

Search Overview

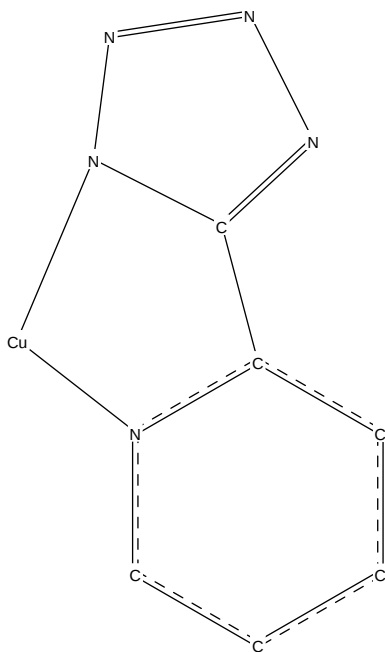
Search:	search1
Date/Time done:	Fri Sep 12 09:25:06 2025
Database(s):	CSD version 5.45 updates (Mar 2024) CSD version 5.45 (November 2023)
Restriction Info:	No refcode restrictions applied
Filters:	None
Percentage Completed:	100%
Number of Hits:	26

Single query used. Search found structures that:

match

Query 1

Query 1



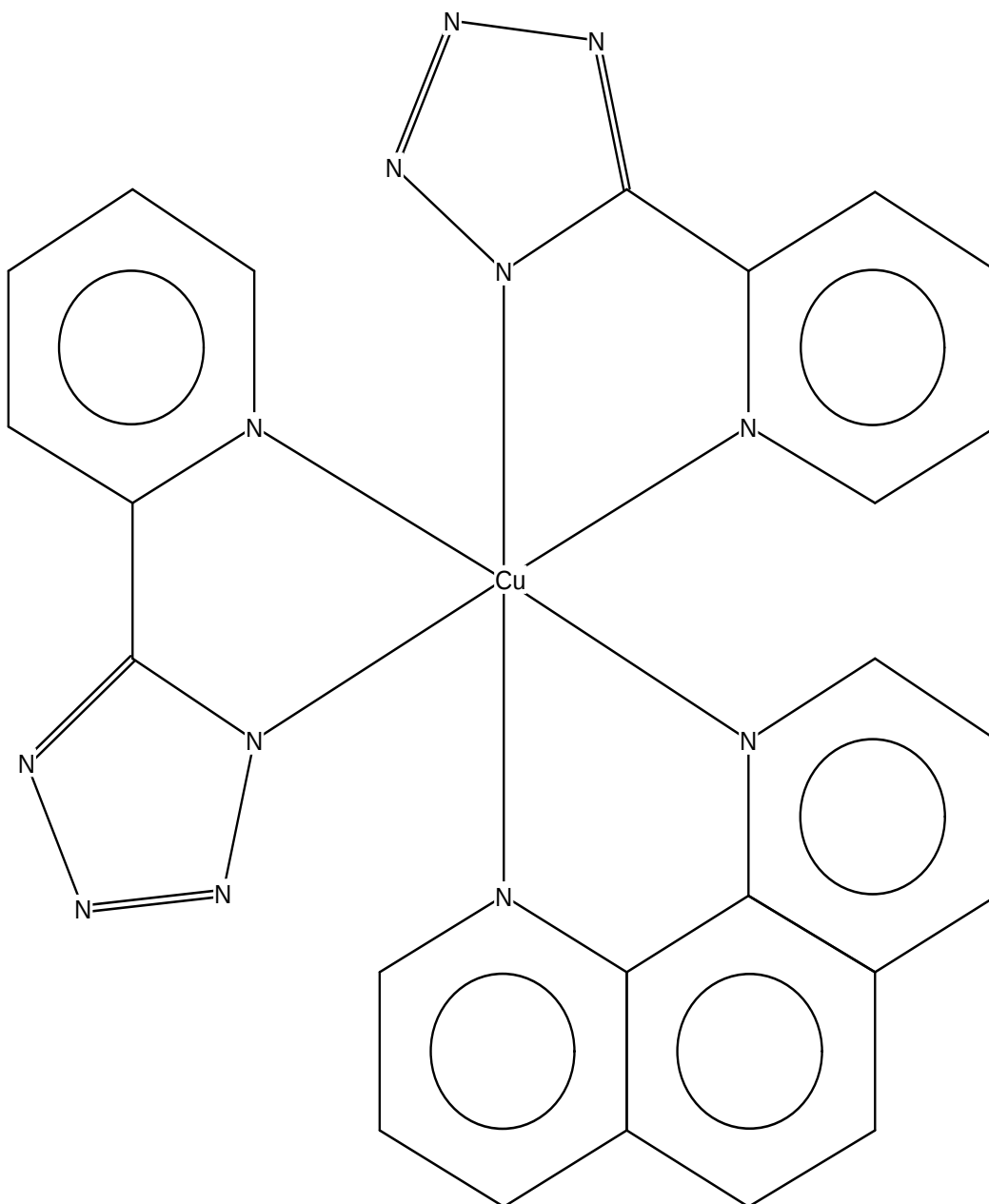
HAVBIS

Reference: M.Saha, K.M.Vyas, L.M.D.R.S.Martins, N.M.R.Martins, A.J.L.Pombeiro, S.M.Mobin, D.Bhattacharjee, K.P.Bhabak, S.Mukhopadhyay (2017) *Polyhedron* ,**132**,53

Formula: C₂₄ H₁₆ Cu₁ N₁₂

Compound Name: (1,10-phenanthroline)-bis(5-(pyridin-2-yl)tetrazol-1-yl)-copper(ii)

Space Group:	Pbcn	Cell:	a 14.247(0)	b 10.106(0)	c 15.772(0)
Space Group No.:	60	(Å, °)	α 90.00	β 90.00	γ 90.00
R-Factor (%):	3.47	Temperature(K):	150	Density(g/cm³):	1.568



Search: search1 (Fri Sep 12 09:25:06 2025): Hit 2

KAHXID

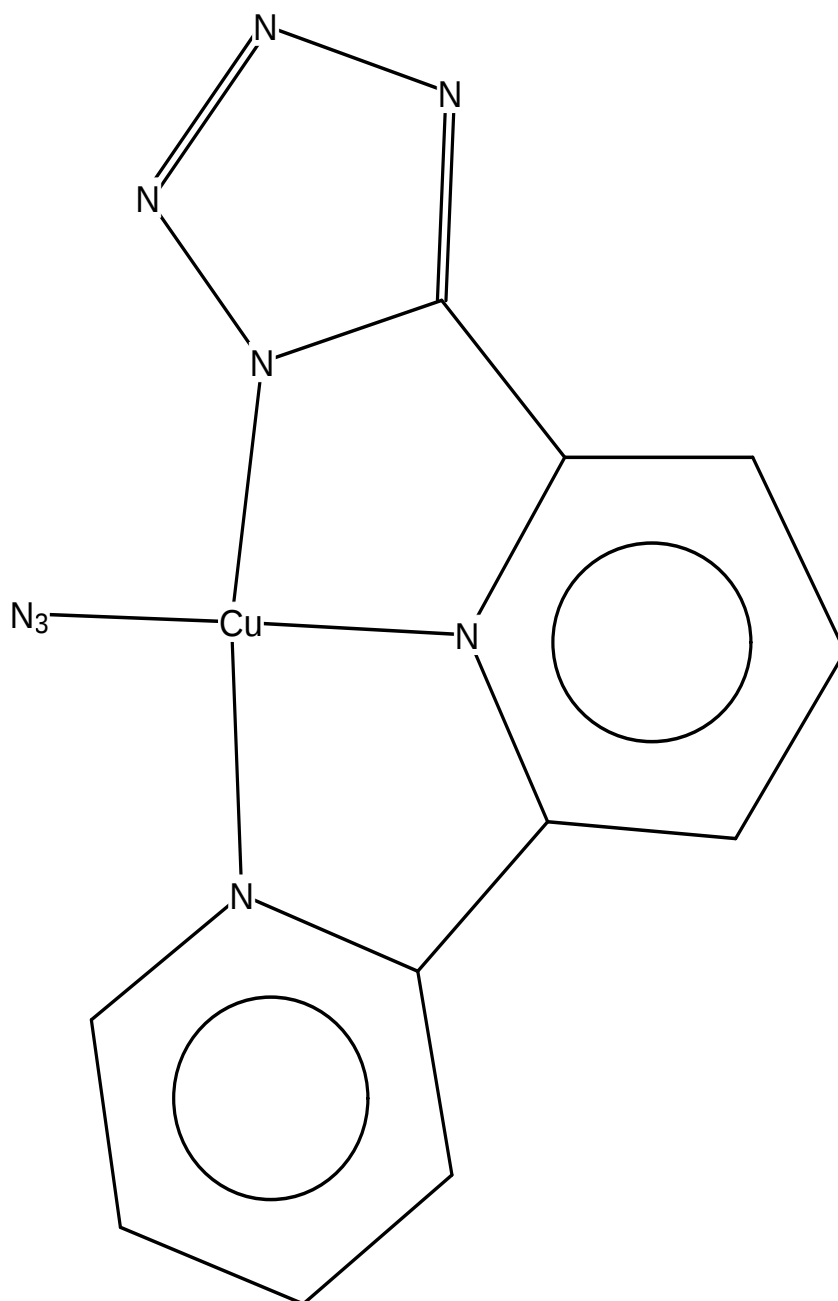
Reference: Jung-Yu Tsao, Jia-Dong Tsai, C.-I. Yang (2016)
Dalton Trans. ,**45**,3388

Formula: C₁₁ H₇ Cu₁ N₉

Compound Name: azido-(6-(1H-tetrazol-5-yl)-2,2'-bipyridinato)-copper(ii)

Space Group:	P21/c	Cell:	a	6.777(0)	b	20.701(1)	c	8.396(0)
Space Group No.:	14	(Å, °)	α	90.00	β	91.21(0)	γ	90.00

R-Factor (%): 4.06 **Temperature(K):** 150 **Density(g/cm³):** 1.854



Search: search1 (Fri Sep 12 09:25:06 2025): Hit 3

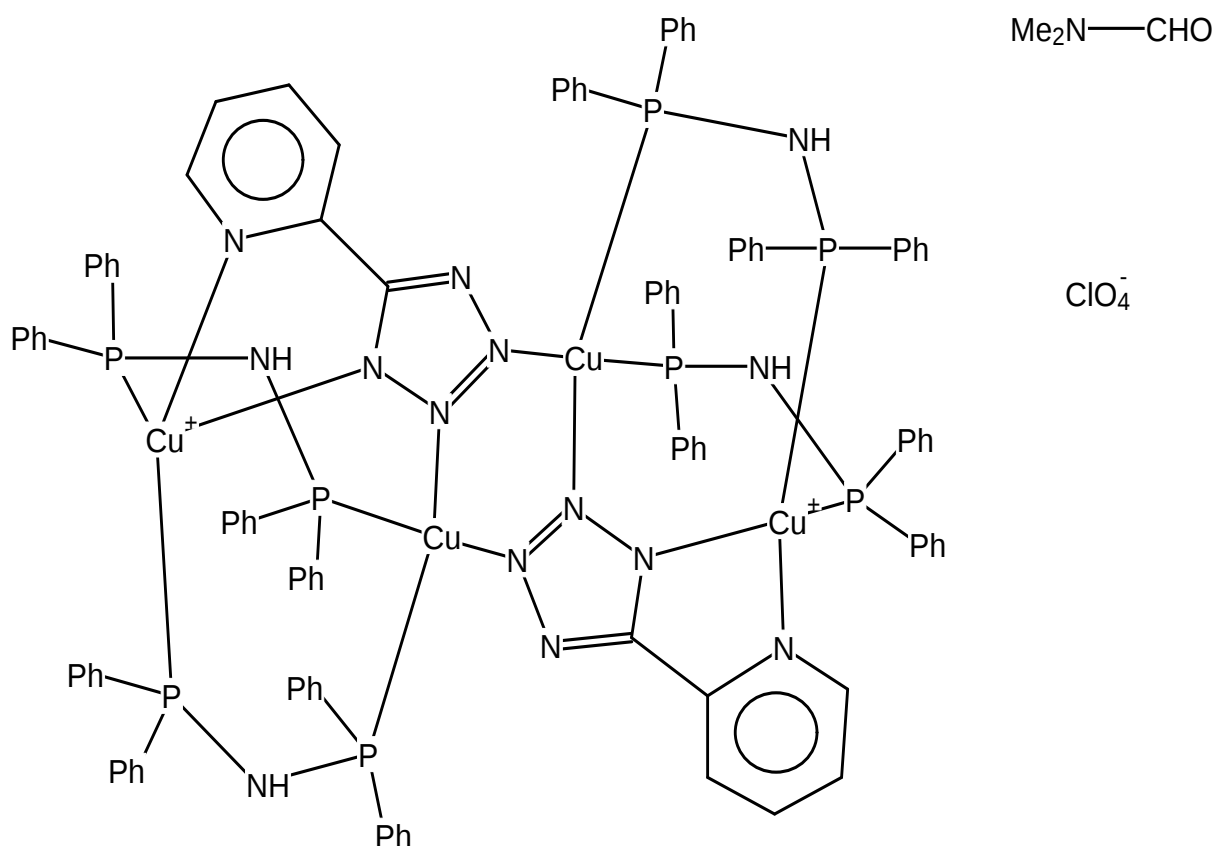
LADDIH

Reference: Dan Peng, Li-Hua He, Peng Ju, Jing-Lin Chen, Heng-Yun Ye, Jin-Yun Wang, Sui-Jun Liu, He-Rui Wen (2020) *Inorg.Chem.* ,**59**,17213

