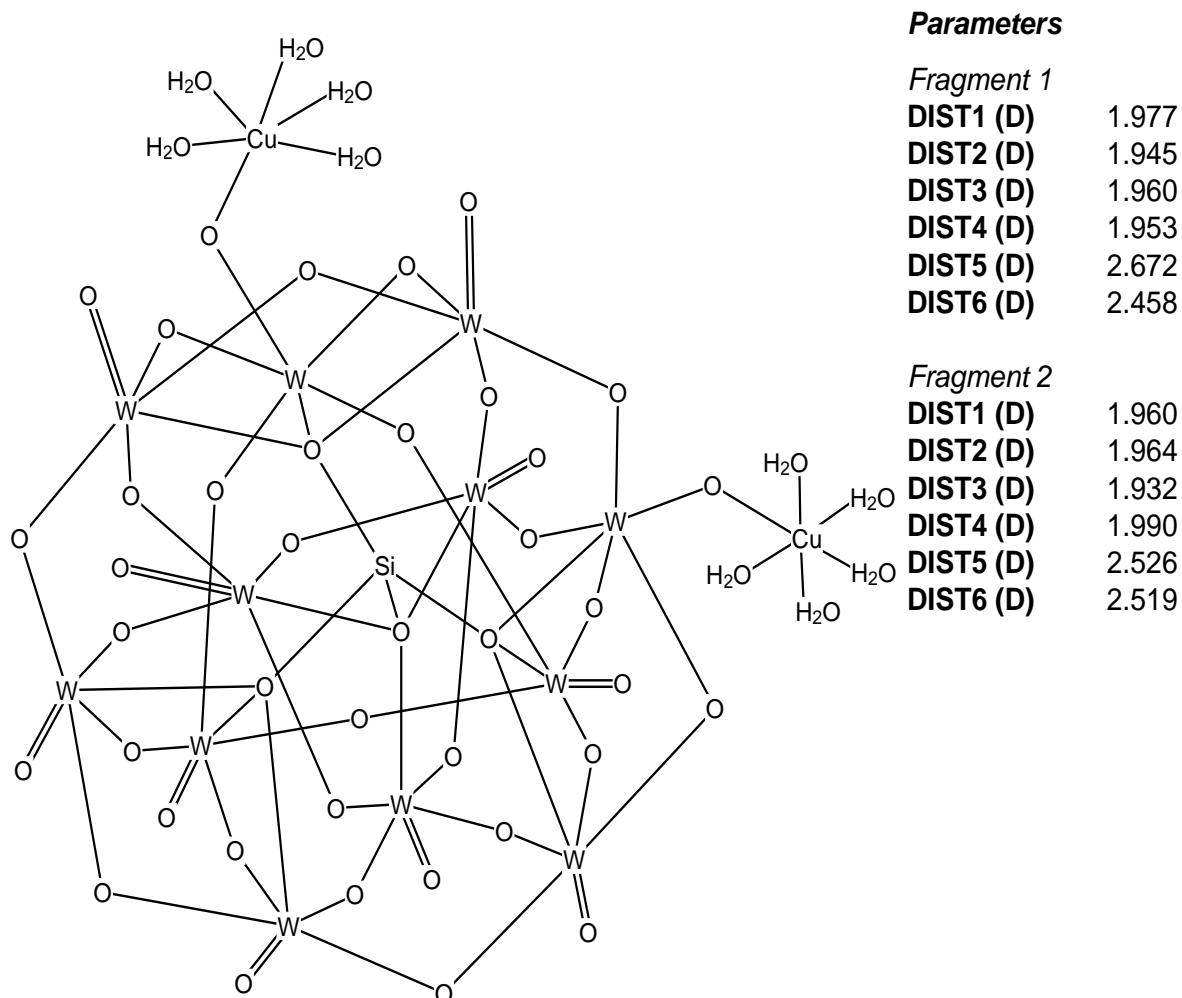
Reference: S.R.Bajpe, S.Henke, Jung-Hoon Lee, P.D.Bristowe, A.K.Cheetham (2016) *CrystEngComm*, **18**,5327

Formula: $H_{20} Cu_2 O_{50} Si_1 W_{12}, 6(H_2 O_1)$

Compound Name: (μ -silicato)-hexacosakis(μ -oxo)-deca-aqua-decaoxo-di-copper-dodeca-tungsten hexahydrate

Space Group: P21/n **Cell:** **a** 12.901(0) **b** 22.195(0) **c** 15.347(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 94.43(0) γ 90.00

R-Factor (%): 2.76 **Temperature(K):** 124 **Density(g/cm³):** 4.987



H₂O

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 188

VITKOA

Reference: R.Koefenstein, C.Robl (2014) *Z.Anorg.Allg.Chem.* ,**640**,310

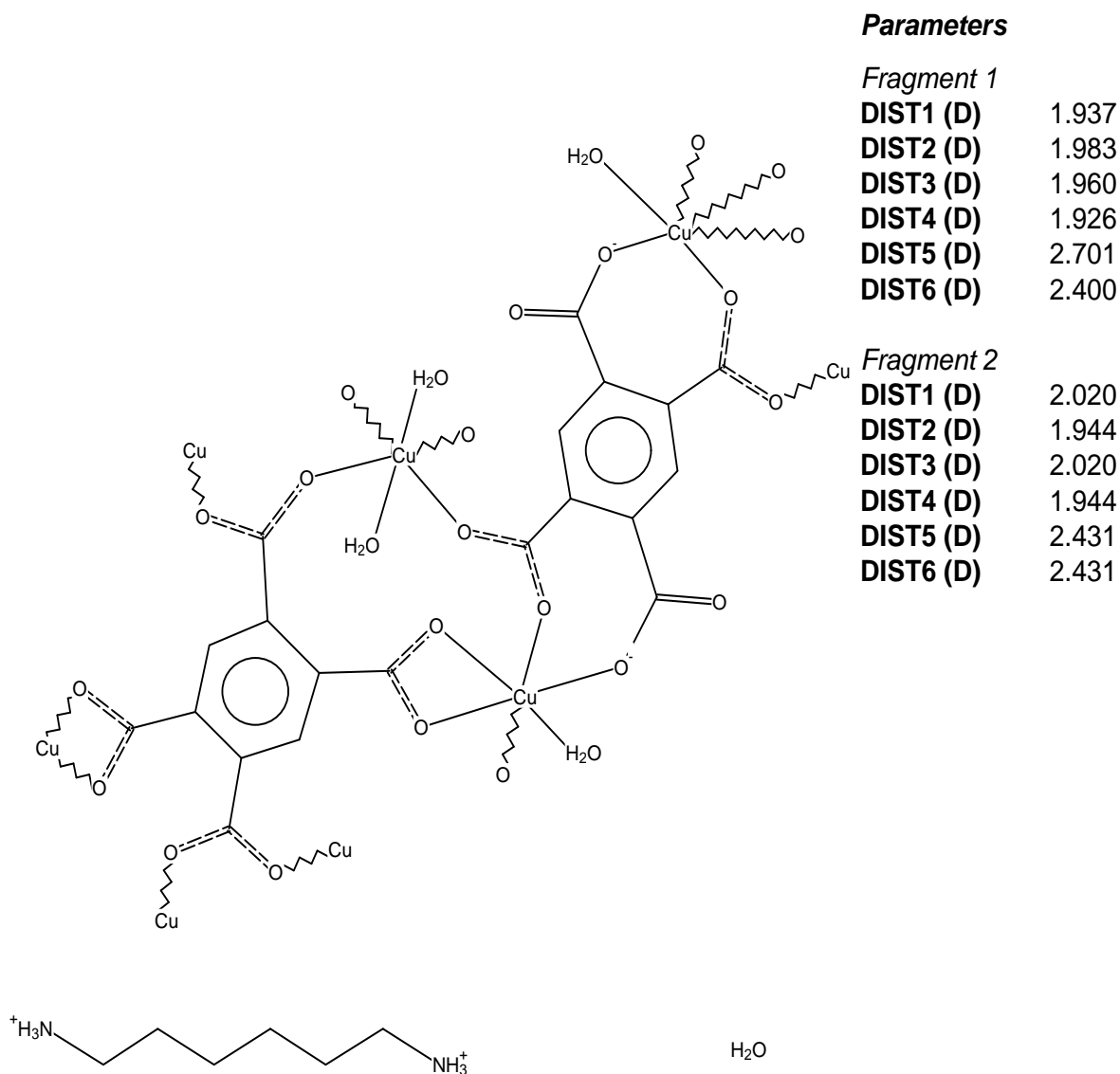
Formula: $(C_{20}H_{12}Cu_3O_{20}^{2-})_n, n(C_6H_{18}N_2^{2+})_n, 6n(H_2O)_1$

Compound Name: catena-[hexane-1,6-diaminium (μ_6 -benzene-1,2,4,5-tetracarboxylato)-(μ_4 -benzene-1,2,4,5-tetracarboxylato)-tetraaqua-tri-copper hexahydrate]

Space Group: P-1 **Cell:** **a** 7.726(0) **b** 11.104(0) **c** 11.120(0)

Space Group No.: 2 **(Å, °)** α 98.72(0) β 108.25(0) γ 95.56(0)

R-Factor (%): 2.58 **Temperature(K):** 293 **Density(g/cm³):** 1.857



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 189

VUBNIP

Reference: G.M.Frankenbach, M.A.Beno, A.M.Kini, J.M.Williams, U.Welp, J.E.Thompson, M.-H.Whangbo (1992) *Inorg.Chim.Acta*, **192**, 195

Formula: (C₄ H₈ Cu₁ O₈)_n

Compound Name: catena-(Tetra-aqua-(μ₂-squarato-O,O')-copper(ii))

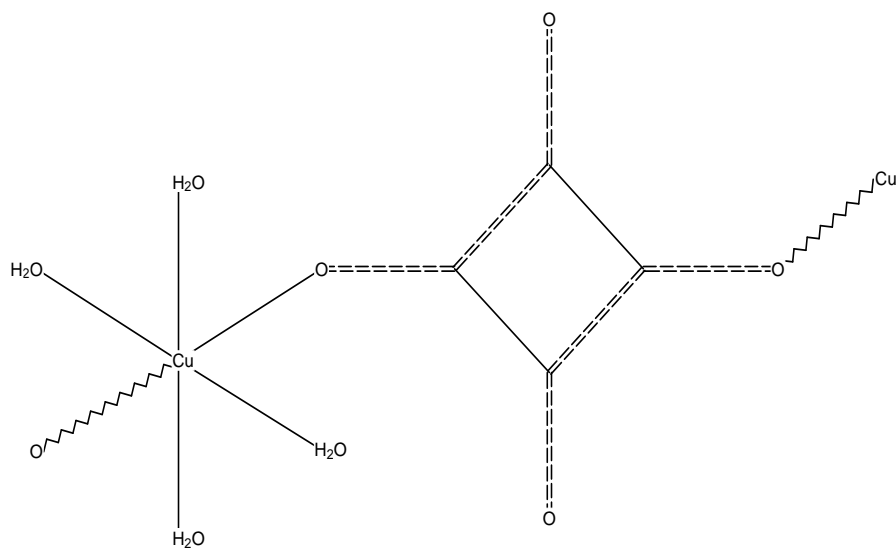
Space Group: P21/c **Cell:** **a** 6.676(2) **b** 7.946(4) **c** 7.668(2)
Space Group No.: 14 **(Å, °)** α 90.00 β 110.39(2) γ 90.00

R-Factor (%): 2.00 **Temperature(K):** 295 **Density(g/cm³):** 2.157

Parameters

Fragment 1

DIST1 (D) 1.961
DIST2 (D) 1.948
DIST3 (D) 1.961
DIST4 (D) 1.948
DIST5 (D) 2.468
DIST6 (D) 2.468



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 190

WAJPAY

Reference: V.Kh.Sabirov, M.A.Porai-Koshits, Yu.T.Struchkov,
A.N.Yunuskhodzhaev, A.F.Dusmatov (1992)
Koord.Khim.(Russ.)(Coord.Chem.), **18**,292

Formula: C₁₂ H₂₄ Cu₁ N₆ O₁₂

Compound Name: Diaqua-bis(2-oxo-1-pyrrolidineacetamide-O)-bis(nitrato-O)-copper(ii)

Synonym: Diaqua-bis(piracetam)-bis(nitrato-O)-copper(ii)

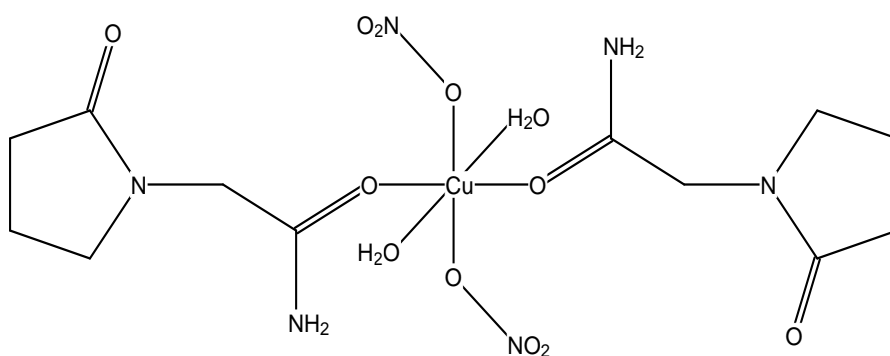
Space Group: P21/n **Cell:** **a** 9.231(2) **b** 6.045(1) **c** 17.759(4)
Space Group No.: 14 **(Å, °)** α 90.00 β 94.70(2) γ 90.00

R-Factor (%): 2.90 **Temperature(K):** 153 **Density(g/cm³):** 1.708

Parameters

Fragment 1

DIST1 (D)	1.941
DIST2 (D)	1.963
DIST3 (D)	1.963
DIST4 (D)	1.941
DIST5 (D)	2.421
DIST6 (D)	2.421



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 191

WEVQOD

Reference: R.Baggio, M.T.Garland, Y.Moreno, O.Pena, M.Perec, E.Spodine (2000) *J.Chem.Soc.,Dalton Trans.* ,2061

Formula: $(C_{24} H_{36} Cu_3 Gd_2 O_{36})_n, 12n(H_2 O)_1$

Compound Name: catena-(hexakis(μ_3 -2,2'-Oxydiacetato)-hexa-aqua-tri-copper(ii)-gadolinium(iii) dodecahydrate)

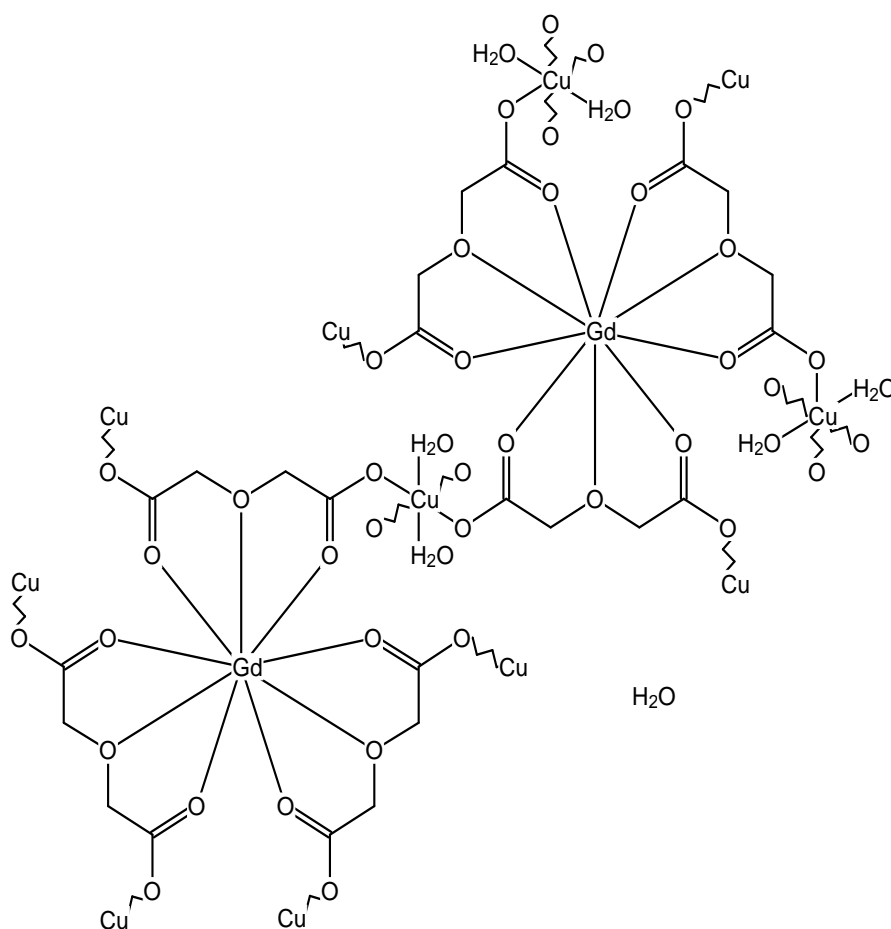
Space Group: P6/mcc **Cell:** **a** 14.717(2) **b** 14.717(2) **c** 15.169(3)
Space Group No.: 192 (**\AA , $^\circ$**) α 90.00 β 90.00 γ 120.00