Formula: $C_{108}H_{92}Cu_4N_{14}P_8^{2+}, 4(C_3H_7N_1O_1), 2(Cl_1O_4^{1-})$

Compound Name: bis(μ -5-(pyridin-2-yl)tetrazolyl)-tetrakis(μ -N,N-bis(diphenylphosphanyl)amine)-tetra-copper(i) diperchlorate N,N-dimethylformamide solvate

Space Group:	P21/c	Cell:	a 14.400(0)	b 22.954(1)	c 18.981(1)
Space Group No.:	14	(Å, °)	α 90.00	β 100.58(0)	γ 90.00
R-Factor (%):	3.88	Temperature(K):	293	Density(g/cm³):	1.389



Search: search1 (Fri Sep 12 09:25:06 2025): Hit 4

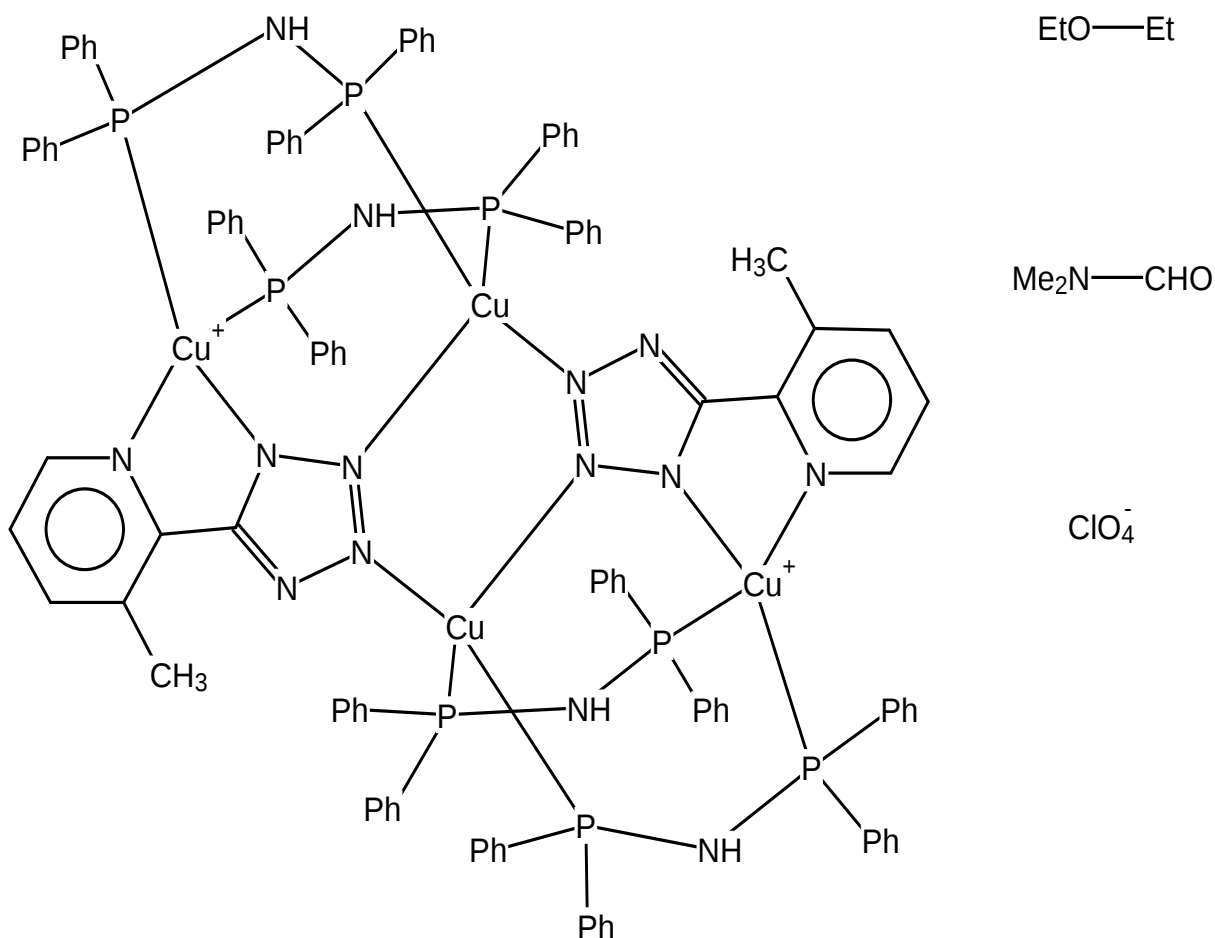
LADDON

Reference: Dan Peng, Li-Hua He, Peng Ju, Jing-Lin Chen, Heng-Yun Ye, Jin-Yun Wang, Sui-Jun Liu, He-Rui Wen (2020) *Inorg.Chem.* ,**59**,17213

Formula: $C_{110}H_{96}Cu_4N_{14}P_8^{2+}, 2(C_4H_{10}O_1), 6(C_3H_7N_1O_1), 2(Cl_1O_4^{1-})$

Compound Name: bis(μ -5-(3-methylpyridin-2-yl)tetrazolyl)-tetrakis(μ -N,N-bis(diphenylphosphanyl)amine)-tetra-copper dperchlorate N,N-dimethylformamide diethyl ether solvate

Space Group:	P21/c	Cell:	a 17.607(1)	b 23.217(2)	c 18.117(1)
Space Group No.:	14	(Å, °)	α 90.00	β 106.37(0)	γ 90.00
R-Factor (%):	5.43	Temperature(K):	293	Density(g/cm³):	1.356



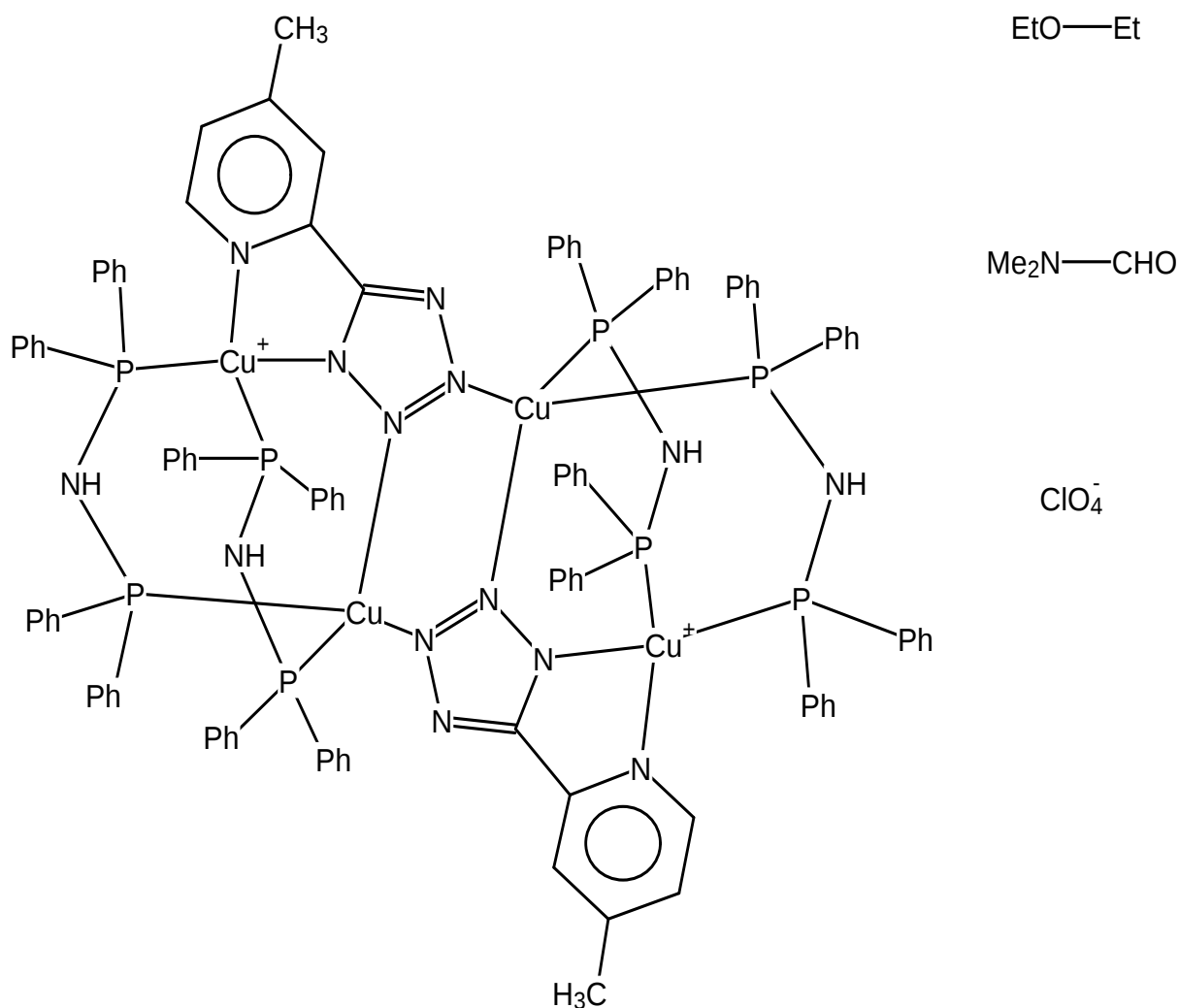
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Reference: Dan Peng, Li-Hua He, Peng Ju, Jing-Lin Chen, Heng-Yun Ye, Jin-Yun Wang, Sui-Jun Liu, He-Rui Wen (2020) *Inorg.Chem.* ,**59**,17213

Formula: $C_{110}H_{96}Cu_4N_{14}P_8^{2+}, 2(C_4H_{10}O_1), 4(C_3H_7N_1O_1), 2(Cl_1O_4^{1-})$

Compound Name: bis(μ -5-(4-methylpyridin-2-yl)tetrazolyl)-tetrakis(μ -N,N-bis(diphenylphosphanyl)amine)-tetra-copper diperchlorate N,N-dimethylformamide diethyl ether solvate

Space Group:	P-1	Cell:	a 15.292(1)	b 15.786(1)	c 16.339(1)
Space Group No.:	2	(Å, °)	α 90.80(0)	β 113.62(0)	γ 108.79(0)
R-Factor (%):	6.87	Temperature(K):	293	Density(g/cm³):	1.356



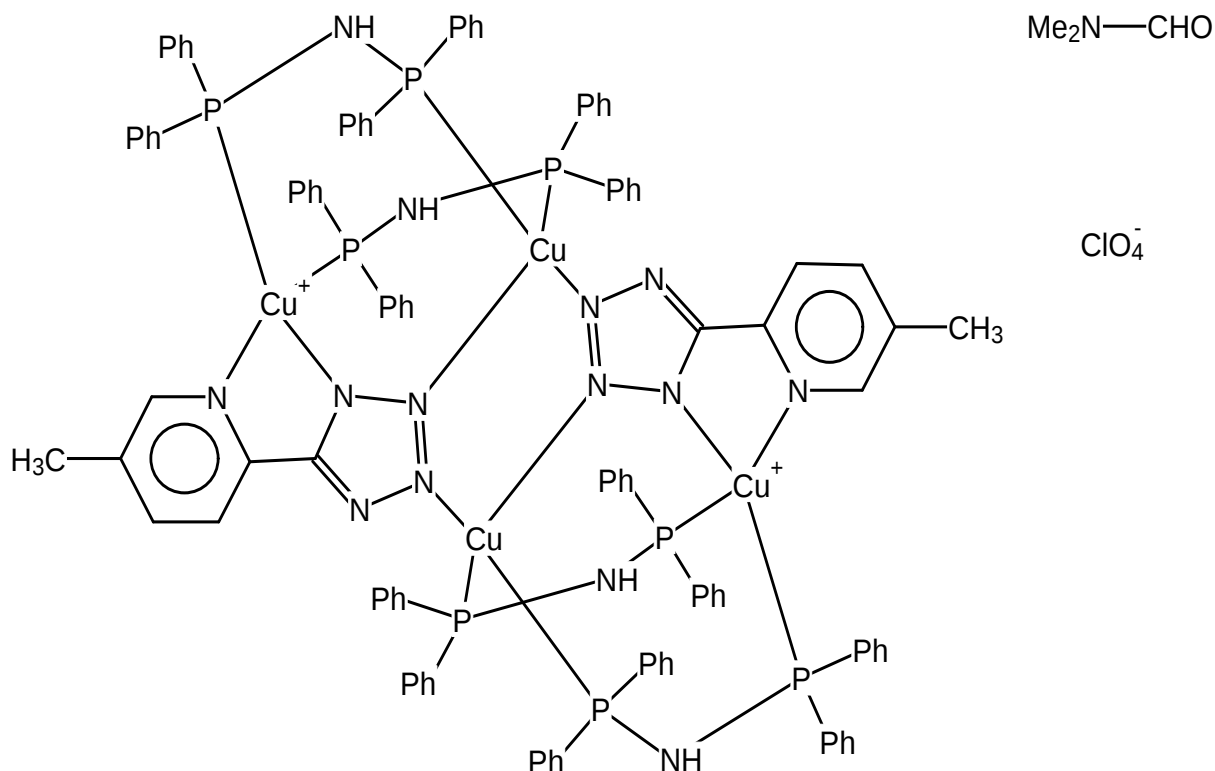
LADFAB

Reference: Dan Peng, Li-Hua He, Peng Ju, Jing-Lin Chen, Heng-Yun Ye, Jin-Yun Wang, Sui-Jun Liu, He-Rui Wen (2020) *Inorg.Chem.* ,**59**,17213

Formula: $C_{110}H_{96}Cu_4N_{14}P_8^{2+}, 10(C_3H_7N_1O_1), 2(Cl_1O_4^{1-})$

Compound Name: bis(μ -5-(5-methylpyridin-2-yl)tetrazolyl)-tetrakis(μ -N,N-bis(diphenylphosphanyl)amine)-tetra-copper diperchlorate N,N-dimethylformamide solvate