R-Factor (%): 2.40 **Temperature(K):** 295 **Density(g/cm³):** 1.893

Parameters

Fragment 1

DIST1 (D)	1.955
DIST2 (D)	1.955
DIST3 (D)	1.955
DIST4 (D)	1.955
DIST5 (D)	2.510
DIST6 (D)	2.510



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 192

WIZGES

Reference: Ming-Lin Guo, Hong-Jun Zang (2008)
Acta Crystallogr., Sect. C: Cryst. Struct. Commun. ,**64**,m173

Formula: (C₁₀ H₁₆ Cu₁ O₁₄ P₂)_n,2n(H₂ O₁)

Compound Name: catena-[bis(μ₂-1-Oxo-2,6,7-trioxa-1-phosphabicyclo(2.2.2)octane-4-carboxylato-O,O')-diaqua-copper(ii) dihydrate]

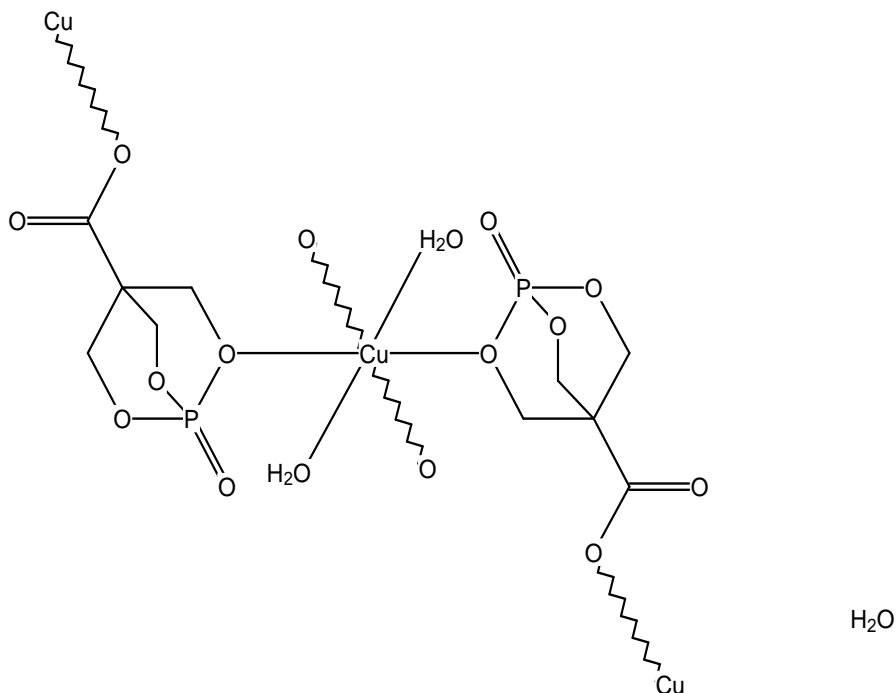
Space Group: P21/c **Cell:** **a** 8.340(3) **b** 8.863(3) **c** 12.565(4)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 99.58(0) **γ** 90.00

R-Factor (%): 2.65 **Temperature(K):** 294 **Density(g/cm³):** 1.892

Parameters

Fragment 1

DIST1 (D)	1.941
DIST2 (D)	1.908
DIST3 (D)	1.908
DIST4 (D)	1.941
DIST5 (D)	2.704
DIST6 (D)	2.704



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 193

WOQMAR

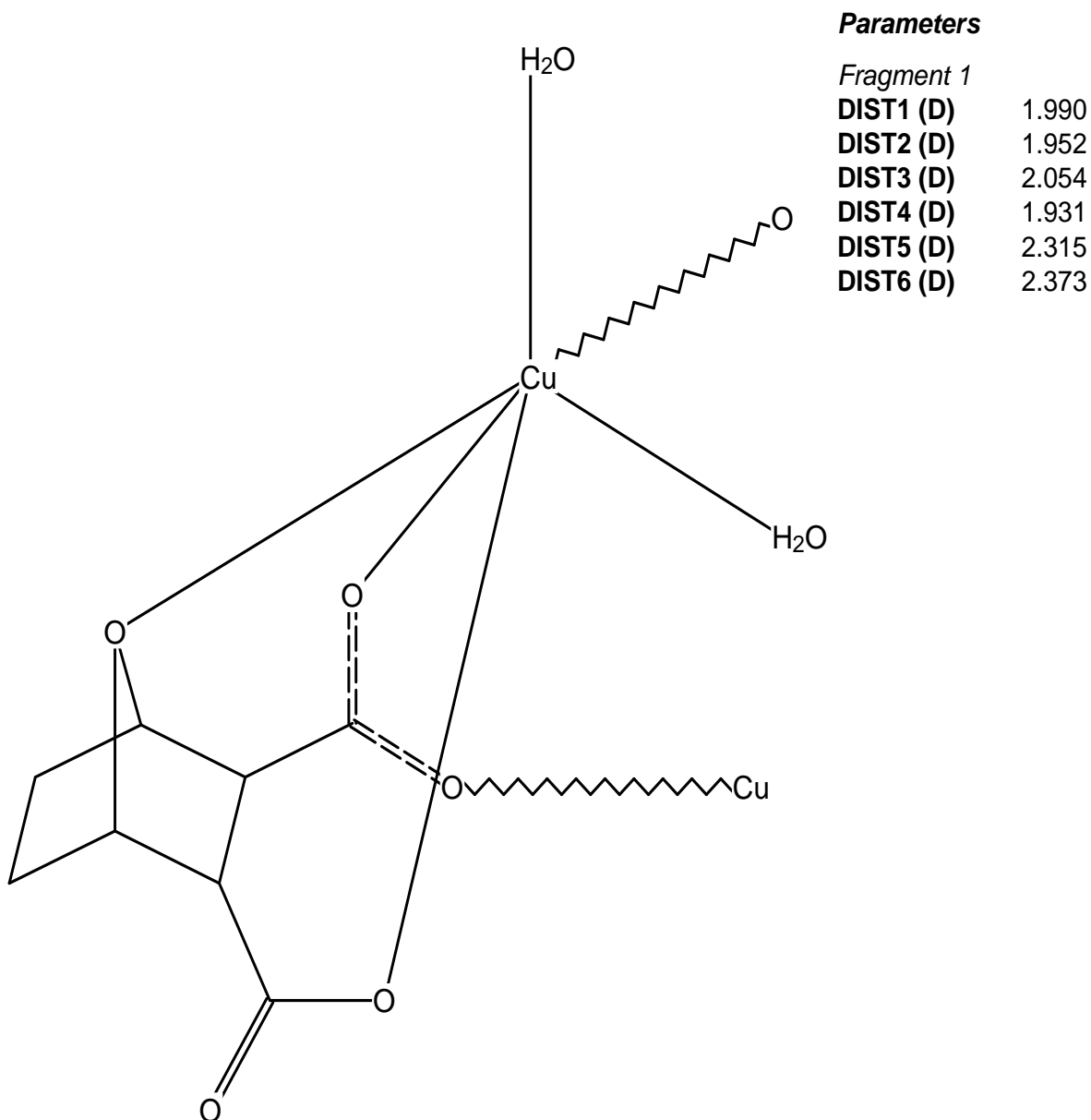
Reference: Yun-Yun Wang, Rui-Ding Hu, Yan-Jun Wang (2009)
Acta Crystallogr., Sect. E: Struct. Rep. Online ,65,m169

Formula: (C₈ H₁₂ Cu₁ O₇)_n

Compound Name: catena-((μ₂-7-Oxabicyclo[2.2.1]heptane-2,3-dicarboxylato-O,O',O'')-
diaqua-copper(ii))

Space Group: Iba2 **Cell:** **a** 10.551(0) **b** 19.339(0) **c** 9.744(0)
Space Group No.: 45 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.23 **Temperature(K):** 296 **Density(g/cm³):** 1.896



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 194

WULSAY

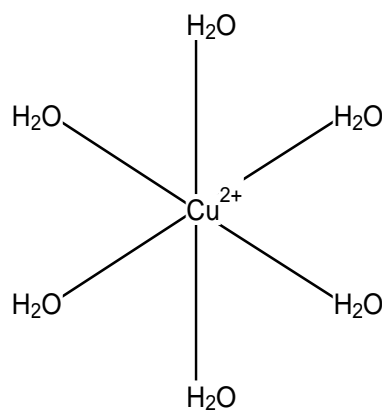
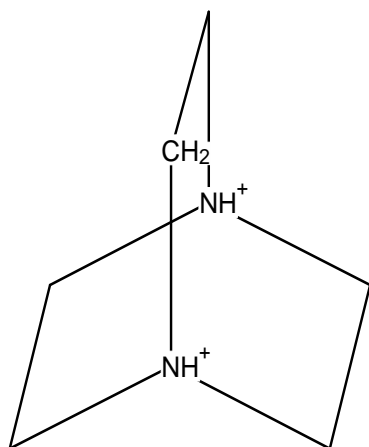
Reference: Wen Zhang, Li-Zhuang Chen, Ren-Gen Xiong, T.Nakamura, S.D.Huang (2009) *J.Am.Chem.Soc.* ,**131**,12544

Formula: $C_6 H_{14} N_2^{2+}, H_{12} Cu_1 O_6^{2+}, 2(O_4 Se_1^{2-})$

Compound Name: 1,4-Diazoniabicyclo[2.2.2]octane hexa-aqua-copper(ii) bis(selenate)

Space Group: P21 **Cell:** **a** 7.147(0) **b** 12.615(0) **c** 9.952(0)
Space Group No.: 4 **(Å, °)** α 90.00 β 91.73(0) γ 90.00

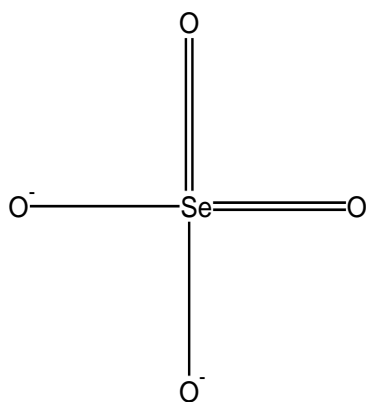
R-Factor (%): 2.81 **Temperature(K):** 103 **Density(g/cm³):** 2.117



Parameters

Fragment 1

DIST1 (D)	1.989
DIST2 (D)	1.964
DIST3 (D)	1.989
DIST4 (D)	1.975
DIST5 (D)	2.375
DIST6 (D)	2.383



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 195

WULSAY02

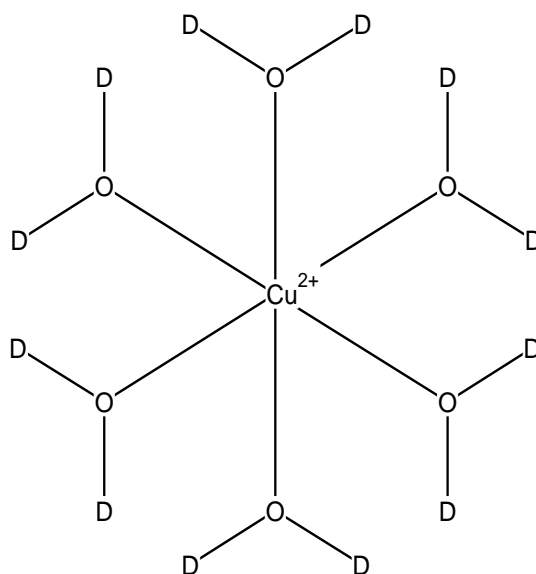
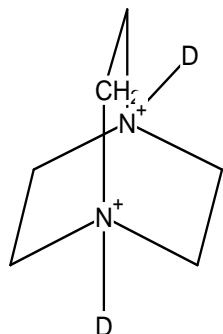
Reference: Wen Zhang, Li-Zhuang Chen, Ren-Gen Xiong, T.Nakamura, S.D.Huang (2009) *J.Am.Chem.Soc.* ,**131**,12544

Formula: $C_6 H_{12} D_2 N_2^{2+}, D_{12} Cu_1 O_6^{2+}, 2(O_4 Se_1^{2-})$

Compound Name: Dideutero-1,4-diazoniabicyclo[2.2.2]octane hexakis(dideuterium oxide)-copper(ii) bis(selenate)

Space Group: P21 **Cell:** **a** 7.140(0) **b** 12.602(0) **c** 9.944(0)
Space Group No.: 4 **(Å, °)** α 90.00 β 91.94(0) γ 90.00

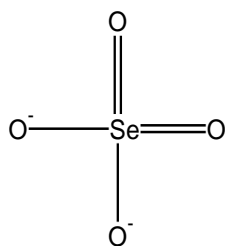
R-Factor (%): 2.66 **Temperature(K):** 93 **Density(g/cm³):** 2.175



Parameters

Fragment 1

DIST1 (D)	1.979
DIST2 (D)	1.971
DIST3 (D)	1.986
DIST4 (D)	1.986
DIST5 (D)	2.390
DIST6 (D)	2.370



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 196

WUZXOF

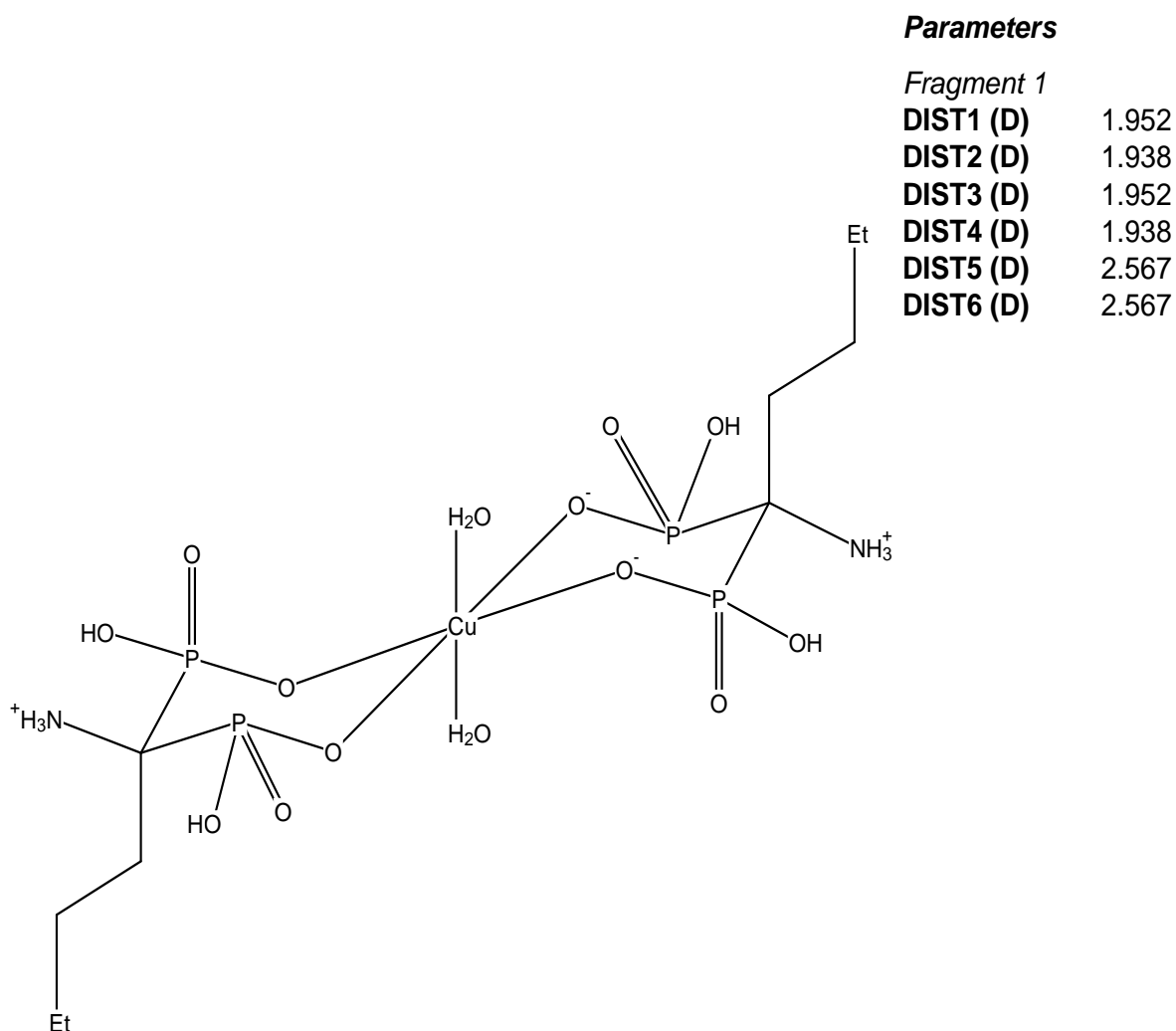
Reference: N.V.Tsaryk, A.V.Dudko, A.N.Kozachkova, V.V.Bon, V.I.Pekhnyo (2010) *Acta Crystallogr., Sect.E:Struct.Rep.Online* ,**66**, m1533

Formula: C₁₀ H₃₂ Cu₁ N₂ O₁₄ P₄

Compound Name: trans-Diaqua-(bis(1,1-bis(phosphono)pentan-1-aminiumato))-copper(ii)

Space Group: P-1 **Cell:** **a** 5.563(0) **b** 10.024(0) **c** 10.524(0)
Space Group No.: 2 **(Å, °)** **α** 69.31(0) **β** 86.67(0) **γ** 88.40(0)

R-Factor (%): 2.34 **Temperature(K):** 173 **Density(g/cm³):** 1.793



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 197

XACMIA

Reference: Xiuli Wang, Danna Liu, Hongyan Lin, Guocheng Liu, Xiang Wang, Mao Le, Xing Rong (2016) *CrystEngComm* ,18,888

Formula: (C₂₄ H₂₂ Cu₂ Mo₈ N₆ O₃₄)_n

Compound Name: catena-(bis(μ₅-Oxo)-hexakis(μ₃-oxo)-bis(μ₂-3-(pyridin-3-ylcarbamoyl)pyridine-2-carboxylato)-bis(μ₂-hydroxo)-tetrakis(μ₂-oxo)-diaqua-dodecaoxo-di-copper-octa-molybdenum)

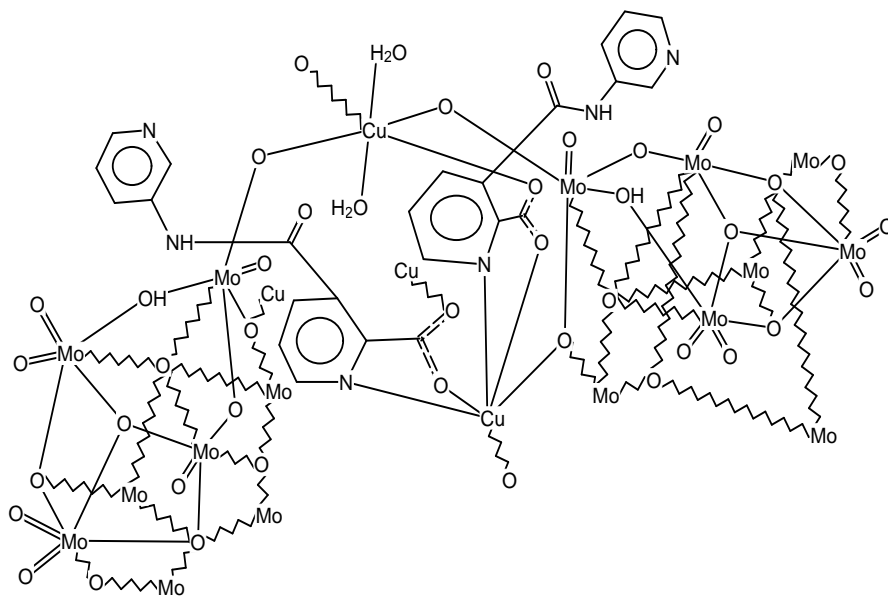
Space Group: P-1 **Cell:** **a** 9.942(0) **b** 10.231(0) **c** 11.093(0)
Space Group No.: 2 **(Å, °)** α 84.35(0) β 89.57(0) γ 88.02(0)

R-Factor (%): 2.43 **Temperature(K):** 296 **Density(g/cm³):** 2.712

Parameters

Fragment 1

DIST1 (D)	1.985
DIST2 (D)	1.976
DIST3 (D)	1.976
DIST4 (D)	1.985
DIST5 (D)	2.390
DIST6 (D)	2.390



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 198

XAXMEO

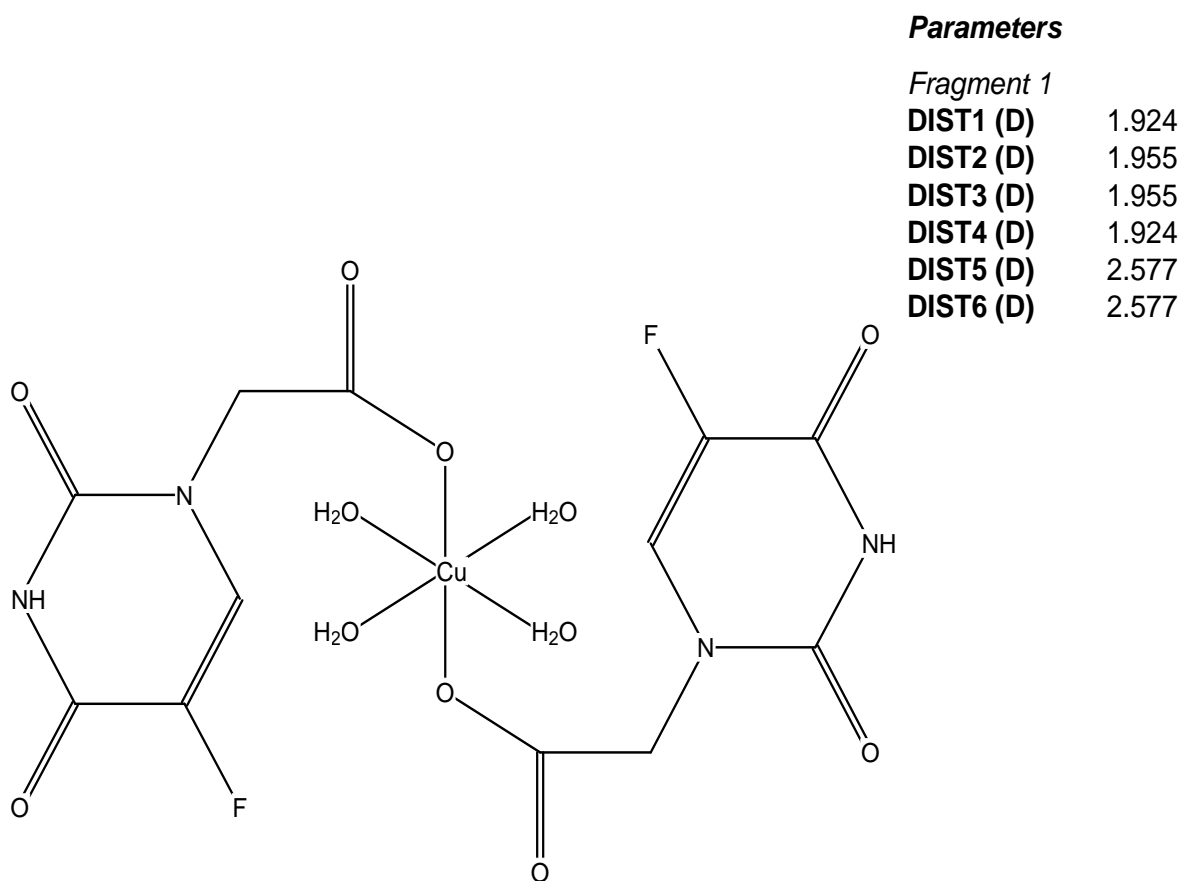
Reference: Jian Huang, Yi-Zhi Li, Gang-Chun Sun, Rong-Bin Dai, Qin-Xi Li, Liu-Fang Wang, Chun-Gu Xia (2000)
Acta Crystallogr., Sect. C: Cryst. Struct. Commun., **56**, e489

Formula: C₁₂ H₁₆ Cu₁ F₂ N₄ O₁₂, 4(H₂ O₁)

Compound Name: Tetra-aqua-bis(5-fluorouracil-1-acetato-O)-copper(ii) tetrahydrate

Space Group: P21/c **Cell:** **a** 8.304(1) **b** 12.044(2) **c** 11.082(2)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 92.47(1) **γ** 90.00

R-Factor (%): 2.00 **Temperature(K):** 295 **Density(g/cm³):** 1.745



H₂O

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 199

XEHTIO

Reference: Yun Gong, Wang Tang, Wenbin Hou, Zhongyong Zha, Changwen Hu (2006) *Inorg.Chem.* ,45,4987

Formula: (C₆ H₂₀ Cu₃ N₂ O₁₆ P₄)_n

Compound Name: catena-(bis(μ₄-3-Ammonium-1-hydroxypropylidene-1,1-bisphosphonato)-diaqua-tri-copper(ii))

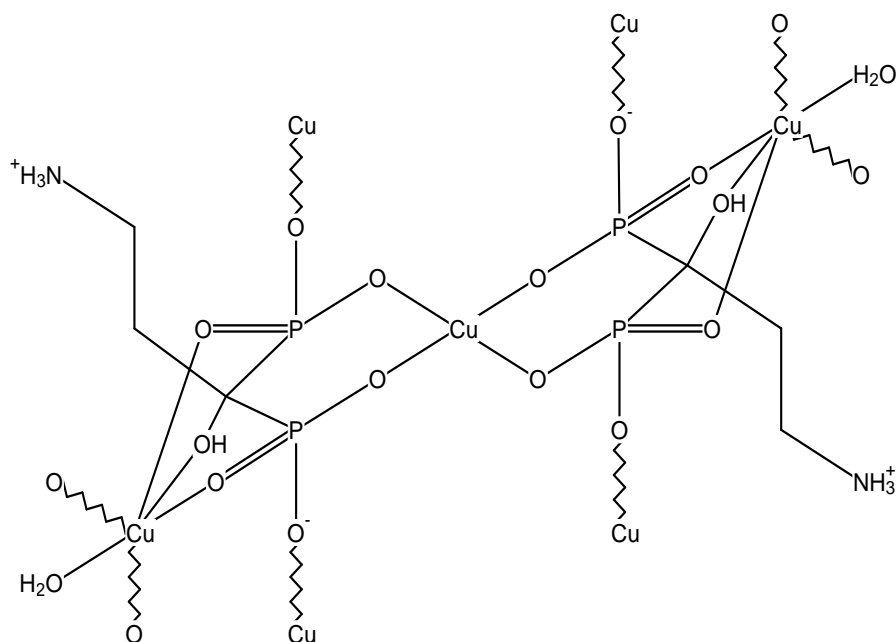
Space Group: P21/n **Cell:** **a** 10.232(4) **b** 7.961(3) **c** 11.016(4)
Space Group No.: 14 **(Å, °)** α 90.00 β 101.45(0) γ 90.00

R-Factor (%): 2.37 **Temperature(K):** 298 **Density(g/cm³):** 2.608

Parameters

Fragment 1

DIST1 (D)	1.954
DIST2 (D)	1.968
DIST3 (D)	2.147
DIST4 (D)	1.975
DIST5 (D)	2.396
DIST6 (D)	2.358



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 200

XOQHIW

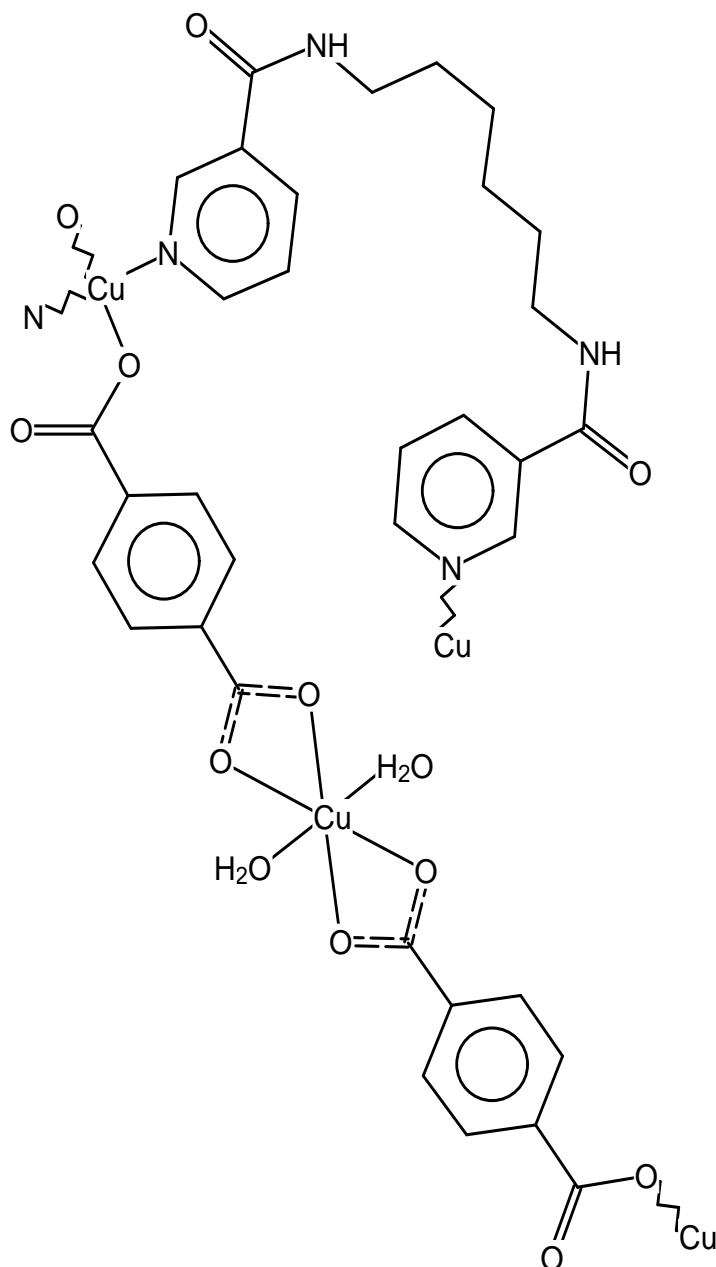
Reference: Qi-Lin Lu, Jian Luan, Xiu-Li Wang, Hong-Yan Lin, Mao Le, Guo-Cheng Liu (2014) *Polyhedron*, **83**,108

Formula: (C₃₄ H₃₄ Cu₂ N₄ O₁₂)_n

Compound Name: catena-((μ₂-N,N'-(Hexane-1,6-diyl)dinicotinamide)-bis(μ₂-terephthalato)-diaqua-di-copper)

Space Group: P-1 **Cell:** **a** 8.540(0) **b** 9.066(0) **c** 11.650(1)
Space Group No.: 2 **(Å, °)** **α** 86.83(0) **β** 69.09(0) **γ** 87.44(0)

R-Factor (%): 2.78 **Temperature(K):** 296 **Density(g/cm³):** 1.615



Parameters

Fragment 1

DIST1 (D)	1.977
DIST2 (D)	1.978
DIST3 (D)	1.978
DIST4 (D)	1.977
DIST5 (D)	2.496
DIST6 (D)	2.496

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 201

XOZVEN

Reference: L.R.Falvello, R.Garde, M.Tomas (2002) *Inorg.Chem.* ,**41**, 4599

Formula: C₆ H₁₀ Cu₁ N₄ O₁₀·2(H₂ O₁)

Compound Name: trans-Diaqua-bis(oxalurato-O,O')-copper(ii) dihydrate

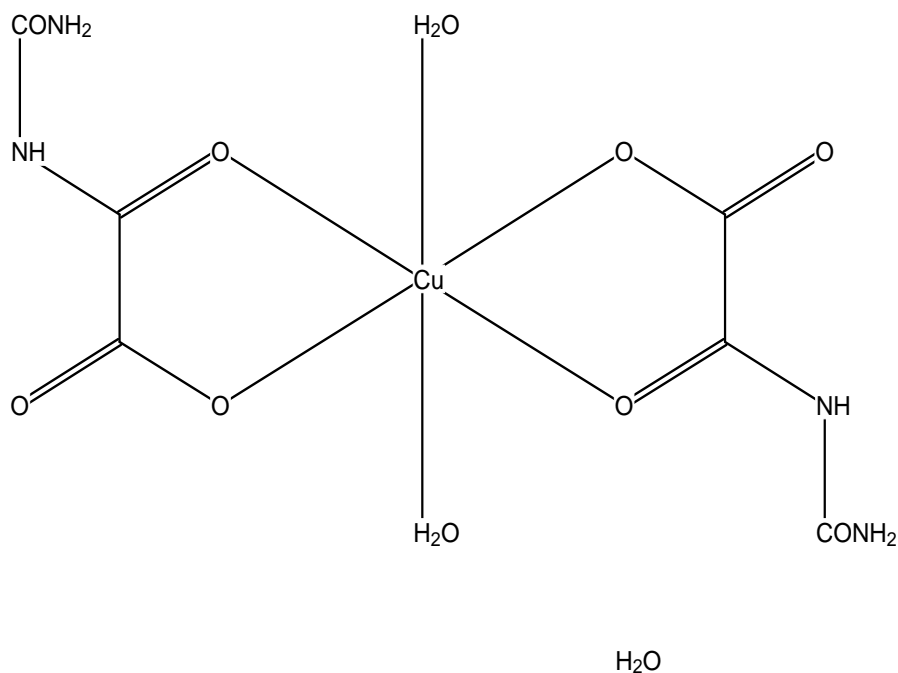
Space Group: P-1 **Cell:** **a** 5.258(0) **b** 6.833(1) **c** 10.314(2)
Space Group No.: 2 **(Å, °)** α 72.69(2) β 83.39(2) γ 71.27(1)

R-Factor (%): 2.82 **Temperature(K):** 148 **Density(g/cm³):** 1.972

Parameters

Fragment 1

DIST1 (D)	1.961
DIST2 (D)	1.957
DIST3 (D)	1.957
DIST4 (D)	1.961
DIST5 (D)	2.379
DIST6 (D)	2.379



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 202

YEDZOX

Reference: Qi-Hua Zhao, Lin Du, Rui-Bing Fang (2006)
Acta Crystallogr., Sect. E: Struct. Rep. Online ,62,m360