Space Group:	P-1	Cell:	a 13.539(3)	b 16.925(3)	c 17.880(3)
Space Group No.:	2	(Å, °)	α 97.60(0)	β 92.87(0)	γ 110.67(0)
R-Factor (%):	5.51	Temperature(K):	293	Density(g/cm³):	1.338



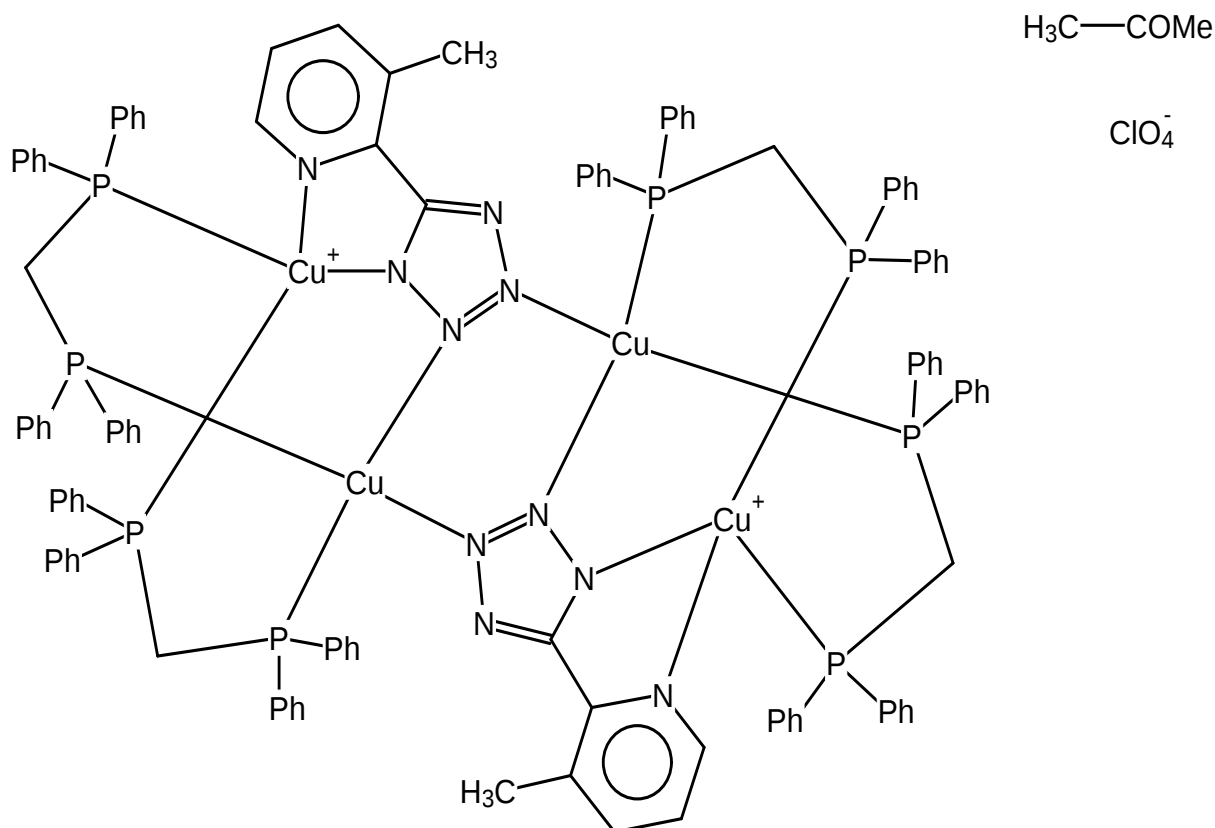
LATHEX

Reference: Ping Yu, Dan Peng, Li-Hua He, Jing-Lin Chen, Jin-Yun Wang, Sui-Jun Liu, He-Rui Wen (2021) *Inorg.Chem.* ,**61**,254

Formula: $C_{114} H_{100} Cu_4 N_{10} P_8^{2+}, 2(C_3 H_6 O_1), 2(Cl_1 O_4^{1-})$

Compound Name: bis(μ -5-(3-methylpyridin-2-yl)tetrazolato)-tetrakis(μ -methylenebis(diphenylphosphine))-tetra-copper(i) bis(perchlorate) acetone solvate

Space Group:	P21/c	Cell:	a 15.815(1)	b 23.277(2)	c 17.318(1)
Space Group No.:	14	(Å, °)	α 90.00	β 112.93(0)	γ 90.00
R-Factor (%):	4.94	Temperature(K):	300	Density(g/cm³):	1.373



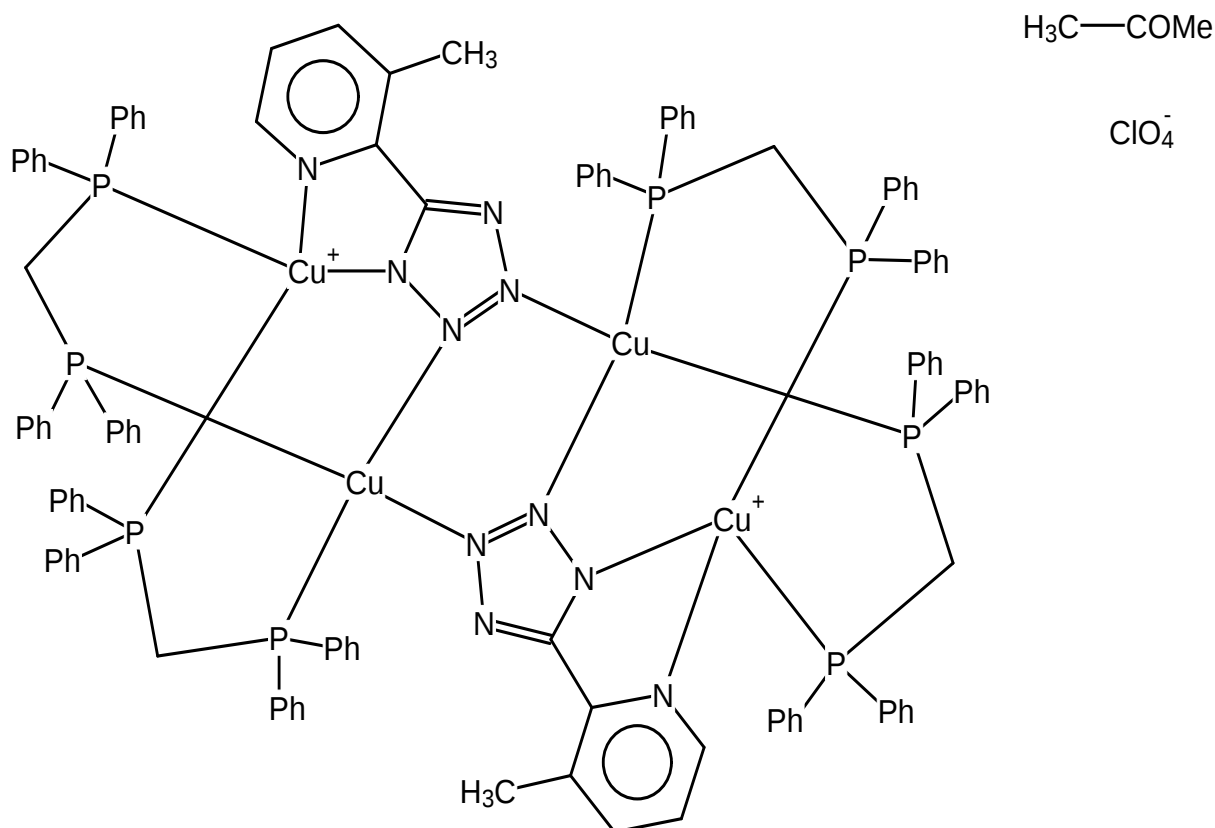
LATHEX01

Reference: Ping Yu, Dan Peng, Li-Hua He, Jing-Lin Chen, Jin-Yun Wang, Sui-Jun Liu, He-Rui Wen (2022) *Inorg.Chem.* ,**61**,254

Formula: $C_{114} H_{100} Cu_4 N_{10} P_8^{2+}, 2(C_3 H_6 O_1), 2(Cl_1 O_4^{1-})$

Compound Name: bis(μ -5-(3-methylpyridin-2-yl)tetrazolato)-tetrakis(μ -methylenebis(diphenylphosphine))-tetra-copper(i) bis(perchlorate) acetone solvate

Space Group:	P21/c	Cell:	a 15.815(1)	b 23.277(2)	c 17.318(1)
Space Group No.:	14	(Å, °)	α 90.00	β 112.93(0)	γ 90.00
R-Factor (%):	4.94	Temperature(K):	300	Density(g/cm³):	1.373



LATHIB

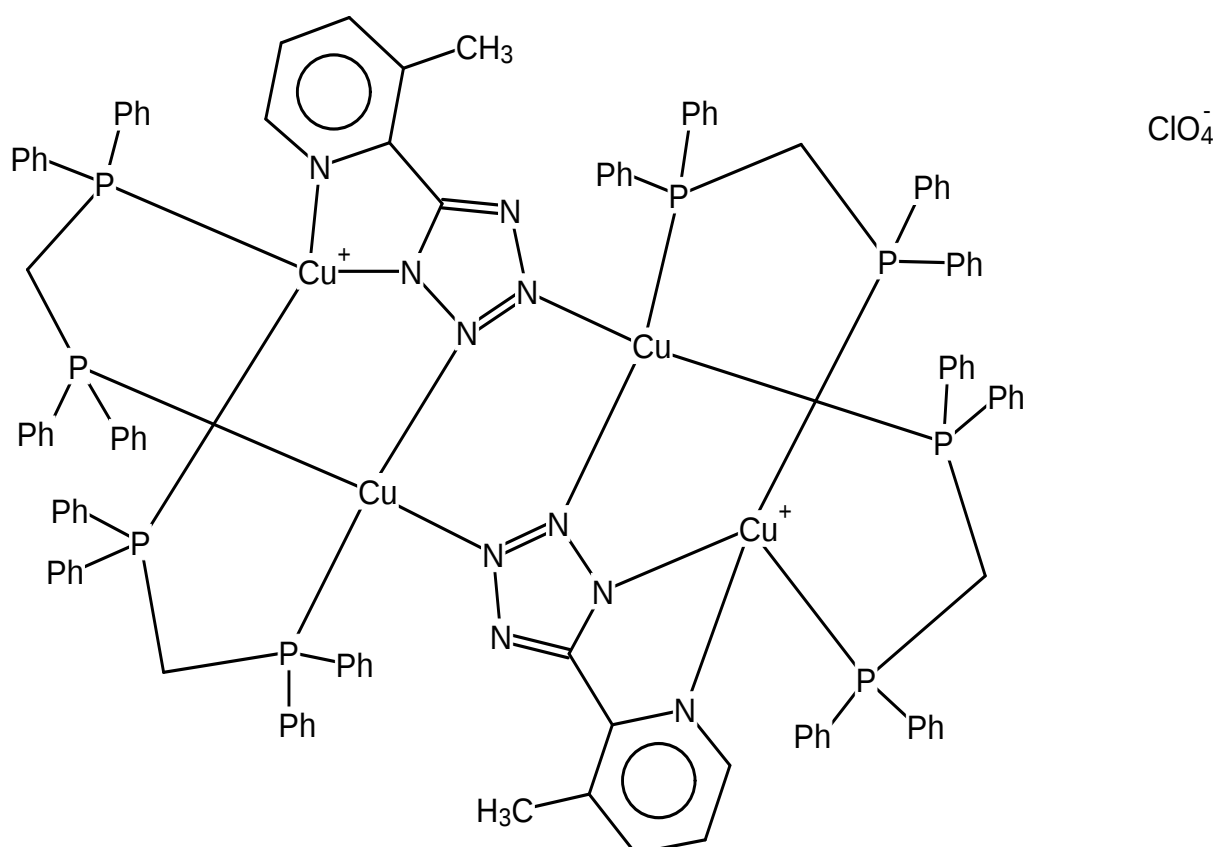
Reference: Ping Yu, Dan Peng, Li-Hua He, Jing-Lin Chen, Jin-Yun Wang, Sui-Jun Liu, He-Rui Wen (2021) *Inorg.Chem.* ,**61**,254

Formula: $C_{114} H_{100} Cu_4 N_{10} P_8^{2+}, 2(Cl_1 O_4^{1-})$

Compound Name: bis(μ -5-(3-methylpyridin-2-yl)tetrazolato)-tetrakis(μ -methylenebis(diphenylphosphine))-tetra-copper(i) bis(perchlorate)

Space Group: P41212 **Cell:** **a** 13.491(0) **b** 13.491(0) **c** 58.805(3)
Space Group No.: 92 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 6.57 **Temperature(K):** 293 **Density(g/cm³):** 1.434



LATHIB01

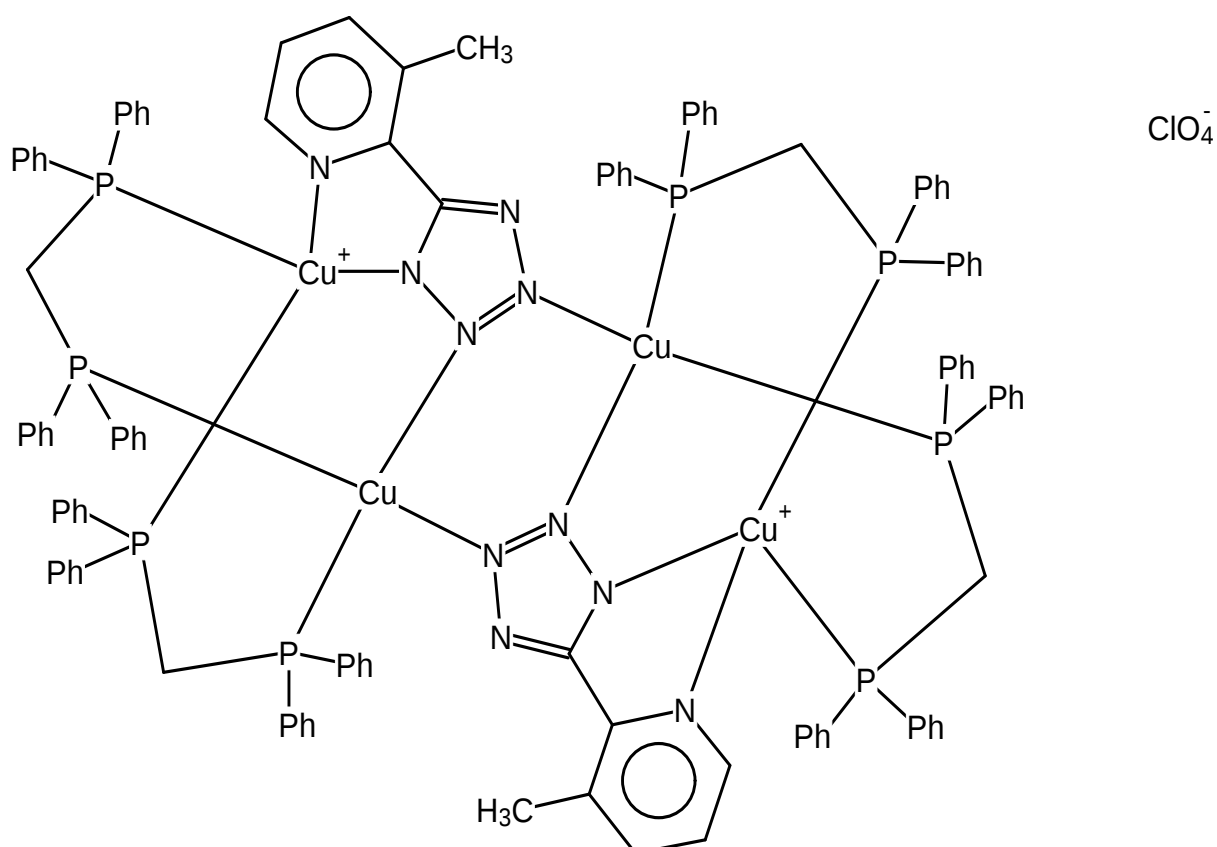
Reference: Ping Yu, Dan Peng, Li-Hua He, Jing-Lin Chen, Jin-Yun Wang, Sui-Jun Liu, He-Rui Wen (2022) *Inorg.Chem.* ,**61**,254

Formula: $C_{114} H_{100} Cu_4 N_{10} P_8^{2+}, 2(Cl_1 O_4^{1-})$

Compound Name: bis(μ -5-(3-methylpyridin-2-yl)tetrazolato)-tetrakis(μ -methylenebis(diphenylphosphine))-tetra-copper(i) bis(perchlorate)

Space Group: P41212 **Cell:** **a** 13.491(0) **b** 13.491(0) **c** 58.805(3)
Space Group No.: 92 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 6.57 **Temperature(K):** 293 **Density(g/cm³):** 1.434



Search: search1 (Fri Sep 12 09:25:06 2025): Hit 11

NEHSOJ

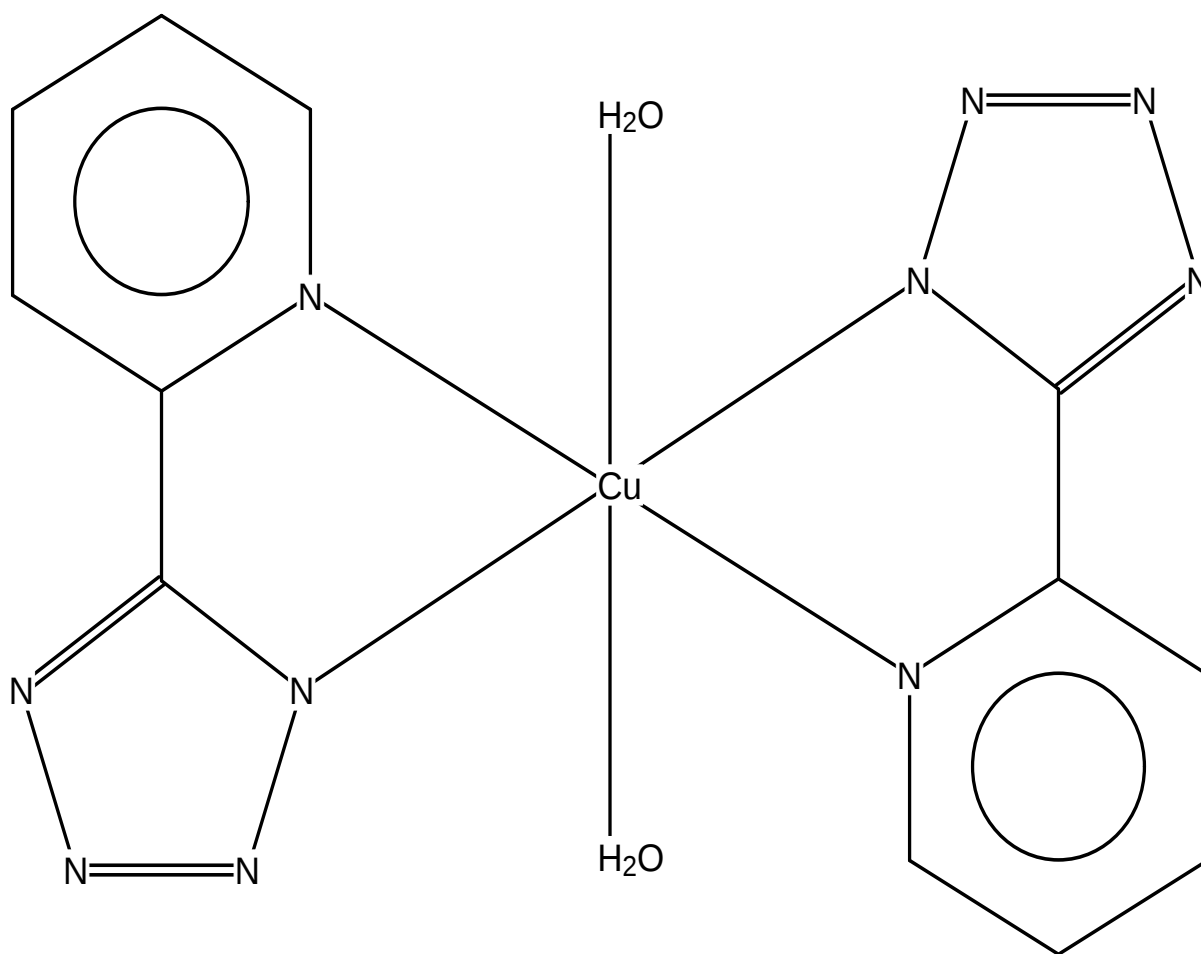
Reference: Xiao-Jie Mo, En-Qing Gao, Zheng He, Wen-Jun Li,
Chun-Hua Yan (2004) *Inorg.Chem.Commun.* ,7,353

Formula: C₁₂ H₁₂ Cu₁ N₁₀ O₂

Compound Name: Diaqua-bis(5-(2-pyridyl)-1H-tetrazolyl)-copper(ii)

Space Group:	P21/c	Cell:	a	8.044(0)	b	12.735(0)	c	7.475(0)
Space Group No.:	14	(Å, °)	α	90.00	β	96.88(0)	γ	90.00

R-Factor (%) :	5.53	Temperature(K) :	295	Density(g/cm³) :	1.712
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NEHSOJ01

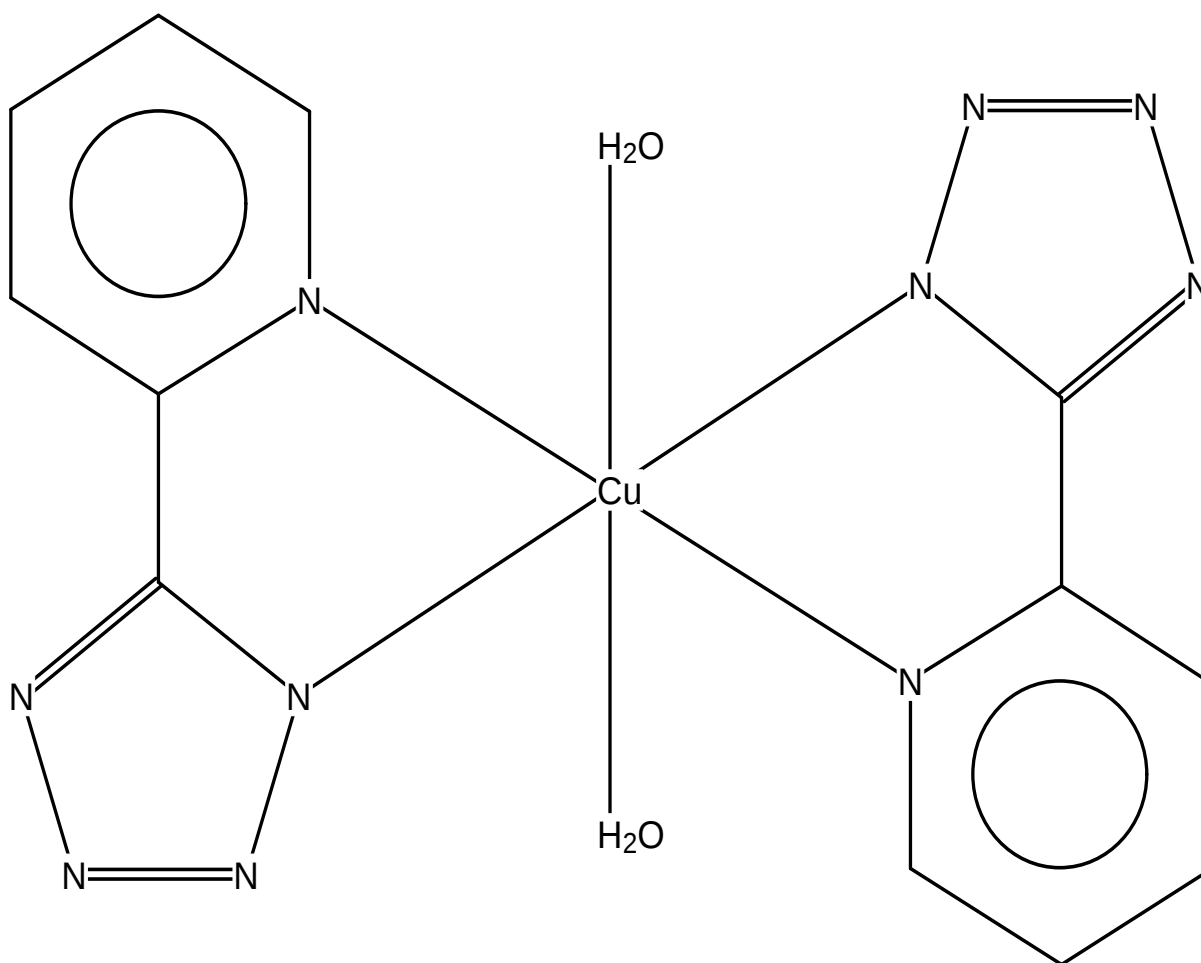
Reference: B.G.Mukhopadhyay, S.Mukhopadhyay, M.F.C.G.da Silva,
M.A.J.Charmier, A.J.L.Pombeiro (2009) *Dalton Trans.* ,4778

Formula: C₁₂ H₁₂ Cu₁ N₁₀ O₂

Compound Name: Diaqua-bis(5-(2-pyridyl)tetrazolato)-copper(ii)

Space Group:	P21/c	Cell:	a	7.989(0)	b	12.709(0)	c	7.391(0)
Space Group No.:	14	(Å, °)	α	90.00	β	97.73(0)	γ	90.00

R-Factor (%):	2.59	Temperature(K):	150	Density(g/cm³):	1.750
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NEHSOJ02