Formula: $2(\text{C}_3\text{H}_{12}\text{N}_2^{2+}), \text{H}_{12}\text{Cu}_1\text{O}_6^{2+}, \text{O}_{28}\text{V}_{10}^{6-}, 7(\text{H}_2\text{O}_1)$

Compound Name: bis(Trimethylenediammonium) hexaaqua-copper(ii) decavanadate heptahydrate

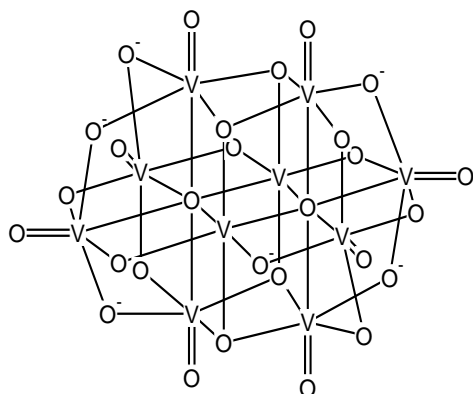
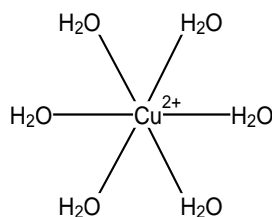
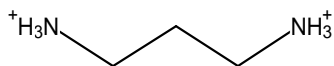
Space Group: P-1 **Cell:** **a** 10.351(2) **b** 11.125(2) **c** 18.536(4)
Space Group No.: 2 **(Å, °)** α 92.62(3) β 103.14(3) γ 100.17(3)

R-Factor (%): 2.76 **Temperature(K):** 253 **Density(g/cm³):** 2.294

Parameters

Fragment 1

DIST1 (D)	2.139
DIST2 (D)	2.080
DIST3 (D)	2.040
DIST4 (D)	2.111
DIST5 (D)	2.098
DIST6 (D)	2.070



H₂O

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 203

YEYTAY

Reference: Ai-E Shi, Bai-Yan Li, Guang-Feng Hou, Jin-Sheng Gao
(2007) *Acta Crystallogr., Sect. E: Struct. Rep. Online* ,63,m471

Formula: C₁₈ H₂₄ Cu₁ N₂ O₁₂·4(H₂ O₁)

Compound Name: trans-Tetraaqua-bis(2,6-dimethylpyridinium-3,5-dicarboxylato)-copper(ii) tetrahydrate

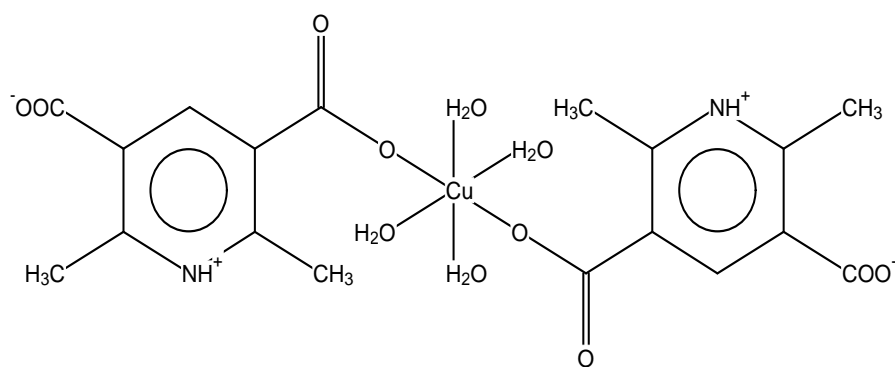
Space Group: P-1 **Cell:** **a** 6.867(5) **b** 9.203(6) **c** 11.108(8)
Space Group No.: 2 **(Å, °)** α 111.22(3) β 102.55(3) γ 96.83(3)

R-Factor (%): 2.90 **Temperature(K):** 291 **Density(g/cm³):** 1.587

Parameters

Fragment 1

DIST1 (D)	1.951
DIST2 (D)	1.954
DIST3 (D)	1.954
DIST4 (D)	1.951
DIST5 (D)	2.503
DIST6 (D)	2.503



H₂O

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 204

YEYTAY01

Reference: Cui-Ling Chen, Ye Zou, Ping Qiu, Yu-Hua Wen, Jun-Yong Li, Ze-Hong Hong, Xiao-Ming Lin, An-Xwu Xu, Yue-Peng Cai (2009) *J.Coord.Chem.* ,62,2480

Formula: C₁₈ H₂₄ Cu₁ N₂ O₁₂·4(H₂ O₁)

Compound Name: Tetra-aqua-bis(2,6-dimethylpyridinium-3,5-dicarboxylato-O)-copper(ii) tetrahydrate

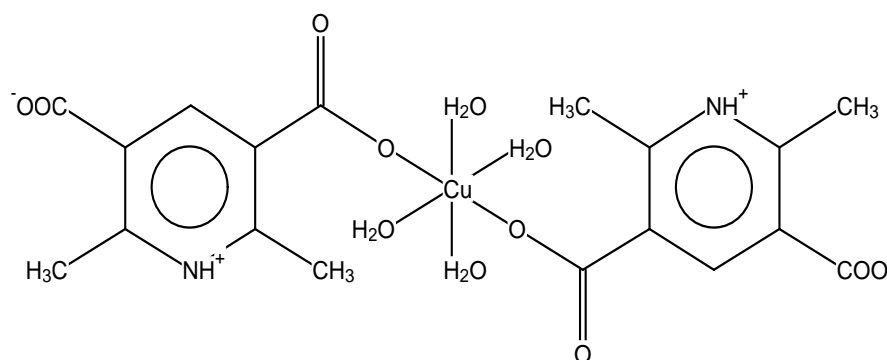
Space Group: P-1 **Cell:** **a** 7.531(0) **b** 8.755(0) **c** 10.828(0)
Space Group No.: 2 **(Å, °)** **α** 69.77(0) **β** 69.67(0) **γ** 83.59(0)

R-Factor (%): 2.67 **Temperature(K):** 298 **Density(g/cm³):** 1.575

Parameters

Fragment 1

DIST1 (D) 2.049
DIST2 (D) 2.046
DIST3 (D) 2.046
DIST4 (D) 2.049
DIST5 (D) 2.210
DIST6 (D) 2.210



H₂O

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 205

YOLFOU

Reference: A.Bouayad, J.-C.Trombe, A.Gleizes (1995)
Inorg.Chim.Acta ,**230**,1

Formula: (C₁₂ H₁₂ Ba₂ Cu₁ O₁₈)_n

Compound Name: catena-((μ₆-Squarato)-bis(μ₃-squarato)-tetrakis(μ₂-aqua)-diaqua-di-barium-copper(ii))

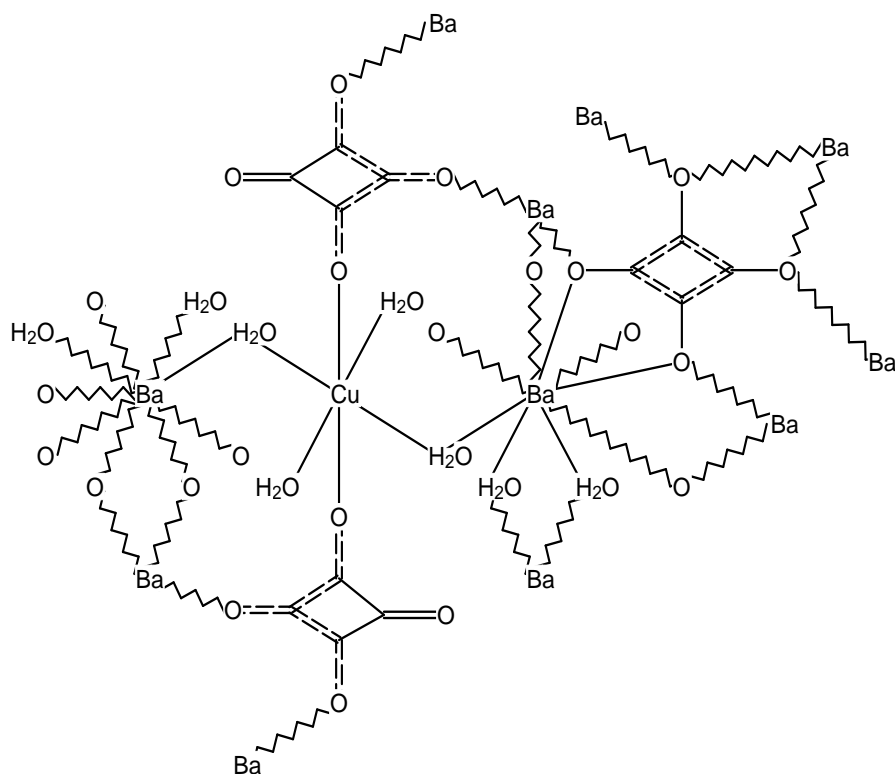
Space Group: P-1 **Cell:** **a** 7.752(1) **b** 10.445(2) **c** 7.420(1)
Space Group No.: 2 (**Å, °**) **α** 99.24(1) **β** 113.20(1) **γ** 109.87(1)

R-Factor (%): 2.60 **Temperature(K):** 295 **Density(g/cm³):** 2.661

Parameters

Fragment 1

DIST1 (D)	1.960
DIST2 (D)	1.945
DIST3 (D)	1.945
DIST4 (D)	1.960
DIST5 (D)	2.533
DIST6 (D)	2.533



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 206

YOXHOK

Reference: I.Bulimestru, S.Shova, N.Popa, P.Roussel, F.Capet, R.-N.Vannier, N.Djelal, L.Burylo, J.-P.Wignacourt, A.Gulea, K.H.Whitmire (2014) *Chem.Mater.* ,26,6092

Formula: $(C_{28} H_{44} Bi_2 Cu_1 N_4 O_{20})_n \cdot n(H_2 O)_1$

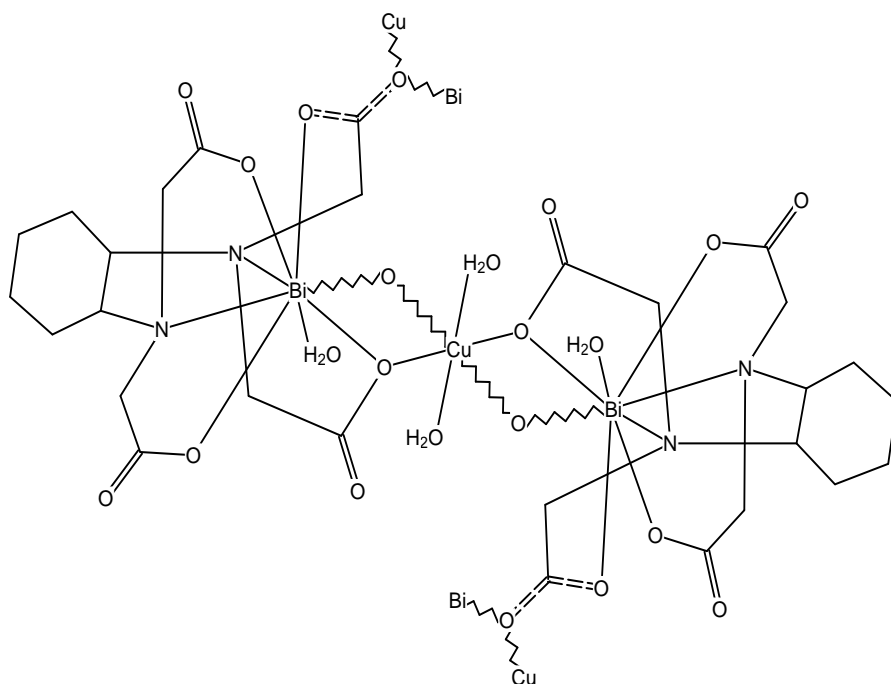
Compound Name: catena-(bis(μ_4 -Cyclohexane-1,2-diamine-N,N,N',N'-tetra-acetato)-tetra-aqua-di-bismuth-copper monohydrate)

Space Group: P-1 **Cell:** **a** 7.323(0) **b** 8.672(0) **c** 14.687(0)
Space Group No.: 2 (**Å, °**) α 94.23(0) β 95.06(0) γ 107.97(0)
R-Factor (%): 1.55 **Temperature(K):** 100 **Density(g/cm³):** 2.374

Parameters

Fragment 1

DIST1 (D) 1.976
DIST2 (D) 1.961
DIST3 (D) 1.976
DIST4 (D) 1.961
DIST5 (D) 2.390
DIST6 (D) 2.390



H₂O

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 207

YUKVOQ

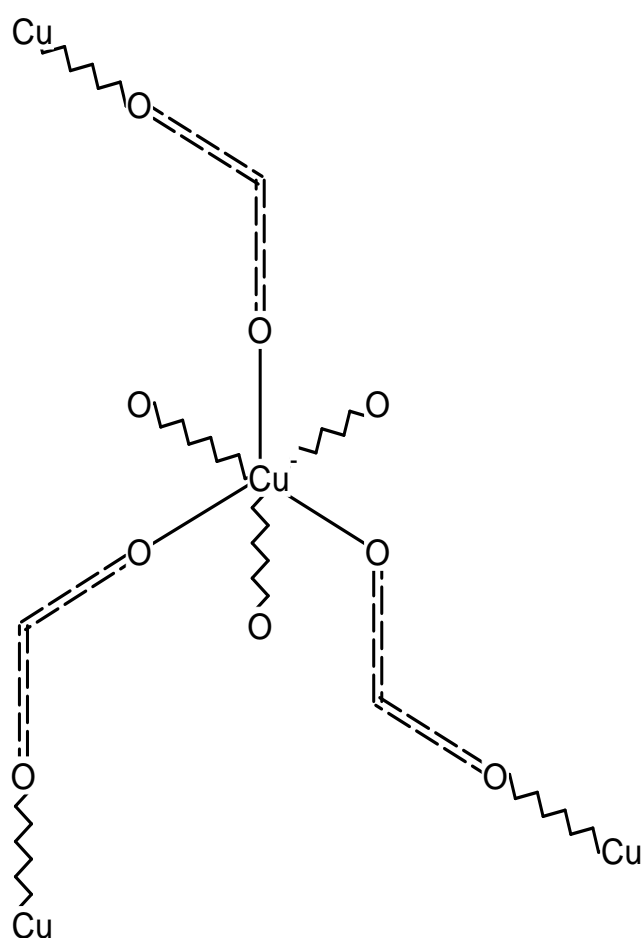
Reference: Ke-Li Hu, M.Kurmoo, Zheming Wang, Song Gao (2009)
Chem.-Eur.J. ,**15**,12050

Formula: (C₃ H₃ Cu₁ O₆¹⁻)_n,n(C₁ H₆ N₃¹⁺)

Compound Name: catena-(Guanidinium tris(μ_2 -formato)-copper(ii))

Space Group: Pna21 **Cell:** **a** 8.521(0) **b** 9.032(0) **c** 11.350(0)
Space Group No.: 33 **(Å, °)** α 90.00 β 90.00 γ 90.00

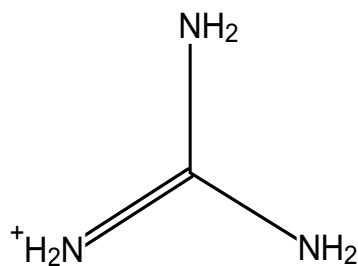
R-Factor (%): 2.80 **Temperature(K):** 293 **Density(g/cm³):** 1.967



Parameters

Fragment 1

DIST1 (D)	1.968
DIST2 (D)	1.996
DIST3 (D)	1.952
DIST4 (D)	2.003
DIST5 (D)	2.383
DIST6 (D)	2.360



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 208

YUNVIM

Reference: N.Barba-Behrens, F.Salazar-Garcia, A.M.Bello-Ramirez, E.Garcia-Baez, M.de.J.Rosales-Hoz, R.Contreras, A.Flores-Parra (1994) *Transition Met.Chem.* ,**19**,575