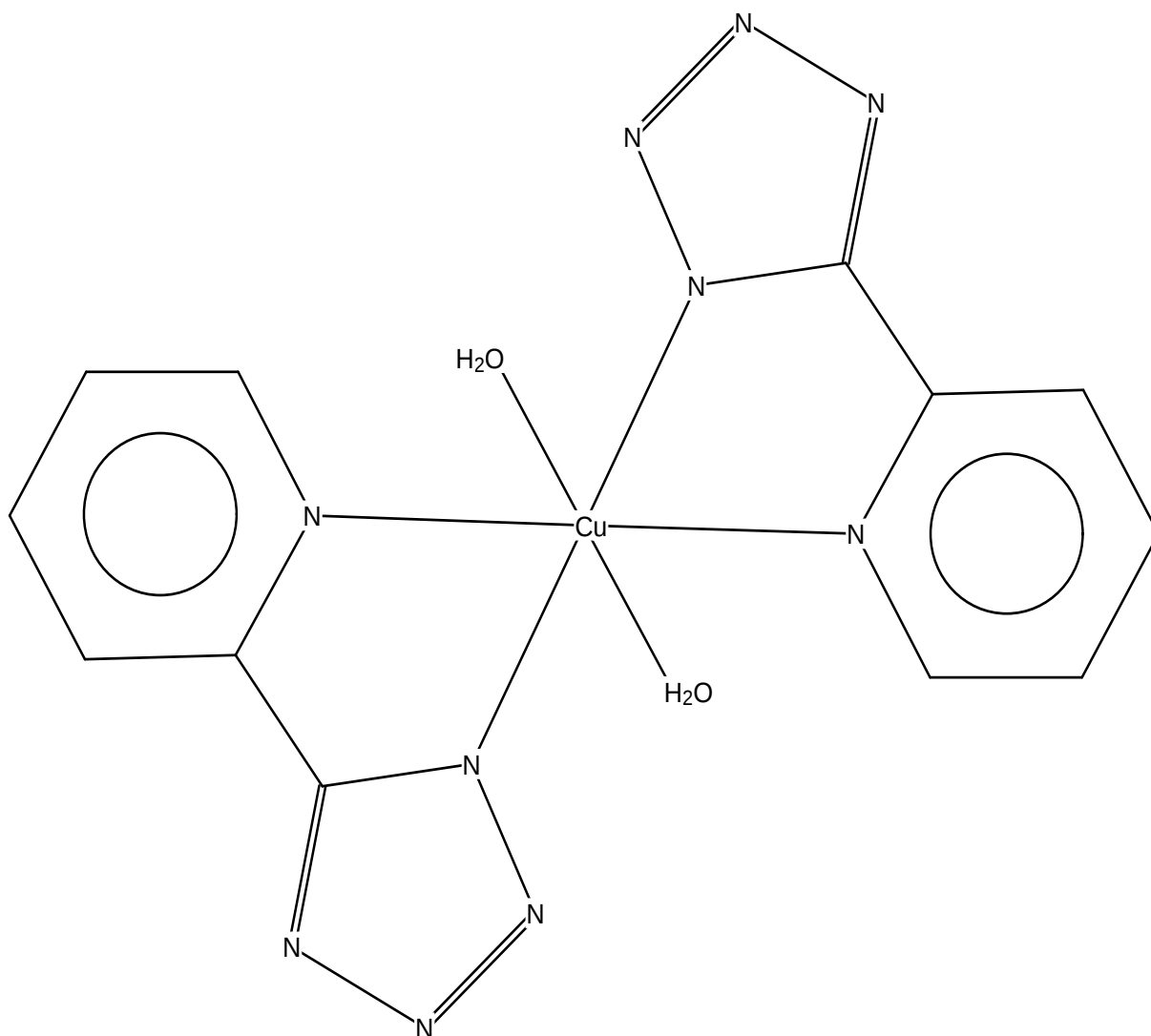
Reference: Arti Chouhan, D.Kumar, G.Pilet, S.Daniele,
Ashutosh Pandey (2022) *Chem. Sel.* ,7,e2022028

Formula: C₁₂ H₁₂ Cu₁ N₁₀ O₂

Compound Name: diaqua-bis(5-(pyridin-2-yl)tetrazolato)-copper(ii)

Space Group:	P21/c	Cell:	a	8.026(0)	b	12.747(0)	c	7.432(0)
Space Group No.:	14	(Å, °)	α	90.00	β	96.86(0)	γ	90.00

R-Factor (%):	2.38	Temperature(K):	293	Density(g/cm³):	1.724
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NIQKUU01

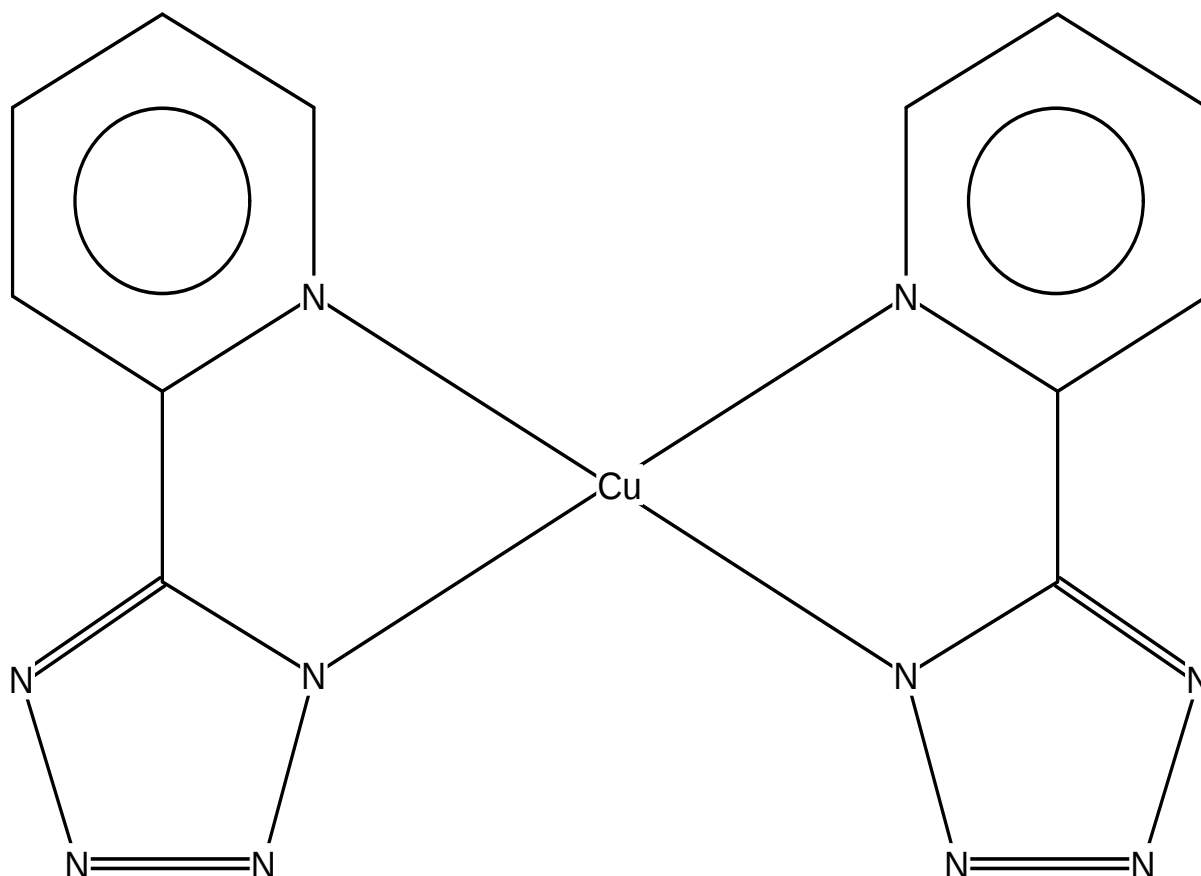
Reference: J.-Q.Li, D.Mu, M.-B.Fan (2014)
Acta Crystallogr., Sect. E: Struct. Rep. Online , **70**, m79

Formula: C₁₂ H₈ Cu₁ N₁₀

Compound Name: bis(2-(1H-tetrazol-5-yl)pyridinato)-copper(ii)

Space Group:	P21/c	Cell:	a	5.539(0)	b	13.128(2)	c	8.795(1)
Space Group No.:	14	(Å, °)	α	90.00	β	97.65(0)	γ	90.00

R-Factor (%) :	3.41	Temperature(K) :	291	Density(g/cm³) :	1.864
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OZILAM

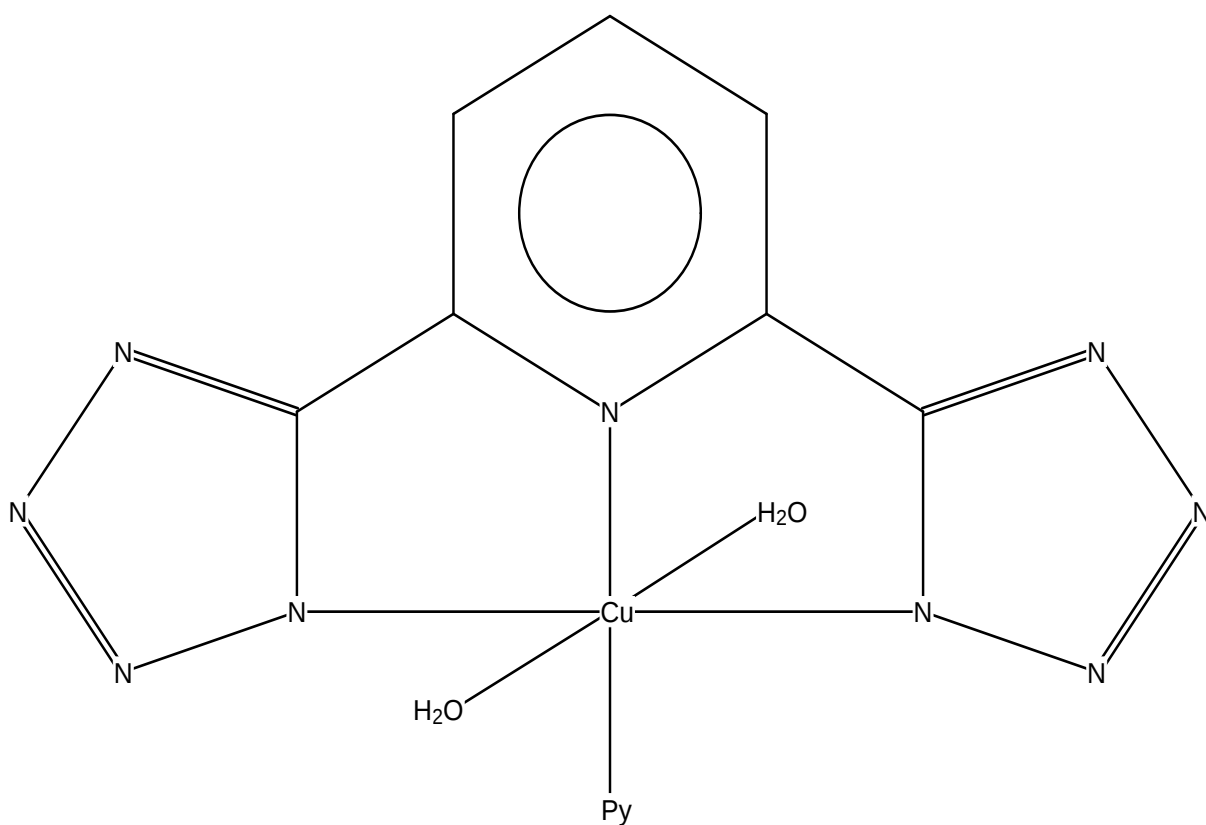
Reference: A.Klein, A.Krest (2016)
CSD Communication(Private Communication) ,

Formula: C₁₂ H₁₂ Cu₁ N₁₀ O₂

Compound Name: diaqua-(5,5'-(pyridine-2,6-diyl)bis(tetrazolyl))-pyridine-copper(ii)

Space Group:	P21	Cell:	a	7.615(1)	b	12.226(1)	c	8.141(1)
Space Group No.:	4	(Å, °)	α	90.00	β	98.62(1)	γ	90.00

R-Factor (%):	3.71	Temperature(K):	293	Density(g/cm³):	1.737
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OZILAM01

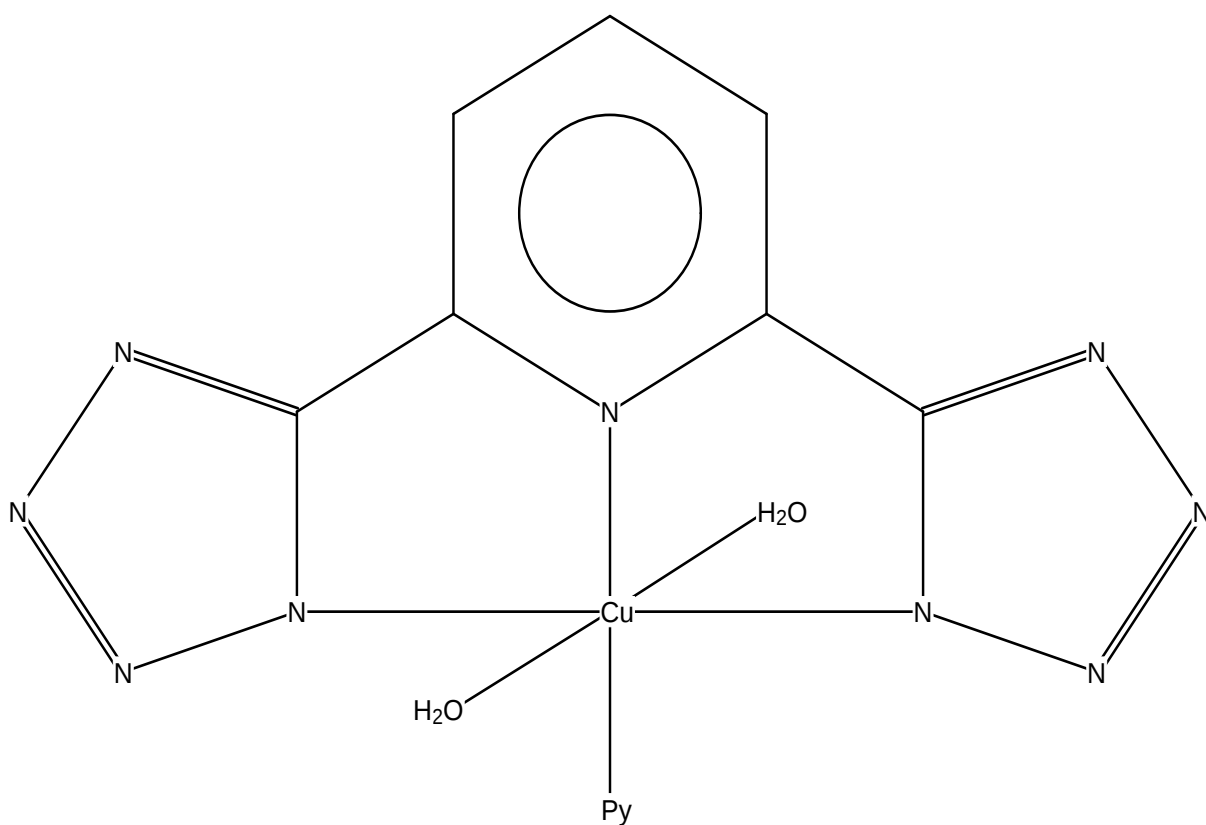
Reference: A.Krest, A.Sandleben, M.Valldor, M.Werker,
Uwe Ruschewitz, A.Klein (2017) *Chem. Sel.* ,2,5849

Formula: C₁₂ H₁₂ Cu₁ N₁₀ O₂

Compound Name: diaqua-(5,5'-(pyridine-2,6-diyl)bis(tetrazolyl))-pyridine-copper(ii)

Space Group:	P21	Cell:	a	7.615(1)	b	12.226(1)	c	8.141(1)
Space Group No.:	4	(Å, °)	α	90.00	β	98.62(1)	γ	90.00

R-Factor (%):	3.71	Temperature(K):	293	Density(g/cm³):	1.737
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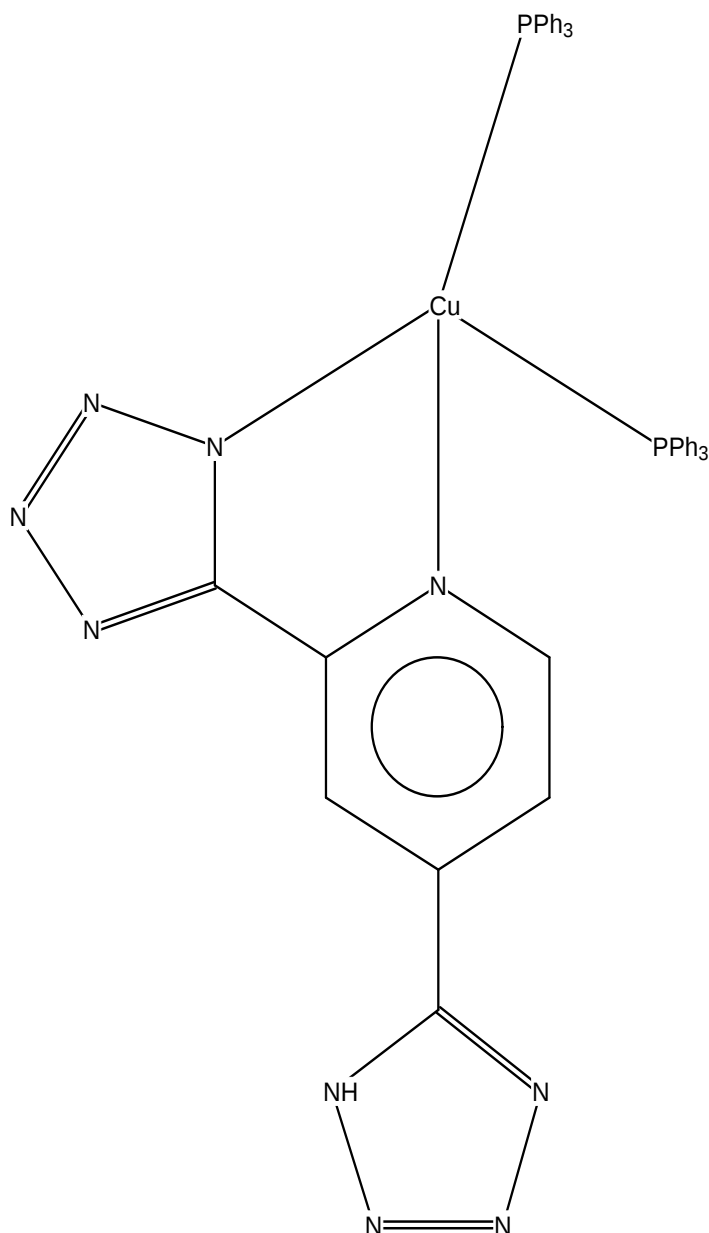
TEQSER

Reference: Jing Xiang Li-Xin Wang, Xu Zhang, De-Sheng Zhu, Lei Wang, Lu-Lu Liu, Chi-Fai Leung, Jing Xiang (2022) *RSC Advances* ,**12**,27267

Formula: C₄₃ H₃₄ Cu₁ N₉ P₂

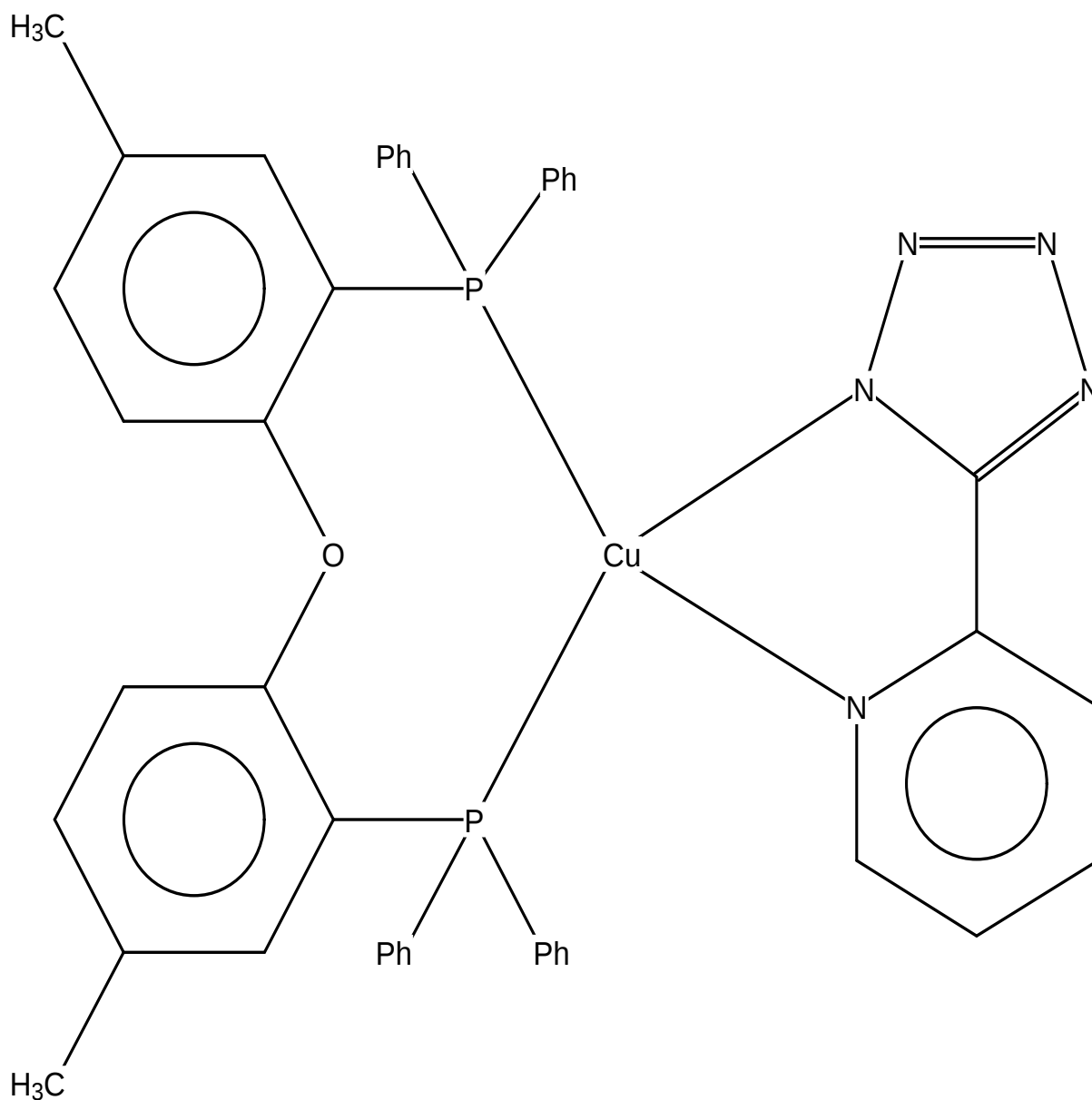
Compound Name: [4-(1H-tetrazol-5-yl)-2-(1H-tetrazol-5-yl)pyridinato]-bis(triphenylphosphine)-copper

Space Group:	P21/n	Cell:	a	18.970(0)	b	10.513(0)	c	19.283(0)
Space Group No.:	14	(Å, °)	α	90.00	β	89.99(0)	γ	90.00
R-Factor (%):	7.70	Temperature(K):	150	Density(g/cm³):	1.386			



VIBCOA

R-Factor (%): 3.07 **Temperature(K)**: 123 **Density(g/cm³)**: 1.350



VIBCUG

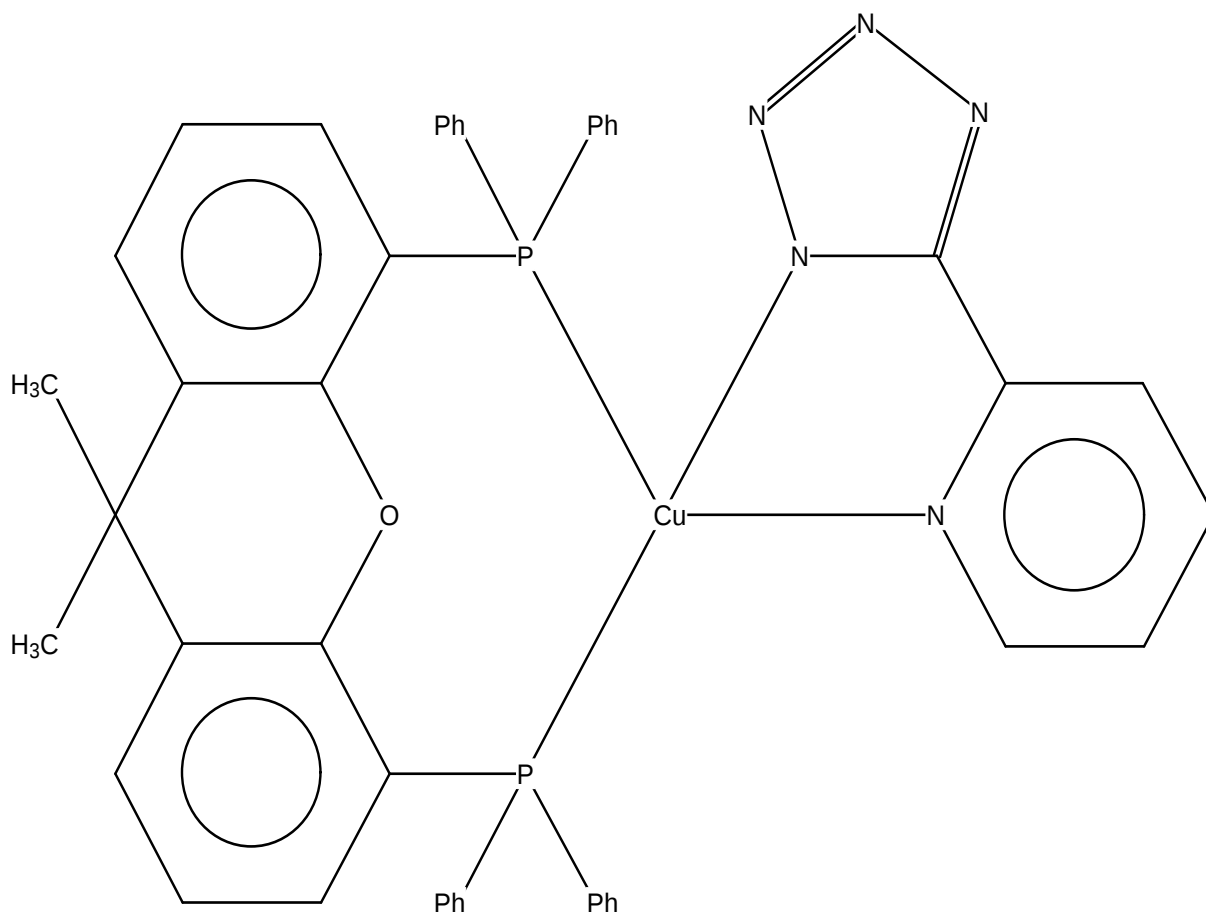
Reference: L.Bergmann, J.Friedrichs, M.Mydlak, T.Baumann,
M.Nieger, S.Bräse (2013) *Chem.Comm.* ,**49**,6507

Formula: C₄₅ H₃₆ Cu₁ N₅ O₁ P₂

Compound Name: (4,5-bis(diphenylphosphino)-9,9-dimethylxanthene)-(5-(pyridin-2-yl)tetrazolato)-copper(i)

Space Group:	P2 ₁ /n	Cell:	a	10.072(0)	b	20.384(1)	c	17.951(1)
Space Group No.:	14	(Å, °)	α	90.00	β	94.18(0)	γ	90.00