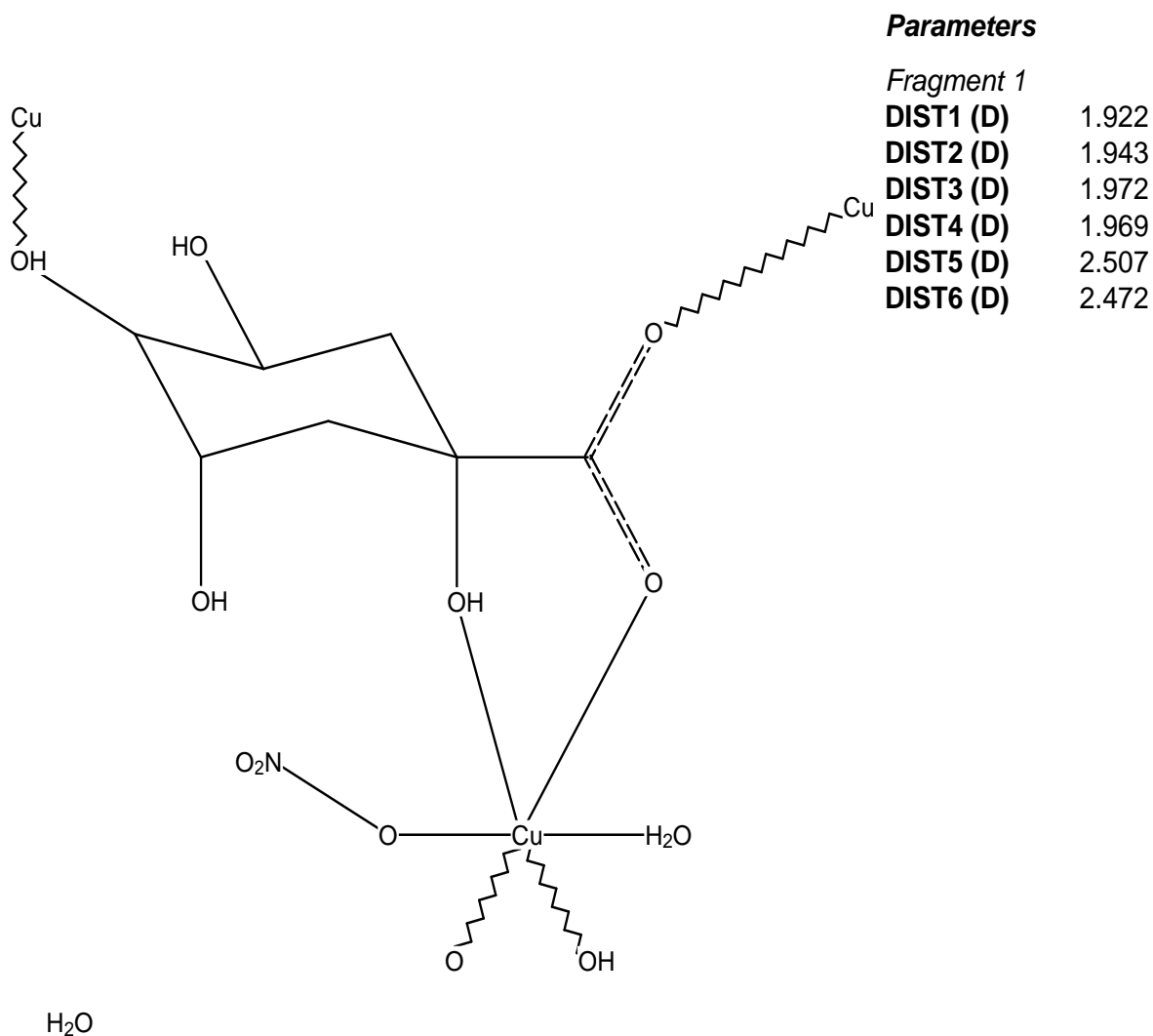
Formula: (C₇ H₁₃ Cu₁ N₁ O₁₀)_n,n(H₂ O₁)

Compound Name: catena-((μ₃-1,3,4,5-Tetrahydroxycyclohexanecarboxylato)-aqua-(nitrate-O)-copper(ii) monohydrate)

Synonym: catena-((μ₃-Quinic acid)-aqua-(nitrate-O)-copper(ii) monohydrate)

Space Group: P212121 **Cell:** **a** 9.721(1) **b** 10.931(1) **c** 11.646(1)
Space Group No.: 19 **(Å, °)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 2.70 **Temperature(K):** 295 **Density(g/cm³):** 1.893



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 209

YURXAM

Reference: J.Landmann, J.A.P.Sprenger, M.Hailmann, V.Bernhardt-Pitchougina, H.Willner, N.Ignat'ev, E.Bernhardt, M.Finze (2015) *Angew.Chem.,Int.Ed.* ,**54**,11259

Formula: C₁₂ H₃₆ Cu₁ O₆ S₆²⁺, C₆ B₂ N₆²⁻

Compound Name: hexakis(dimethyl sulfoxide)-copper(ii) hexacyanodiborate

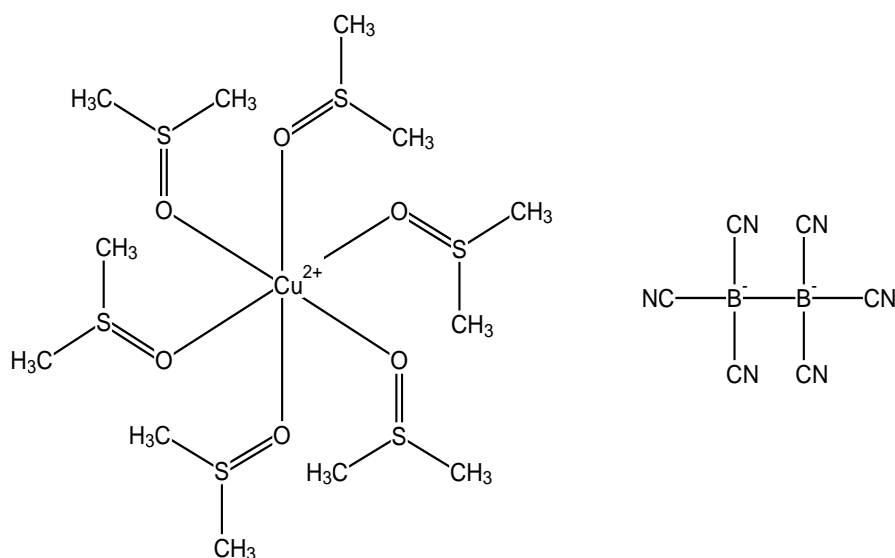
Space Group: P-1 **Cell:** **a** 8.990(1) **b** 9.580(1) **c** 9.642(1)
Space Group No.: 2 **(Å, °)** **α** 87.55(0) **β** 83.57(0) **γ** 89.00(0)

R-Factor (%): 2.87 **Temperature(K):** 100 **Density(g/cm³):** 1.430

Parameters

Fragment 1

DIST1 (D)	1.982
DIST2 (D)	1.996
DIST3 (D)	1.982
DIST4 (D)	1.996
DIST5 (D)	2.387
DIST6 (D)	2.387



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 210

YUSNIK

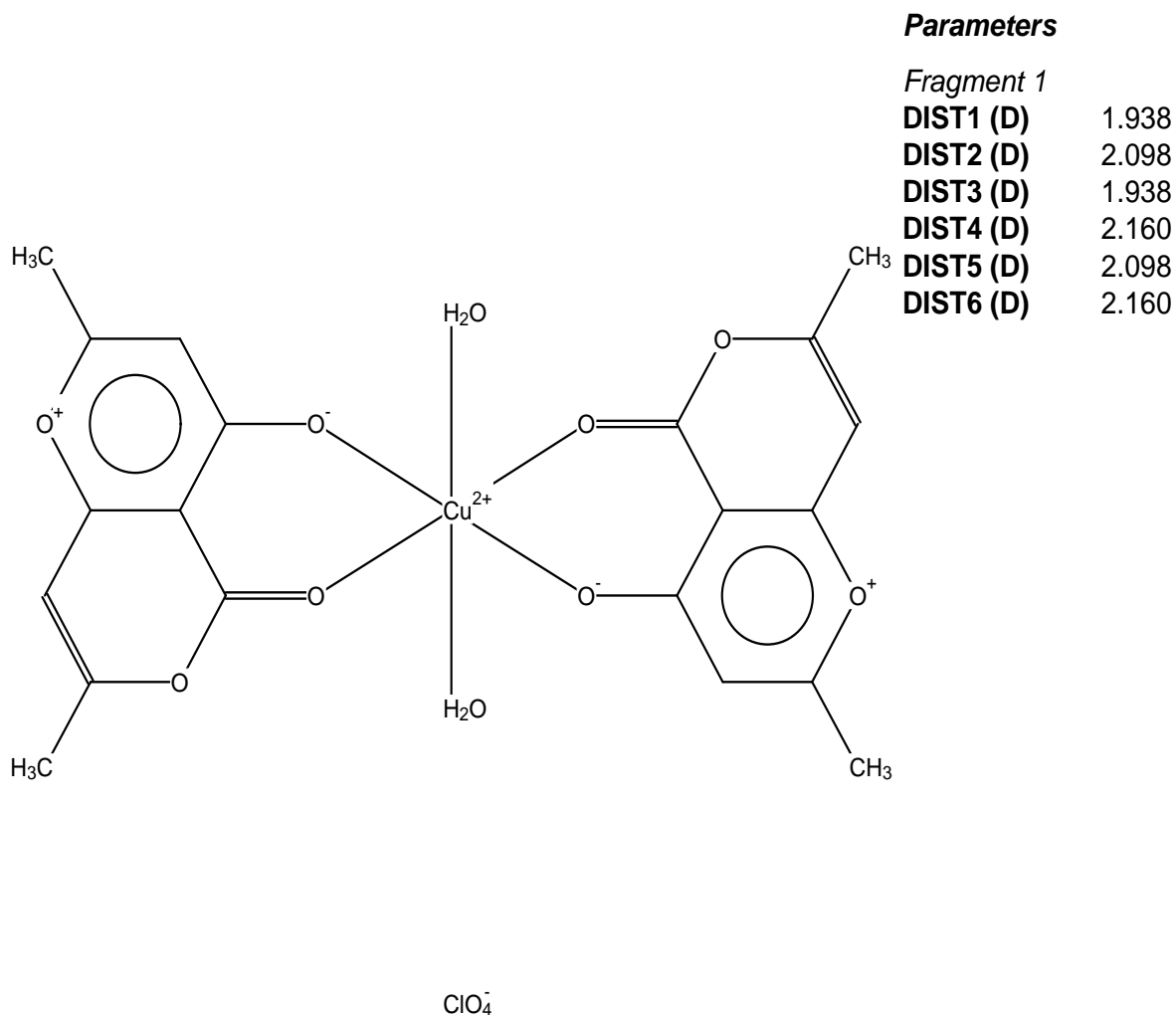
Reference: K.V.Waynant, J.D.White, L.Zakharov (2010)
Chem.Commun. ,46,5304

Formula: C₂₀ H₂₀ Cu₁ O₁₀²⁺, 2(Cl₁ O₄¹⁻)

Compound Name: DIAQUA-BIS(2,7-DIMETHYL-5-OXO-5H-PYRANO(4,3-B)PYRAN-1-IUM-4-OLATO-O,O')-copper(ii) diperchlorate

Space Group: P21/n **Cell:** **a** 9.945(1) **b** 12.641(1) **c** 10.459(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 95.36(0) γ 90.00

R-Factor (%): 2.38 **Temperature(K):** 173 **Density(g/cm³):** 1.732



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 211

YUWHII

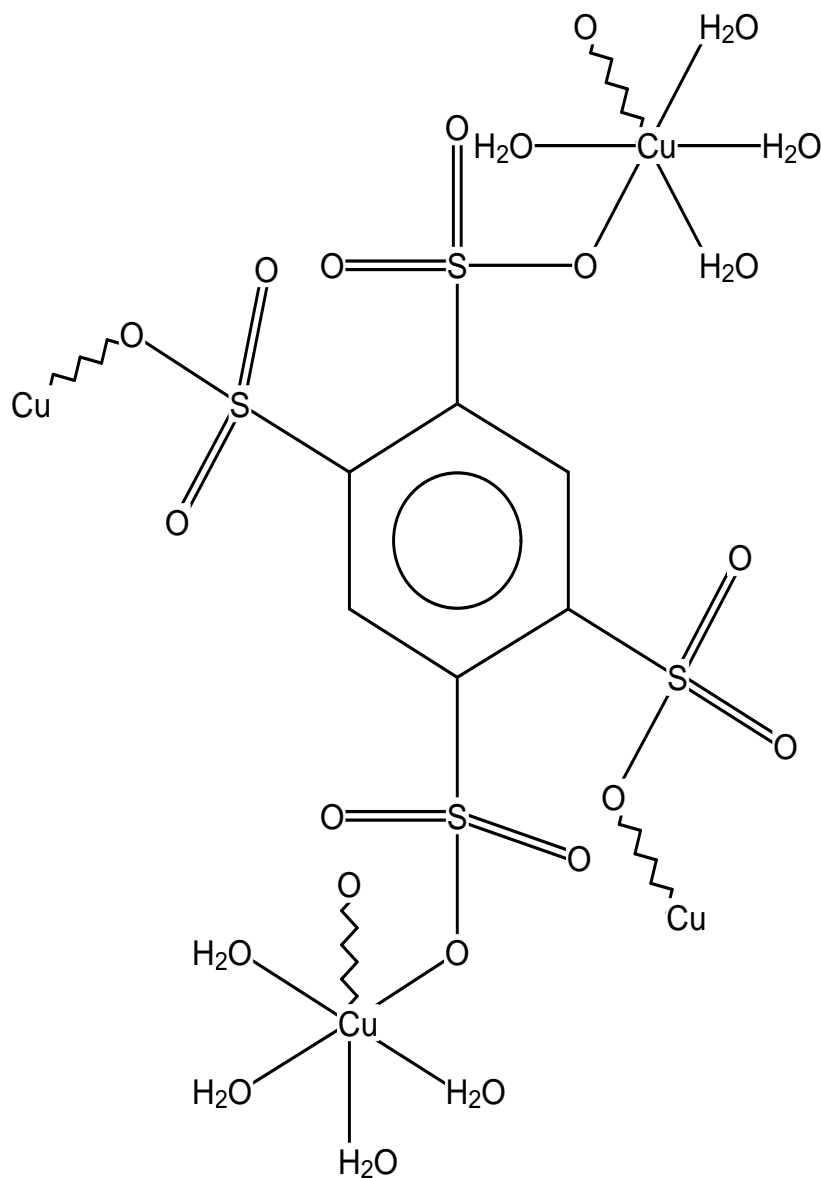
Reference: T.W.T.Muesmann, A.Mietrach, J.Christoffers,
M.S.Wickleder (2010) *Z.Anorg.Allg.Chem.* ,**636**,1307

Formula: $(C_6 H_{18} Cu_2 O_{20} S_4)_n, 0.5n(H_2 O)_1$

Compound Name: catena-((μ_4 -Benzene-1,2,4,5-tetrasulfonato)-octa-aqua-di-copper(ii) hemihydrate)

Space Group: P-1 **Cell:** **a** 7.099(1) **b** 7.137(1) **c** 10.771(1)
Space Group No.: 2 (**Å, °**) α 98.42(1) β 102.91(1) γ 100.69(1)

R-Factor (%): 2.47 **Temperature(K):** 293 **Density(g/cm³):** 2.185



Parameters

Fragment 1

DIST1 (D)	1.965
DIST2 (D)	1.925
DIST3 (D)	1.966
DIST4 (D)	1.960
DIST5 (D)	2.393
DIST6 (D)	2.408

H₂O

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 212

ZADTEG

Reference: Haiyan An, Lin Wang, Ying Hu, Tieqi Xu, Yujiao Hou (2016) *Inorg.Chem.* ,**55**,144

Formula: $H_4 Co_2 Mo_{10} O_{38}^{6-}, H_{12} Cu_1 O_6^{2+}, 4(C_8 H_8 N_1 O_2^{1+}), 5(H_2 O_1)$

Compound Name: tetrakis(4-(2-carboxyethenyl)pyridin-1-ium) hexaaqua-copper tetrakis(μ -hydroxo)-tetradecakis(μ -oxo)-icosaoxo-di-cobalt-deca-molybdenum pentahydrate

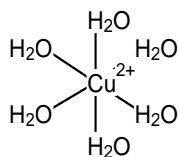
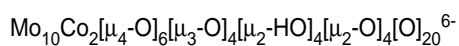
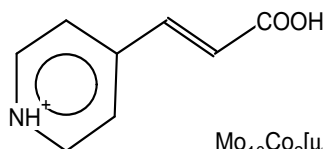
Space Group: P1 **Cell:** **a** 10.016(2) **b** 13.492(2) **c** 13.691(2)
Space Group No.: 1 **(Å, °)** α 104.13(1) β 94.27(1) γ 104.85(1)

R-Factor (%): 2.87 **Temperature(K):** 296 **Density(g/cm³):** 2.470

Parameters

Fragment 1

DIST1 (D)	1.981
DIST2 (D)	2.009
DIST3 (D)	1.988
DIST4 (D)	2.015
DIST5 (D)	2.303
DIST6 (D)	2.296



H₂O

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 213

ZEHLED

Reference: C.Vansant, H.O.Dessey, V.Tangoulis, C.P.Raptopoulou, A.Terzis, S.P.Perlepes (1995) *Polyhedron* ,14,2115

Formula: $C_6 H_{12} Cu_1 N_2 O_8$

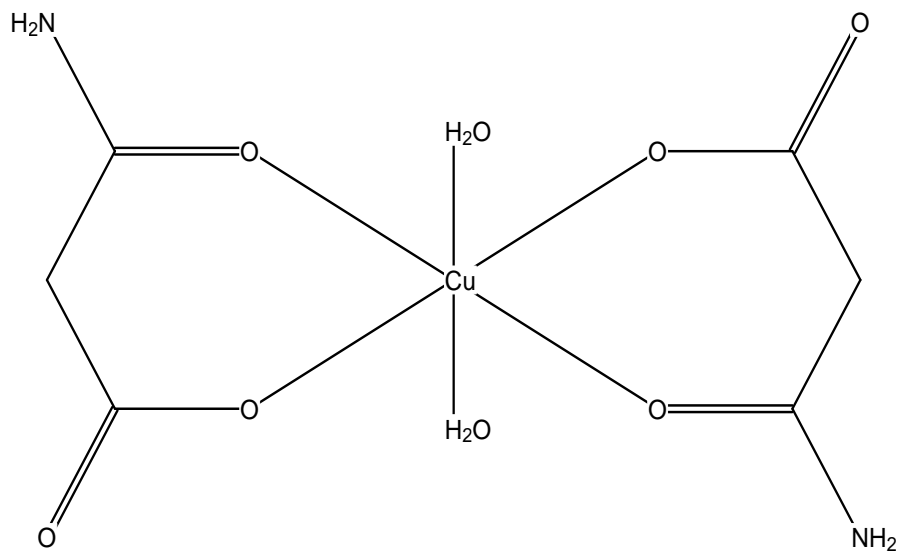
Compound Name: trans-Diaqua-bis(malonamato-O,O')-copper(ii)