R-Factor (%):	2.70	Temperature(K):	123	Density(g/cm³):	1.424
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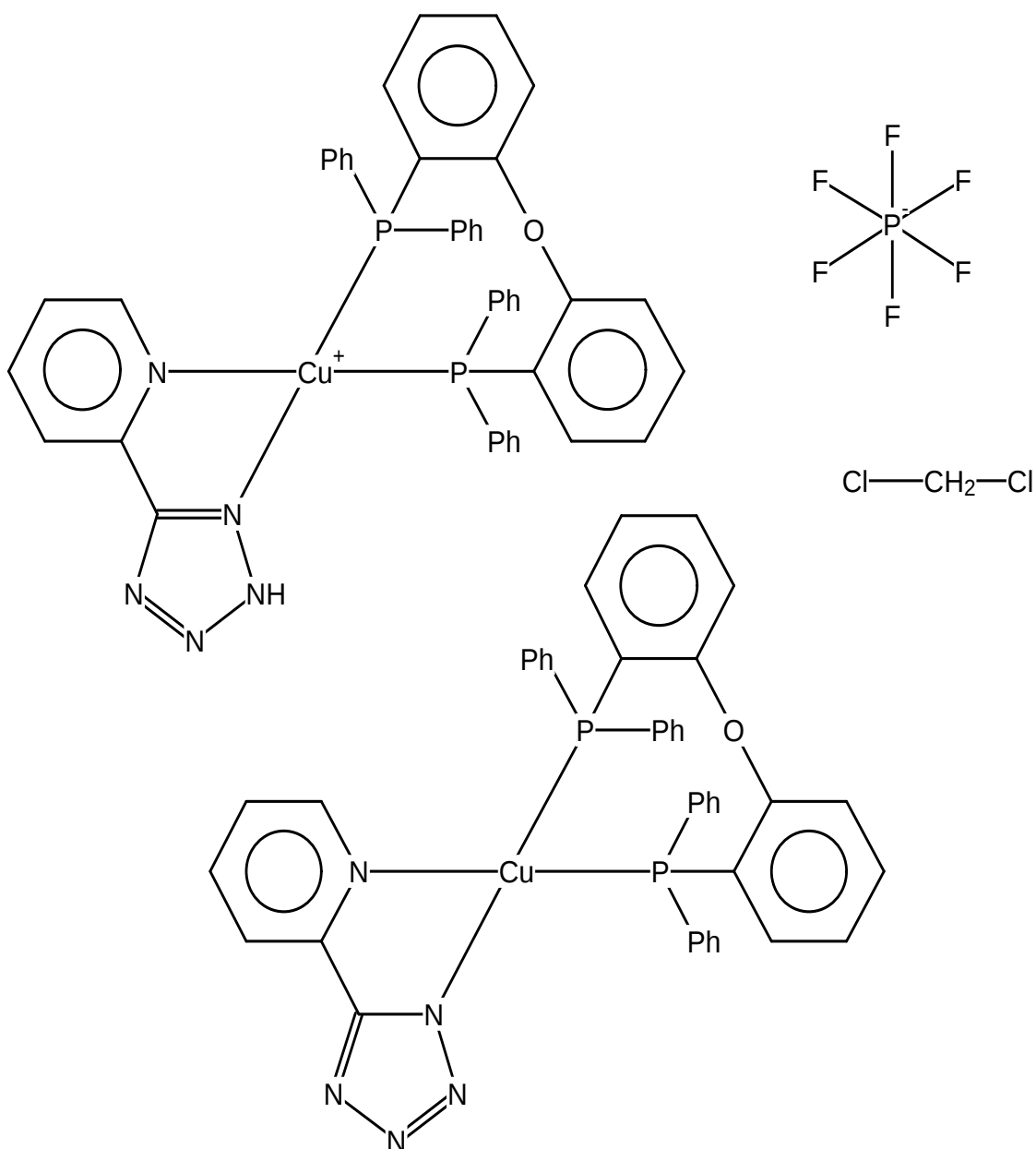
VIBDAN

Reference: L.Bergmann, J.Friedrichs, M.Mydlak, T.Baumann, M.Nieger, S.Bräse (2013) *Chem.Comm.* ,**49**,6507

Formula: $C_{42}H_{33}Cu_1N_5O_1P_2^{1+}, F_6P_1^{1-}, 2(C_1H_2Cl_2), C_{42}H_{32}Cu_1N_5O_1P_2$

Compound Name: (bis(2-(diphenylphosphino)phenyl) ether)-(5-(pyridin-2-yl)-2H-tetrazole)-copper(i) (bis(2-(diphenylphosphino)phenyl) ether)-(5-(pyridin-2-yl) tetrazolato)-copper(i) hexafluorophosphate dichloromethane solvate

Space Group:	P-1	Cell:	a 12.294(1)	b 13.170(1)	c 14.471(1)
Space Group No.:	2	(Å, °)	α 71.00(1)	β 85.67(1)	γ 69.54(1)
R-Factor (%):	5.65	Temperature(K):	123	Density(g/cm³):	1.451



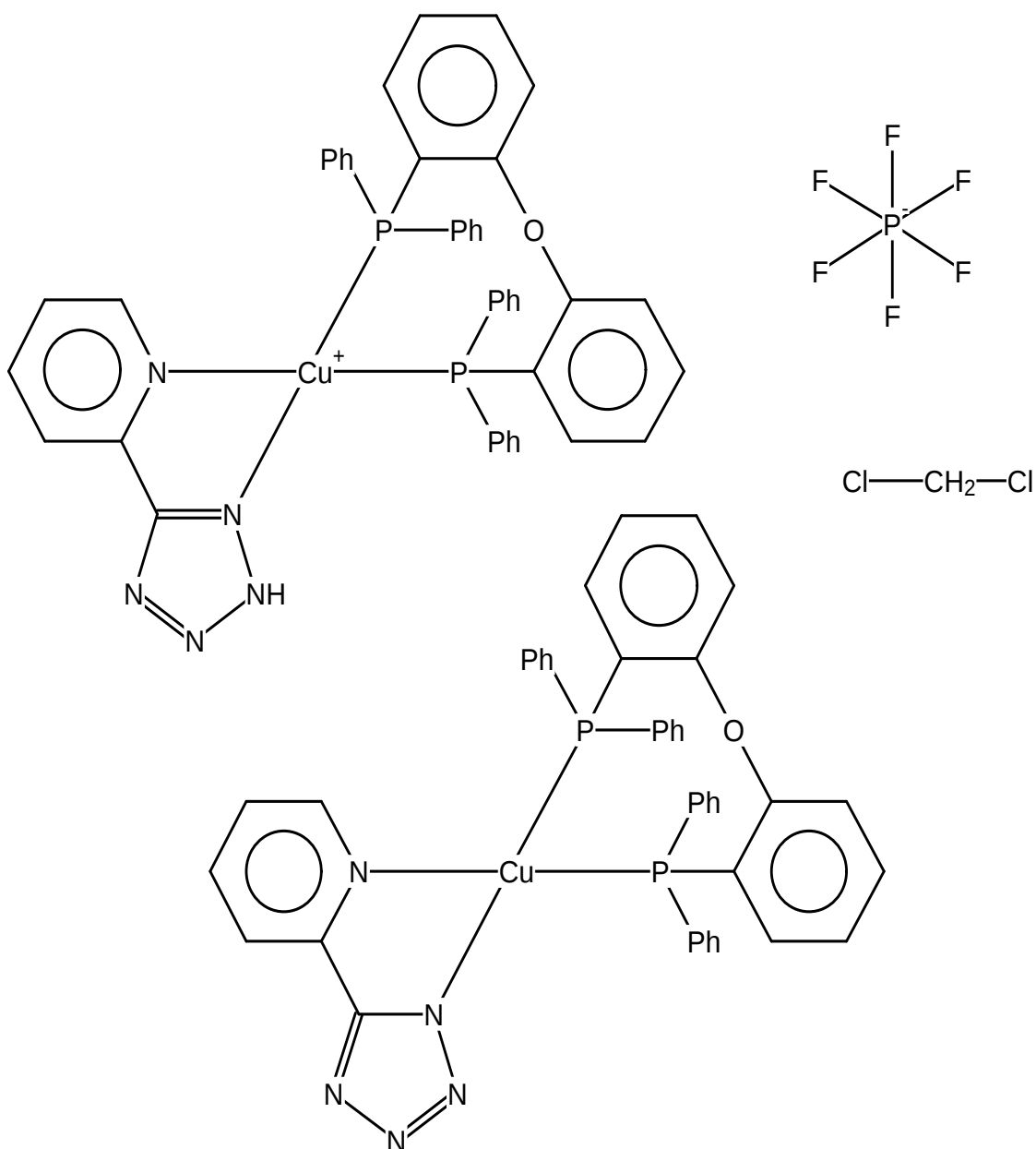
VIBDAN01

Reference: L.Bergmann, C.Braun, M.Nieger, S.Bräse (2018)
Dalton Trans. ,**47**,608

Formula: $C_{42}H_{33}Cu_1N_5O_1P_2^{1+}, F_6P_1^{1-}, 2(C_1H_2Cl_2), C_{42}H_{32}Cu_1N_5O_1P_2$

Compound Name: (bis(2-(diphenylphosphino)phenyl) ether)-(5-(pyridin-2-yl)-2H-tetrazole)-copper(i) (bis(2-(diphenylphosphino)phenyl) ether)-(5-(pyridin-2-yl) tetrazolato)-copper(i) hexafluorophosphate dichloromethane solvate

Space Group:	P-1	Cell:	a 12.294(1)	b 13.170(1)	c 14.471(1)
Space Group No.:	2	(Å, °)	α 71.00(1)	β 85.67(1)	γ 69.54(1)
R-Factor (%):	5.65	Temperature(K):	123	Density(g/cm³):	1.451



VIBDER

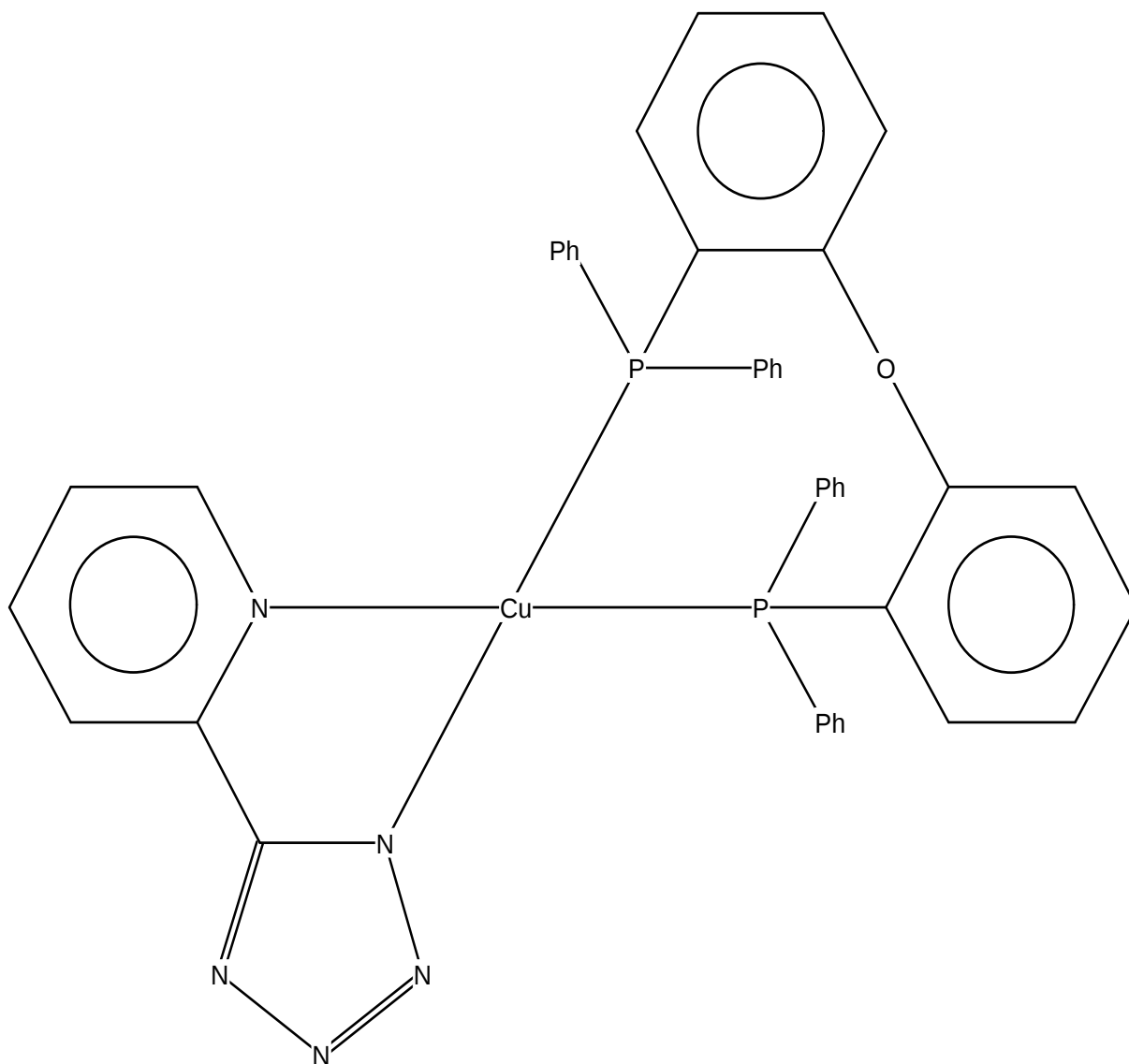
Reference: L.Bergmann, J.Friedrichs, M.Mydlak, T.Baumann,
M.Nieger, S.Bräse (2013) *Chem.Commun.* ,**49**,6507

Formula: C₄₂ H₃₂ Cu₁ N₅ O₁ P₂

Compound Name: (bis(2-(diphenylphosphino)phenyl) ether)-(5-(pyridin-2-yl)tetrazolato)-copper(i)

Space Group:	P21/n	Cell:	a	9.016(0)	b	17.810(1)	c	22.358(1)
Space Group No.:	14	(Å, °)	α	90.00	β	90.65(0)	γ	90.00

R-Factor (%):	3.43	Temperature(K):	123	Density(g/cm³):	1.384
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VIBDER01

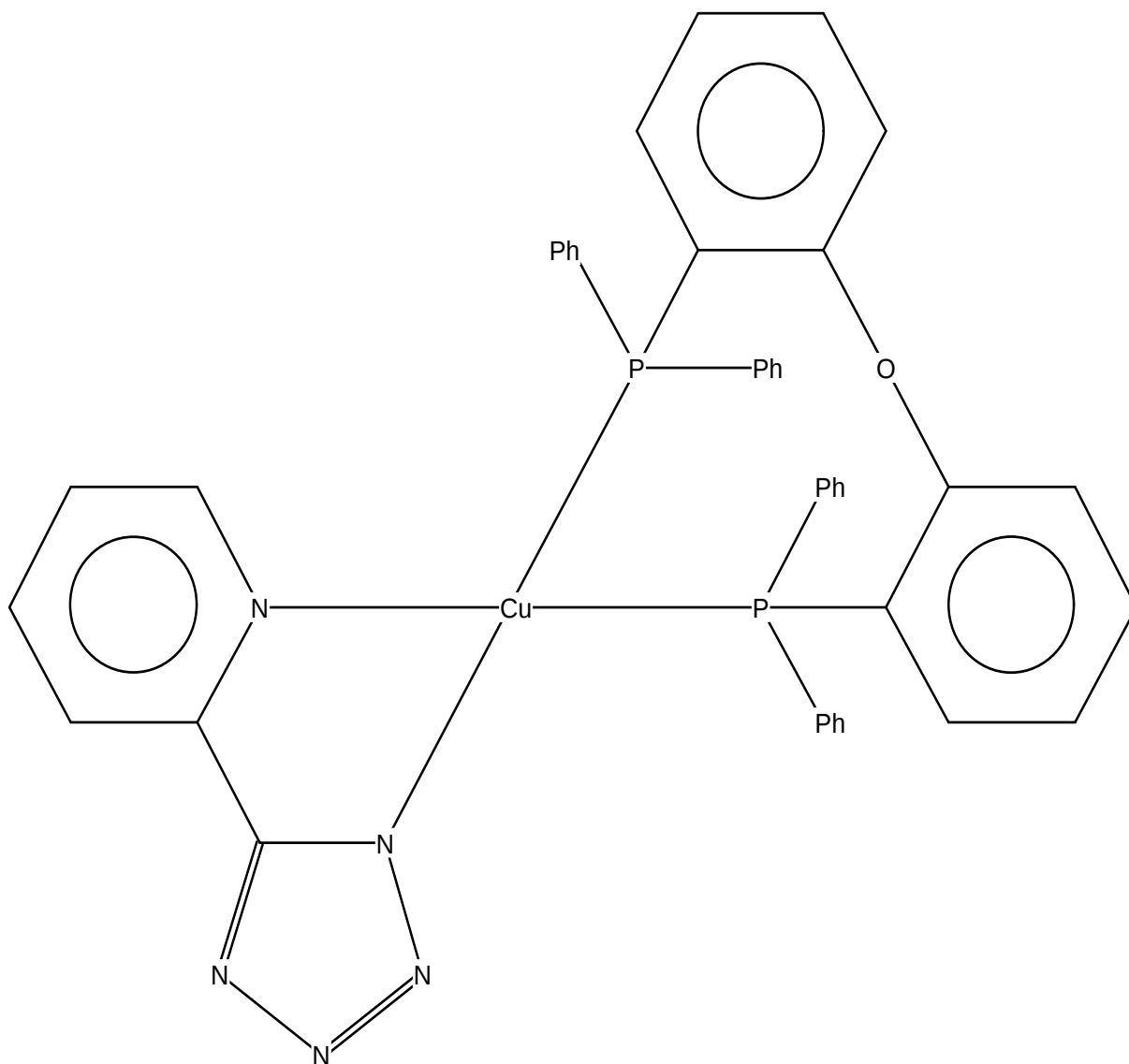
Reference: L.Bergmann, C.Braun, M.Nieger, S.Bräse (2018)
Dalton Trans. ,**47**,608

Formula: C₄₂ H₃₂ Cu₁ N₅ O₁ P₂

Compound Name: (bis(2-(diphenylphosphino)phenyl) ether)-(5-(pyridin-2-yl)tetrazolato)-copper(i)

Space Group:	P21/n	Cell:	a	9.016(0)	b	17.810(1)	c	22.358(1)
Space Group No.:	14	(Å, °)	α	90.00	β	90.65(0)	γ	90.00

R-Factor (%):	3.43	Temperature(K):	123	Density(g/cm³):	1.384
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Search: search1 (Fri Sep 12 09:25:06 2025): Hit 24

VIBDOB

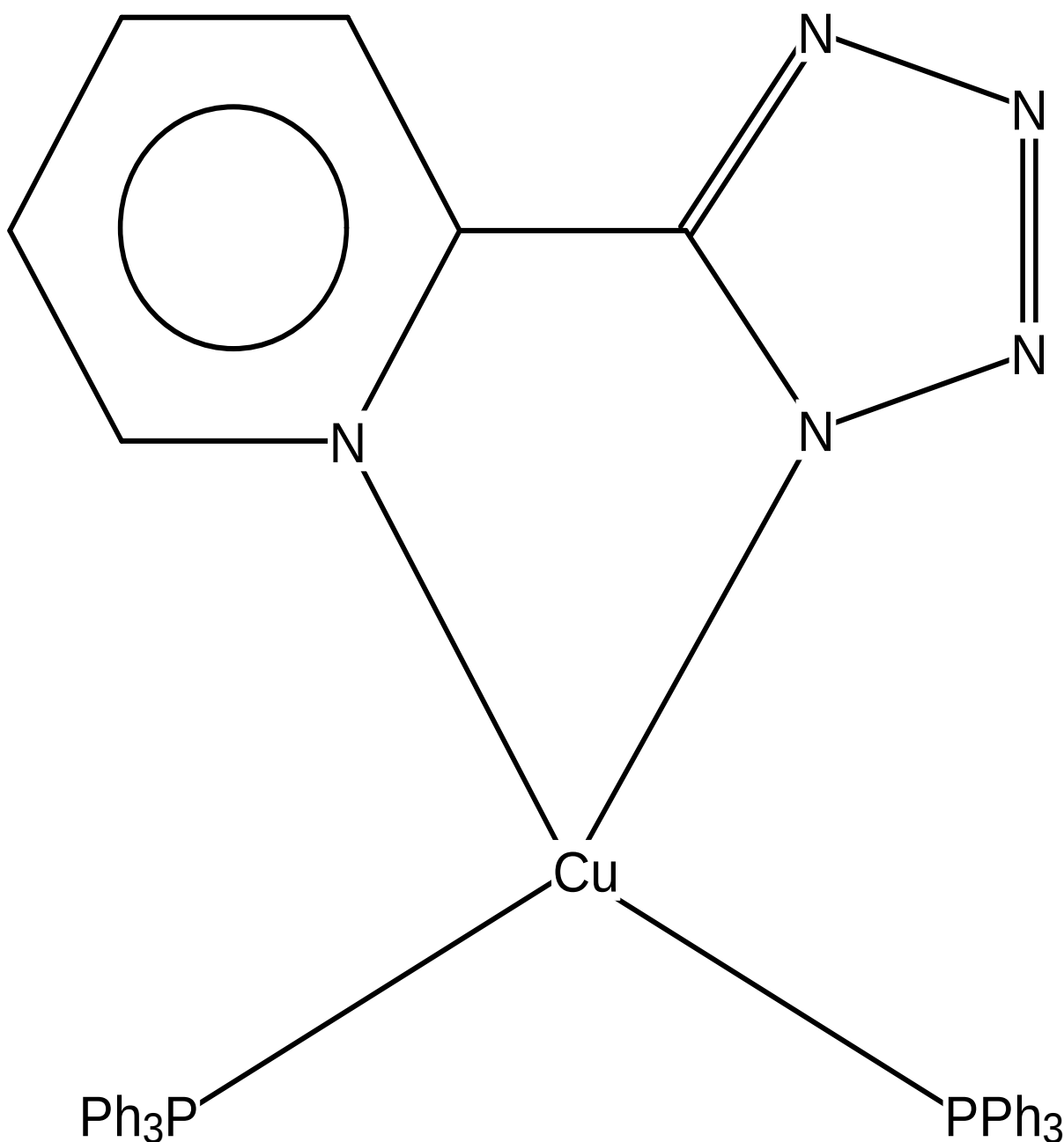
Reference: L.Bergmann, J.Friedrichs, M.Mydlak, T.Baumann,
M.Nieger, S.Bräse (2013) *Chem.Commun.* ,**49**,6507

Formula: C₄₂ H₃₄ Cu₁ N₅ P₂

Compound Name: (5-(pyridin-2-yl)tetrazolato)-bis(triphenylphosphine)-copper(i)

Space Group:	P21/n	Cell:	a	9.082(0)	b	18.255(0)	c	22.236(0)
Space Group No.:	14	(Å, °)	α	90.00	β	91.36(0)	γ	90.00

R-Factor (%): 7.65 **Temperature(K):** 123 **Density(g/cm³):** 1.323



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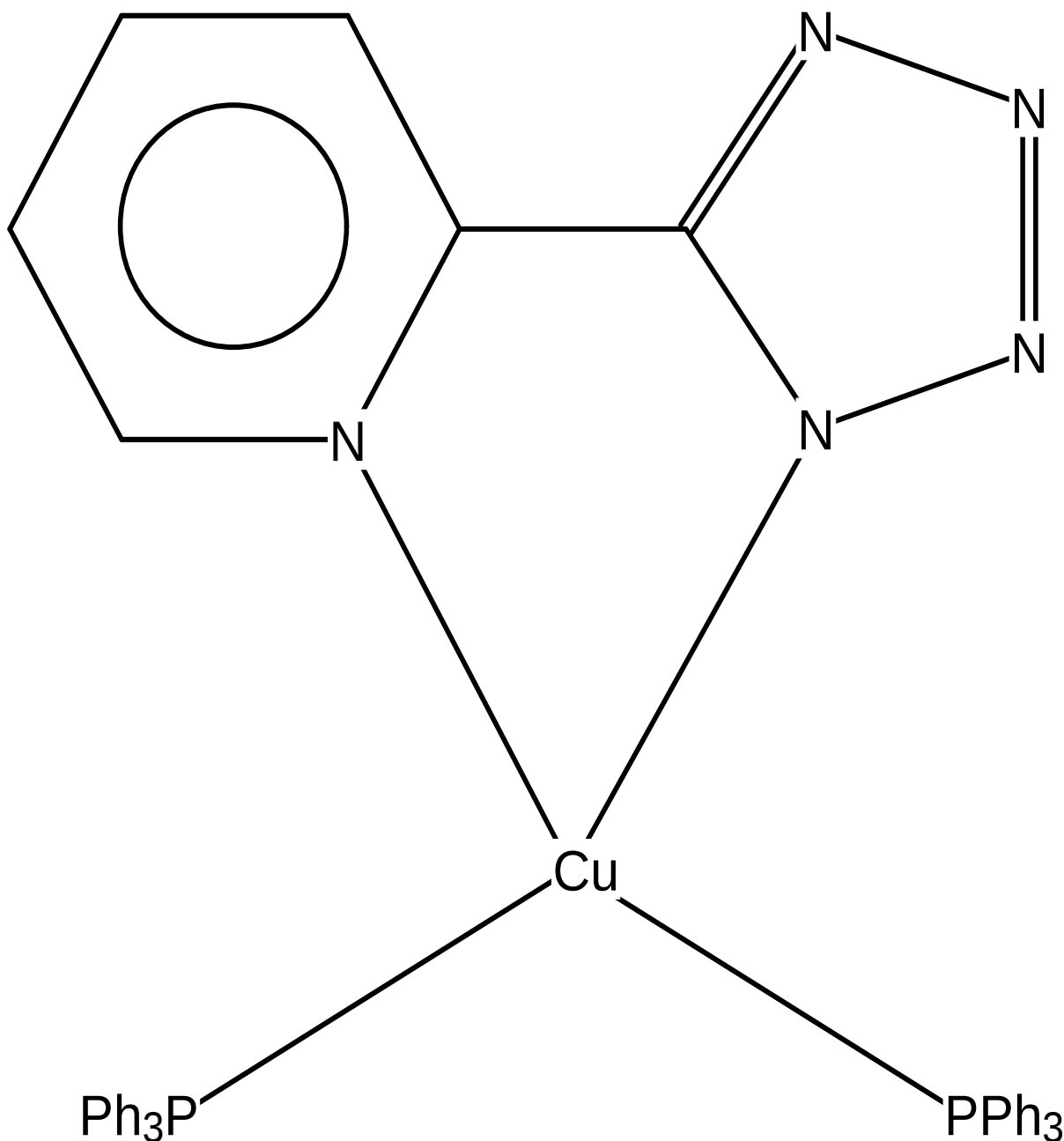
Reference: L.Bergmann, C.Braun, M.Nieger, S.Bräse (2018)
Dalton Trans. ,**47**,608

Formula: C₄₂ H₃₄ Cu₁ N₅ P₂

Compound Name: (5-(pyridin-2-yl)tetrazolato)-bis(triphenylphosphine)-copper(i)

Space Group:	P2 ₁ /n	Cell:	a	9.082(0)	b	18.255(0)	c	22.236(0)
Space Group No.:	14	(Å, °)	α	90.00	β	91.36(0)	γ	90.00

R-Factor (%): 7.65 **Temperature(K):** 123 **Density(g/cm³):** 1.323



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Reference: A.P.Mosalkova, S.V.Voitekhovich, A.S.Lyakhov, L.S.Ivashkevich, J.Lach, B.Kersting, P.N.Gaponik, O.A.Ivashkevich (2013) *Dalton Trans.* ,**42**,2985

Formula: C₃₂ H₄₄ Cu₂ Mn₁ N₁₀ O₁₂

Compound Name: hexakis(μ₂-Acetato)-bis(2-t-butyl-5-(2-pyridyl)-2H-tetrazole)-di-copper(ii)-manganese(ii)

Space Group:	P-1	Cell:	a	8.566(0)	b	9.940(0)	c	12.778(0)
Space Group No.:	2	(Å, °)	α	81.76(0)	β	75.09(0)	γ	70.82(0)
R-Factor (%):	2.33	Temperature(K):	100	Density(g/cm³):	1.580			