Space Group: P21/n **Cell:** **a** 7.068(1) **b** 7.502(1) **c** 9.682(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 100.90(1) γ 90.00

R-Factor (%): 1.90 **Temperature(K):** 295 **Density(g/cm³):** 2.001

Parameters

Fragment 1
DIST1 (D) 1.966
DIST2 (D) 1.934
DIST3 (D) 1.966
DIST4 (D) 1.934
DIST5 (D) 2.480
DIST6 (D) 2.480



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 214

ZUCYON

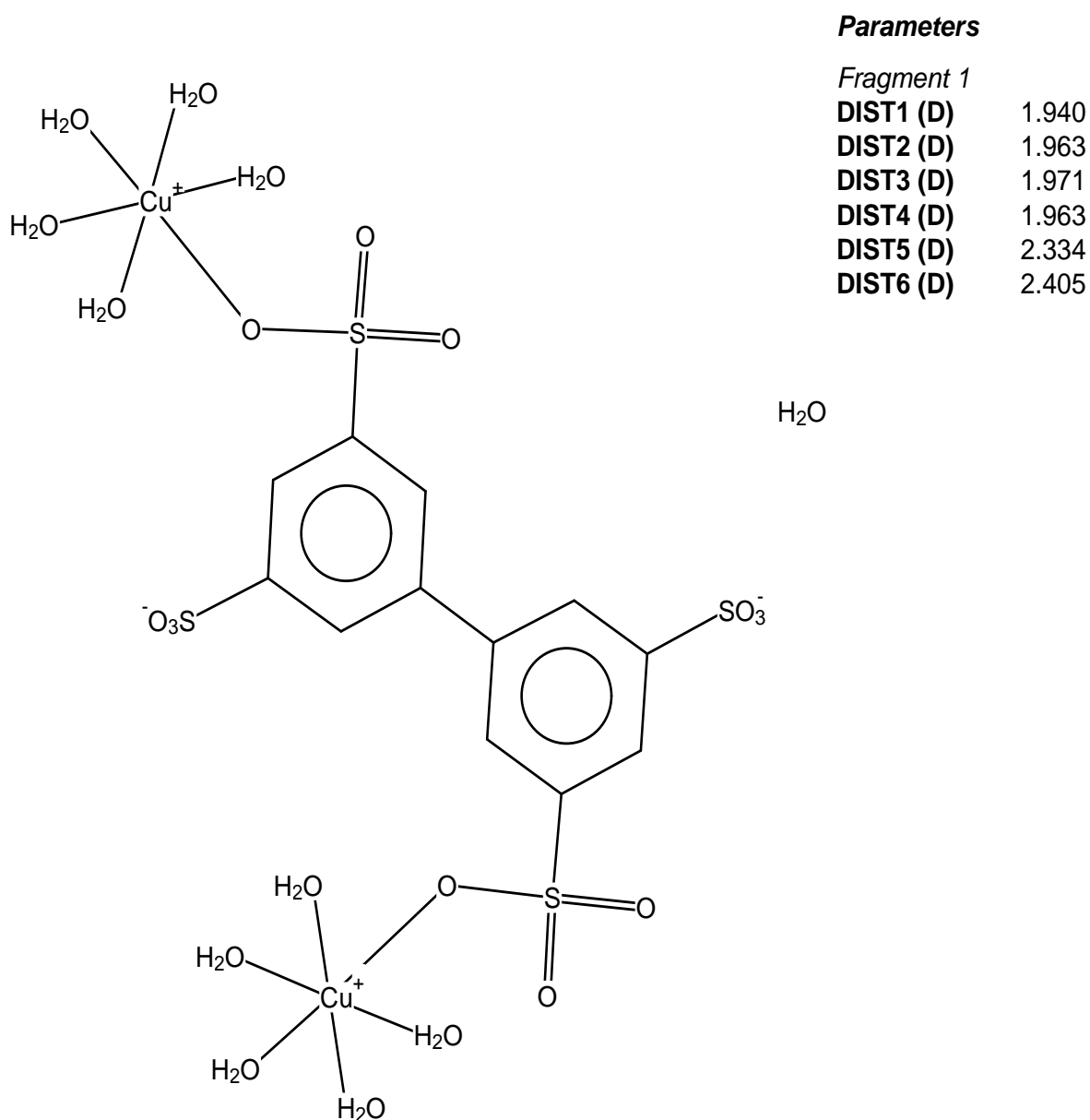
Reference: F.Behler, M.S.Wickleder, J.Christoffers (2015) *ARKIVOC*, 16,64-2

Formula: C₁₂ H₂₆ Cu₂ O₂₂ S₄·2(H₂ O₁)

Compound Name: decaqua-(μ-biphenyl-3,3',5,5'-tetrasulfonato)-di-copper(ii) dihydrate

Space Group: P21/c **Cell:** **a** 5.842(0) **b** 11.265(0) **c** 20.995(1)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 97.50(0) **γ** 90.00

R-Factor (%): 2.37 **Temperature(K):** 120 **Density(g/cm³):** 1.973



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 215

DAMTOD

Reference: A.I.Nicasio, F.Montilla, E.Alvarez, R.P.Colodrero, A.Galindo (2017) *Dalton Trans.* ,46,471

Formula: (C₁₈ H₂₂ Cu₁ N₄ O₈)_n

Compound Name: catena-(bis(μ-(S,S)-2-(3-(1-carboxylatoethyl)-1H-imidazol-3-ium-1-yl)propanoato)-copper)

Space Group: P21212 **Cell:** **a** 13.706(1) **b** 14.275(1) **c** 10.326(0)
Space Group No.: 18 **(Å, °)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 1.92 **Temperature(K):** 193 **Density(g/cm³):** 1.598

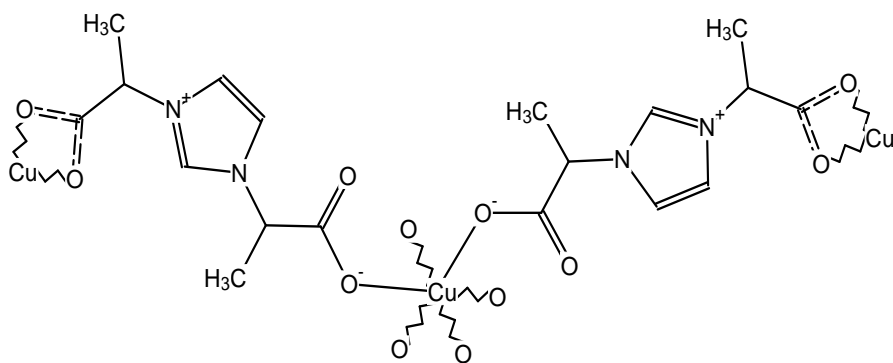
Parameters

Fragment 1

DIST1 (D) 1.973
DIST2 (D) 1.952
DIST3 (D) 1.952
DIST4 (D) 1.973
DIST5 (D) 2.582
DIST6 (D) 2.582

Fragment 2

DIST1 (D) 2.008
DIST2 (D) 1.960
DIST3 (D) 1.960
DIST4 (D) 2.008
DIST5 (D) 2.629
DIST6 (D) 2.629



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 216

IYODEH

Reference: Bowen Cong, Zhanhua Su, Zhifeng Zhao, Wenqi Zhao, Lin Xia, Baibin Zhou (2016) *Polyhedron* ,

Formula: $4(\text{C}_7\text{H}_{11}\text{N}_2^{1+}), \text{As}_6\text{Cu}_1\text{Mo}_6\text{O}_{30}^{4-}$

Compound Name: tetrakis(4-(dimethylamino)pyridinium) octadecakis(μ -oxo)-dodeca-oxo-hexa-arsenic(iii)-copper(ii)-hexa-molybdenum(vi)

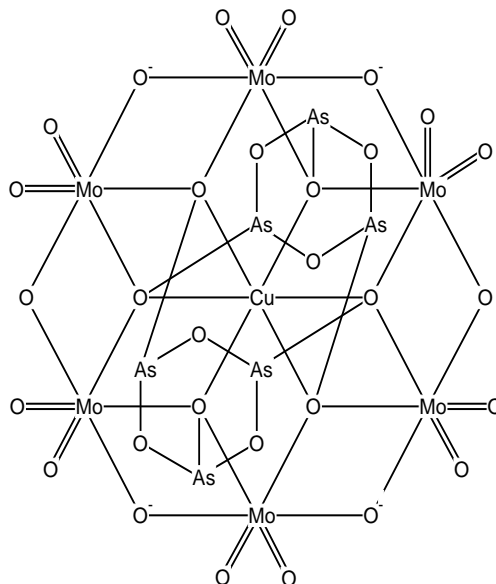
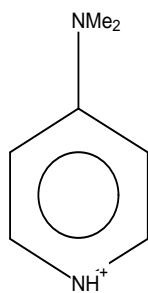
Space Group: P21/c **Cell:** **a** 9.391(0) **b** 19.964(1) **c** 14.837(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 95.98(0) γ 90.00

R-Factor (%): 2.74 **Temperature(K):** 296 **Density(g/cm³):** 2.475

Parameters

Fragment 1

DIST1 (D) 2.057
DIST2 (D) 1.992
DIST3 (D) 2.057
DIST4 (D) 1.992
DIST5 (D) 2.201
DIST6 (D) 2.201



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 217

IZAHUO

Reference: S.Adhikari, A.Sahana, B.Kumari, Durba Ganguly, S.Das, P.P.Banerjee, G.Banerjee, A.Chattopadhyay, M.Fondo, J.S.Matalobos, P.Brandao, V.Felix, D.Das (2016) *New J.Chem.* ,**40**,10378

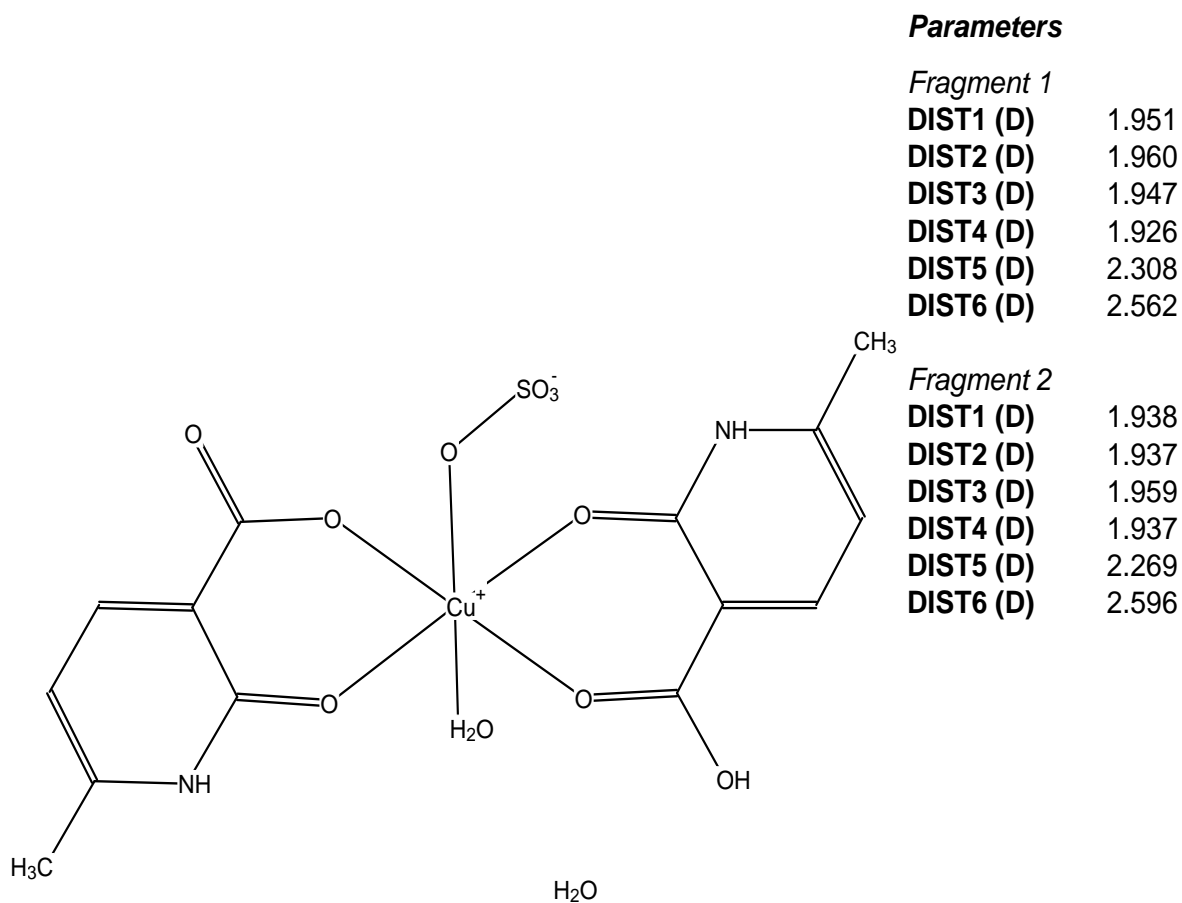
Formula: C₁₄ H₁₅ Cu₁ N₂ O₁₁ S_{1,2}(H₂ O₁)

Compound Name: aqua-(6-methyl-2-(oxo)-1,2-dihydropyridine-3-carboxylato)-(6-methyl-2-(oxo)-1,2-dihydropyridine-3-carboxylic acid)-(sulfato)-copper dihydrate

Space Group: P21 **Cell:** **a** 8.773(0) **b** 13.745(0) **c** 16.607(0)

Space Group No.: 4 **(Å, °)** **α** 90.00 **β** 93.65(0) **γ** 90.00

R-Factor (%): 2.55 **Temperature(K):** 100 **Density(g/cm³):** 1.725



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 218

IZERIQ

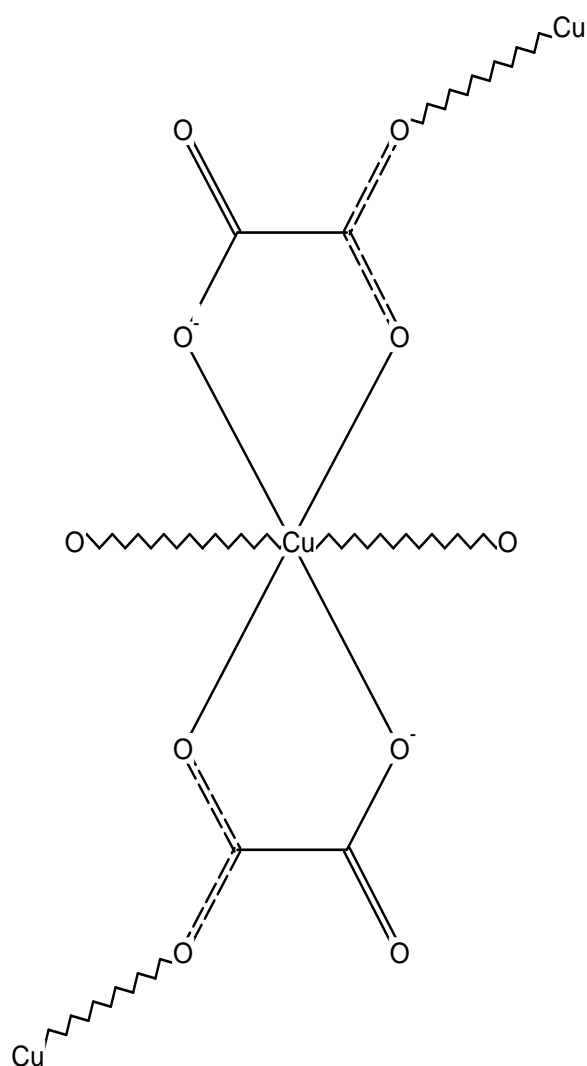
Reference: D.A.Dickie, R.A.Kemp (2016)
Acta Crystallogr., Sect.E:Cryst.Commun. ,72,1780

Formula: $(C_4 Cu_1 O_8^{2-})_n \cdot 2(H_4 N_1^{1+})$

Compound Name: catena-(bis(ammonium) bis(μ -oxalato)-copper(ii))

Space Group: P21/c **Cell:** **a** 4.856(0) **b** 13.519(0) **c** 6.721(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 96.99(0) γ 90.00

R-Factor (%): 1.79 **Temperature(K):** 100 **Density(g/cm³):** 2.090



Parameters

Fragment 1

DIST1 (D)	1.933
DIST2 (D)	1.930
DIST3 (D)	1.933
DIST4 (D)	1.930
DIST5 (D)	2.706
DIST6 (D)	2.706

NH₄⁺

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 219

TEMPIM01

Reference: Zhang Bin (2016)
CSD Communication(Private Communication) ,

Formula: $2(\text{C}_4\text{H}_{12}\text{N}_1^{1+}), (\text{C}_4\text{Cu}_1\text{O}_8^{2-})_n, \text{H}_2\text{O}_1$

Compound Name: catena-[bis(tetramethylammonium) (μ -oxalato)-(oxalato)-copper monohydrate]

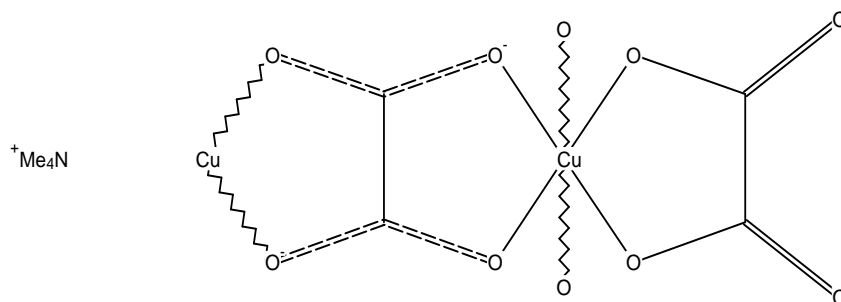
Space Group: Pbcu **Cell:** **a** 11.246(0) **b** 10.139(0) **c** 30.992(0)
Space Group No.: 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.73 **Temperature(K):** 293 **Density(g/cm³):** 1.526

Parameters

Fragment 1

DIST1 (D) 1.968
DIST2 (D) 1.954
DIST3 (D) 1.981
DIST4 (D) 1.975
DIST5 (D) 2.319
DIST6 (D) 2.432



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 220

UCADEK

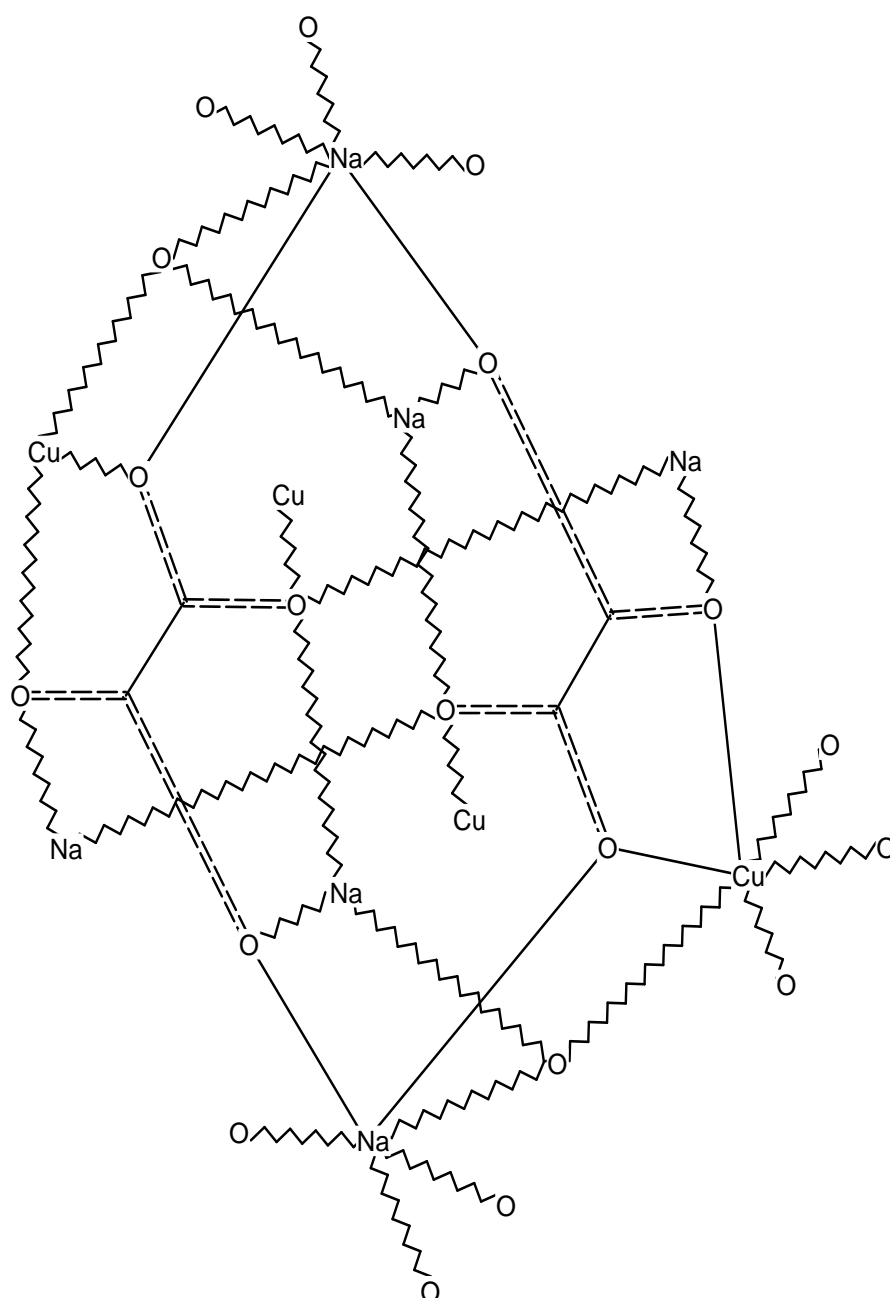
Reference: Wenjiao Yao, A.Robert Armstrong, Philip Lightfoot (2016)
Z.Anorg.Allg.Chem. ,**642**,1345

Formula: $(C_4 Cu_1 Na_2 O_8)_n$

Compound Name: catena-[bis(μ -oxalato)-copper(ii)-di-sodium(i)]

Space Group: P21/n **Cell:** **a** 7.258(0) **b** 5.771(0) **c** 8.660(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 106.95(0) γ 90.00

R-Factor (%): 2.00 **Temperature(K):** 173 **Density(g/cm³):** 2.733



Parameters

Fragment 1

DIST1 (D)	1.939
DIST2 (D)	1.962
DIST3 (D)	1.939
DIST4 (D)	1.962
DIST5 (D)	2.652
DIST6 (D)	2.652

Search: search2 (Wed Jul 26 09:11:25 2017): Hit 221

UXETAU

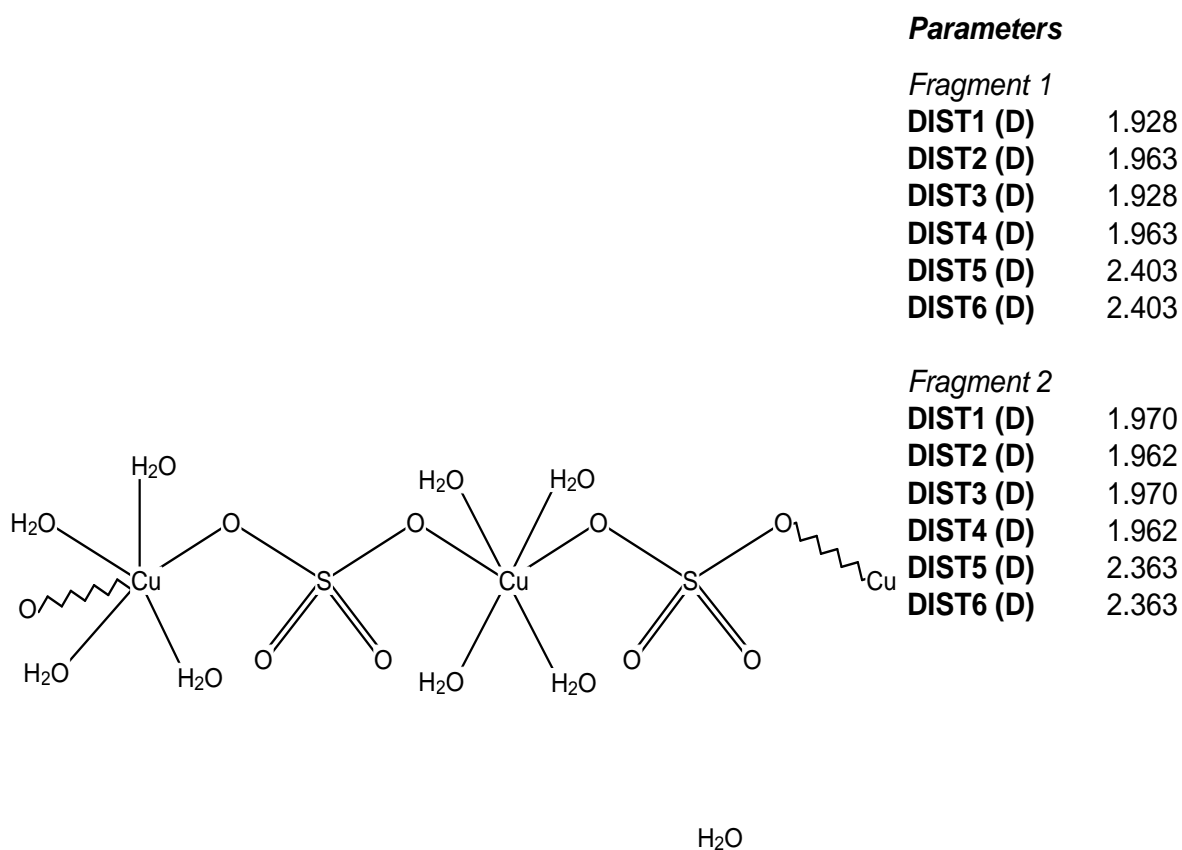
Reference: A.I.Vinokur, I.A.Guzei (2016)
CSD Communication(Private Communication) ,

Formula: $(H_{16} Cu_2 O_{16} S_2)_n \cdot 2(H_2 O)_1$

Compound Name: catena-[bis(μ -sulfato)-octa-aquadi-copper(ii) dihydrate]

Space Group: P-1 **Cell:** **a** 5.963(1) **b** 6.084(1) **c** 10.623(2)
Space Group No.: 2 **(Å, °)** α 77.23(3) β 82.56(3) γ 72.50(3)

R-Factor (%): 2.77 **Temperature(K):** 100 **Density(g/cm³):** 2.318



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 222

UXISAX

Reference: S.Yoneyama, T.Kodama, K.Kikuchi, T.Fujisawa,
A.Yamaguchi, A.Sumiyama, Yoshiaki Shuku, Shinobu Aoyagi, W.Fujita
(2016) *Dalton Trans.* ,**45**,16774

Formula: (C₄ H₆ Cu₁ O₆)_n

Compound Name: catena-[bis(μ-glycolato)-copper(ii)]

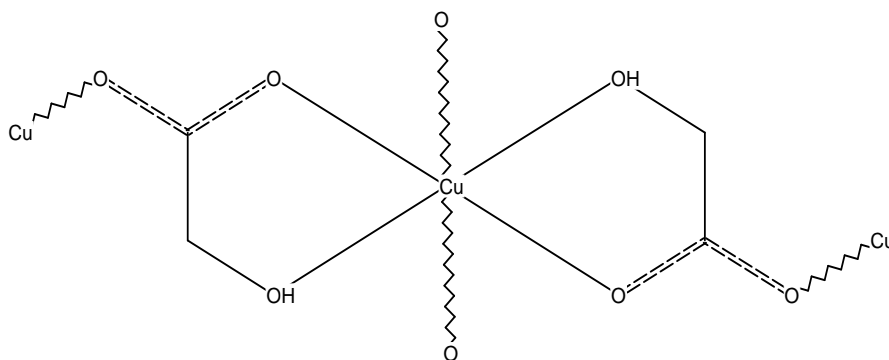
Space Group: P21/n **Cell:** **a** 5.185(1) **b** 7.252(1) **c** 8.875(3)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 100.86(0) **γ** 90.00

R-Factor (%): 2.13 **Temperature(K):** 173 **Density(g/cm³):** 2.165

Parameters

Fragment 1

DIST1 (D) 1.928
DIST2 (D) 1.966
DIST3 (D) 1.928
DIST4 (D) 1.966
DIST5 (D) 2.435
DIST6 (D) 2.435



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 223

UXISAX01

Reference: S.Yoneyama, T.Kodama, K.Kikuchi, T.Fujisawa, A.Yamaguchi, A.Sumiyama, Yoshiaki Shuku, Shinobu Aoyagi, W.Fujita (2016) *Dalton Trans.* ,**45**,16774

Formula: (C₄ H₆ Cu₁ O₆)_n

Compound Name: catena-[bis(μ-glycolato)-copper(ii)]

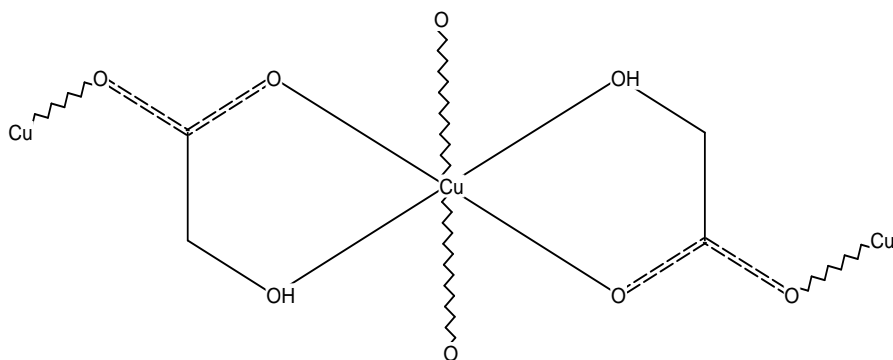
Space Group: P21/n **Cell:** **a** 5.079(0) **b** 8.692(0) **c** 7.705(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 107.34(0) γ 90.00

R-Factor (%): 2.28 **Temperature(K):** 230 **Density(g/cm³):** 2.185

Parameters

Fragment 1

DIST1 (D) 1.922
DIST2 (D) 1.932
DIST3 (D) 1.922
DIST4 (D) 1.932
DIST5 (D) 2.522
DIST6 (D) 2.522



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 224

UXISAX02

Reference: S.Yoneyama, T.Kodama, K.Kikuchi, T.Fujisawa,
A.Yamaguchi, A.Sumiyama, Yoshiaki Shuku, Shinobu Aoyagi, W.Fujita
(2016) *Dalton Trans.* ,**45**,16774

Formula: (C₄ H₆ Cu₁ O₆)_n

Compound Name: catena-[bis(μ-glycolato)-copper(ii)]

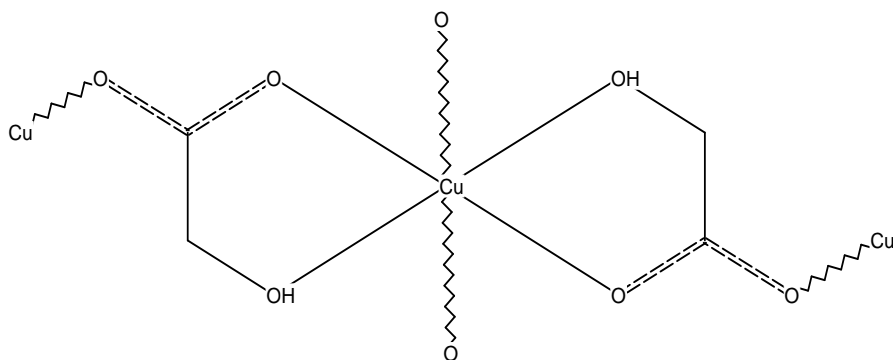
Space Group: P21/n **Cell:** **a** 5.201(4) **b** 7.356(5) **c** 8.839(6)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 101.17(0) **γ** 90.00

R-Factor (%): 2.68 **Temperature(K):** 290 **Density(g/cm³):** 2.139

Parameters

Fragment 1

DIST1 (D)	1.926
DIST2 (D)	1.960
DIST3 (D)	1.926
DIST4 (D)	1.960
DIST5 (D)	2.439
DIST6 (D)	2.439



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 225

UXISAX04

Reference: S.Yoneyama, T.Kodama, K.Kikuchi, T.Fujisawa, A.Yamaguchi, A.Sumiyama, Yoshiaki Shuku, Shinobu Aoyagi, W.Fujita (2016) *Dalton Trans.* ,**45**,16774

Formula: (C₄ H₆ Cu₁ O₆)_n

Compound Name: catena-[bis(μ-glycolato)-copper(ii)]

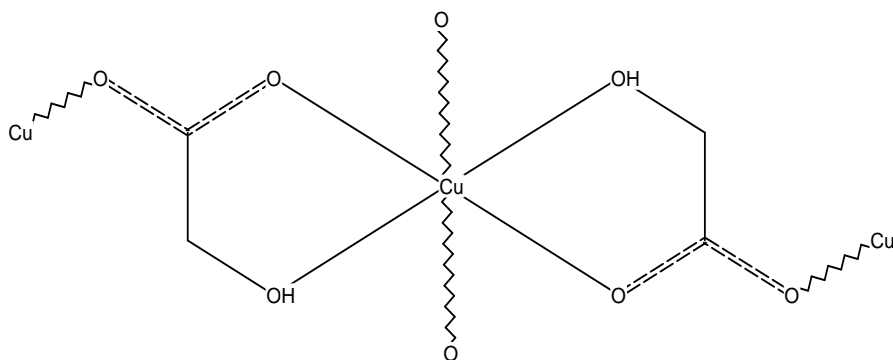
Space Group: P21/n **Cell:** **a** 5.101(3) **b** 8.673(5) **c** 7.747(5)
Space Group No.: 14 **(Å, °)** α 90.00 β 106.93(0) γ 90.00

R-Factor (%): 2.81 **Temperature(K):** 290 **Density(g/cm³):** 2.164

Parameters

Fragment 1

DIST1 (D)	1.919
DIST2 (D)	1.932
DIST3 (D)	1.919
DIST4 (D)	1.932
DIST5 (D)	2.538
DIST6 (D)	2.538



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 226

UXISAX05

Reference: S.Yoneyama, T.Kodama, K.Kikuchi, T.Fujisawa,
A.Yamaguchi, A.Sumiyama, Yoshiaki Shuku, Shinobu Aoyagi, W.Fujita
(2016) *Dalton Trans.* ,**45**,16774

Formula: (C₄ H₆ Cu₁ O₆)_n

Compound Name: catena-[bis(μ-glycolato)-copper(ii)]

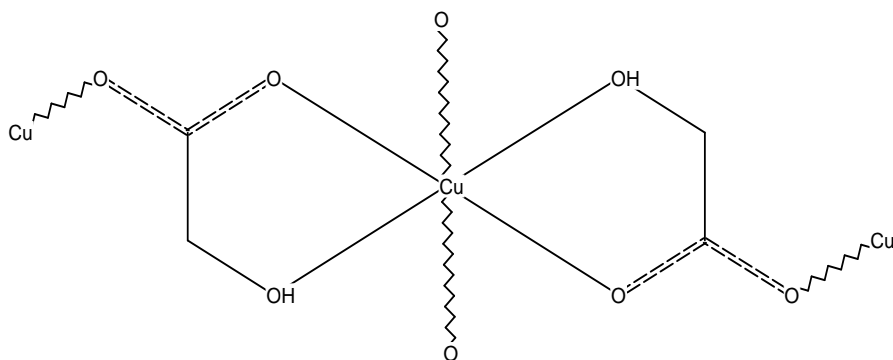
Space Group: P21/n **Cell:** **a** 5.110(6) **b** 8.680(1) **c** 7.748(9)
Space Group No.: 14 **(Å, °)** α 90.00 β 106.73(1) γ 90.00

R-Factor (%): 2.64 **Temperature(K):** 290 **Density(g/cm³):** 2.156

Parameters

Fragment 1

DIST1 (D)	1.917
DIST2 (D)	1.936
DIST3 (D)	1.917
DIST4 (D)	1.936
DIST5 (D)	2.542
DIST6 (D)	2.542



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 227

UXISAX06

Reference: S.Yoneyama, T.Kodama, K.Kikuchi, T.Fujisawa,
A.Yamaguchi, A.Sumiyama, Yoshiaki Shuku, Shinobu Aoyagi, W.Fujita
(2016) *Dalton Trans.* ,**45**,16774

Formula: (C₄ H₆ Cu₁ O₆)_n

Compound Name: catena-[bis(μ-glycolato)-copper(ii)]

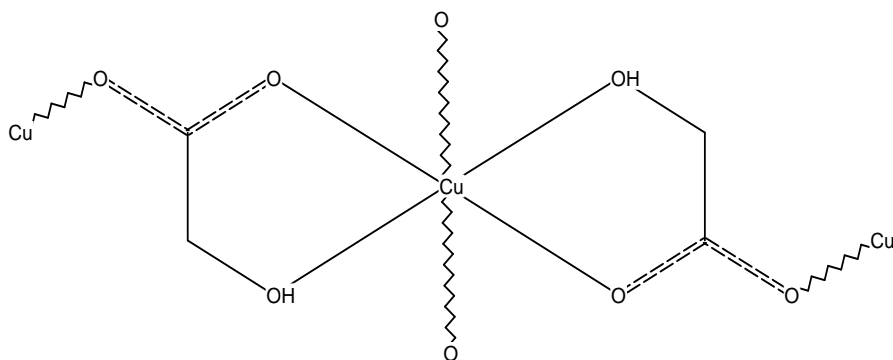
Space Group: P21/n **Cell:** **a** 5.108(2) **b** 8.677(3) **c** 7.755(3)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 106.81(0) **γ** 90.00

R-Factor (%): 2.65 **Temperature(K):** 290 **Density(g/cm³):** 2.156

Parameters

Fragment 1

DIST1 (D)	1.919
DIST2 (D)	1.935
DIST3 (D)	1.919
DIST4 (D)	1.935
DIST5 (D)	2.539
DIST6 (D)	2.539



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 228

HARKOD

Reference: F.Zhang, B.-G.Zhang (2017)
Acta Crystallogr., Sect.E:Cryst. Commun. ,73,835

Formula: (C₁₈ H₁₀ Ca₂ Cu₁ O₁₄)_n

Compound Name: catena-[bis(μ-benzene-1,3,5-tricarboxylato)-diaqua-di-calcium(ii)-copper(ii)]

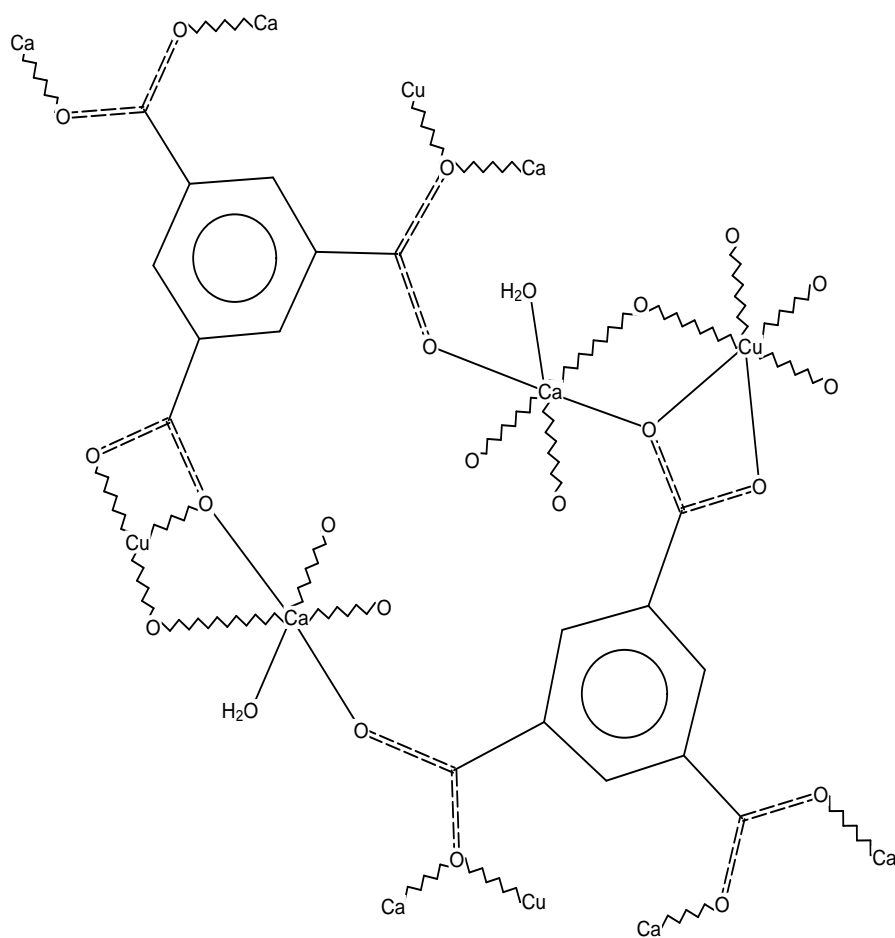
Space Group: P-1 **Cell:** **a** 6.664(3) **b** 8.754(4) **c** 8.925(4)
Space Group No.: 2 **(Å, °)** **α** 103.06(0) **β** 110.14(0) **γ** 92.78(0)

R-Factor (%): 2.87 **Temperature(K):** 296 **Density(g/cm³):** 2.091

Parameters

Fragment 1

DIST1 (D)	1.980
DIST2 (D)	1.943
DIST3 (D)	1.943
DIST4 (D)	1.980
DIST5 (D)	2.770
DIST6 (D)	2.770



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 229

KARHOD

Reference: G.Smith, U.D.Wermuth (2017)
Acta Crystallogr., Sect. C: Cryst. Struct. Chem., **73**, 325

Formula: $2(\text{C}_6\text{H}_9\text{As}_1\text{N}_1\text{O}_3^{1+}), \text{H}_{12}\text{Cu}_1\text{O}_6^{2+}, 2(\text{O}_4\text{S}_1^{2-}), 2(\text{H}_2\text{O}_1)$

Compound Name: hexaaqua-copper(ii) bis(4-arsonoanilinium) disulfate dihydrate

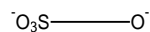
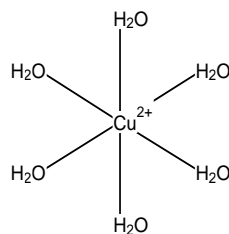
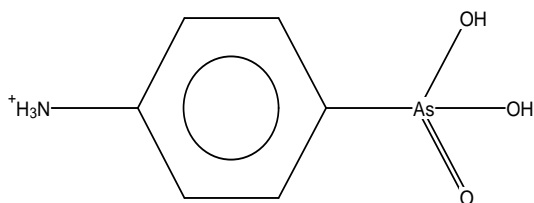
Space Group: P21/c **Cell:** **a** 15.078(0) **b** 11.230(0) **c** 8.676(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 99.31(0) γ 90.00

R-Factor (%): 2.74 **Temperature(K):** 200 **Density(g/cm³):** 1.915

Parameters

Fragment 1

DIST1 (D)	1.946
DIST2 (D)	2.013
DIST3 (D)	1.946
DIST4 (D)	2.013
DIST5 (D)	2.270
DIST6 (D)	2.270



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 230

KEDJAG04

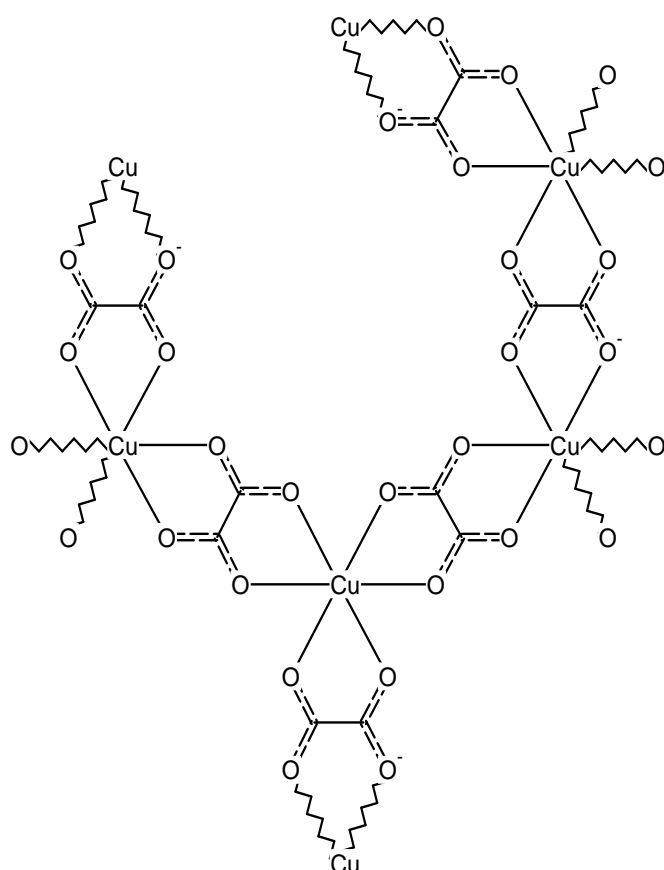
Reference: Zhang Bin (2017)
CSD Communication(Private Communication) ,

Formula: $(C_{12} Cu_4 O_{24}^{4-})_n, 4(C_6 H_{16} N_1^{1+})$

Compound Name: catena-(tetrakis(Triethylammonium) hexakis(μ_2 -oxalato)-tetra-copper)

Space Group: P21/c **Cell:** **a** 8.682(0) **b** 34.180(0) **c** 8.582(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 107.60(0) γ 90.00

R-Factor (%): 2.85 **Temperature(K):** 93 **Density(g/cm³):** 1.630



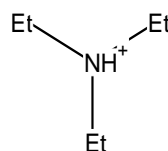
Parameters

Fragment 1

DIST1 (D)	1.992
DIST2 (D)	1.986
DIST3 (D)	1.957
DIST4 (D)	1.991
DIST5 (D)	2.258
DIST6 (D)	2.318

Fragment 2

DIST1 (D)	1.976
DIST2 (D)	1.997
DIST3 (D)	1.955
DIST4 (D)	1.995
DIST5 (D)	2.228
DIST6 (D)	2.331



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 231

KEDJAG10

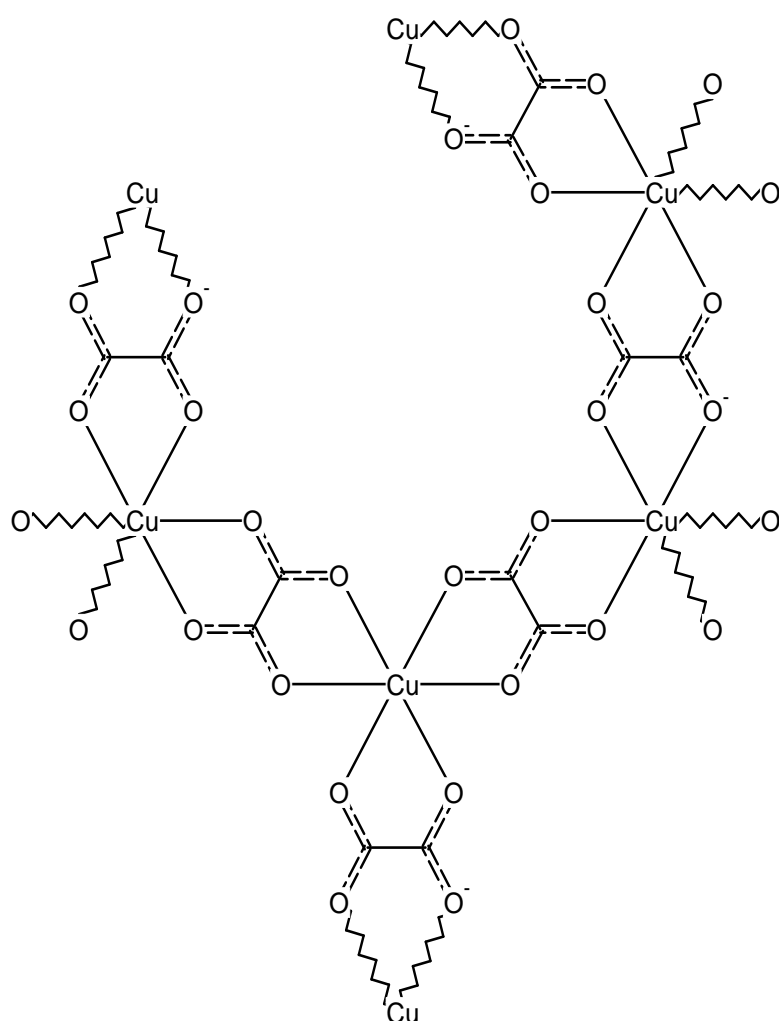
Reference: Zhang Bin (2017)
CSD Communication(Private Communication) ,

Formula: $(C_{12} Cu_4 O_{24}^{4-})_n, 4(C_6 H_{16} N_1^{1+})$

Compound Name: catena-(tetrakis(Triethylammonium) hexakis(μ_2 -oxalato)-tetra-copper)

Space Group: P21/c **Cell:** **a** 8.716(0) **b** 34.081(0) **c** 8.636(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 107.63(0) γ 90.00

R-Factor (%): 2.90 **Temperature(K):** 155 **Density(g/cm³):** 1.618



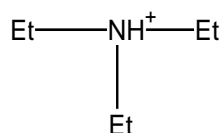
Parameters

Fragment 1

DIST1 (D)	2.011
DIST2 (D)	2.007
DIST3 (D)	1.958
DIST4 (D)	1.989
DIST5 (D)	2.240
DIST6 (D)	2.293

Fragment 2

DIST1 (D)	1.976
DIST2 (D)	2.020
DIST3 (D)	1.958
DIST4 (D)	2.013
DIST5 (D)	2.209
DIST6 (D)	2.304



Search: search2 (Wed Jul 26 09:11:25 2017): Hit 232

LAVFEW

Reference: M.Puchonova, M.Mazur, Jan Moncol, Z.Ruzickova,
D.Valigura (2017) *J.Mol.Struct.* ,**1137**,706

Formula: (C₁₄ H₁₀ Br₄ Cu₁ O₈)_n

Compound Name: catena-(bis(μ -3,5-dibromo-2-hydroxybenzoato)-diaqua-copper(ii))

Space Group: C2/c **Cell:** **a** 32.419(7) **b** 4.516(0) **c** 13.126(3)
Space Group No.: 15 **(Å, °)** α 90.00 β 106.75(3) γ 90.00

R-Factor (%): 2.79 **Temperature(K):** 150 **Density(g/cm³):** 2.488

