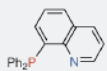
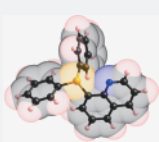


Orange and Yellow Crystals of Copper(I) Complexes Bearing 8-(Diphenylphosphino)quinoline: A Pair of Distortion Isomers of an Intrinsic Tetrahedral Complex

8-(Diphenylphosphino)quinoline



Ph₂P : Ph₂Pqn

Unsymmetrical bidentate ligands

- > Electronic differentiation
- > Planar five-membered chelate ring
- > Stacking interaction by quinolyl and phenyl rings

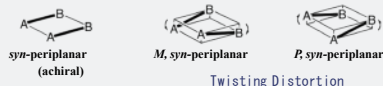


- ◇ Stabilization of unusual coordination geometry
- ◇ and oxidation state of the metal center

- ◇ Distortion of ideal coordination geometry

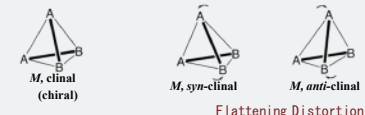
Distortion of Coordination Geometry

Square-Planar Complex with two (A-B) ligands



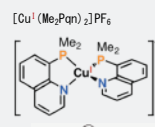
Twisting Distortion

Tetrahedral Complex with two (A-B) ligands

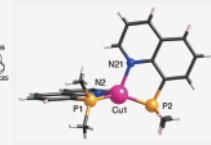
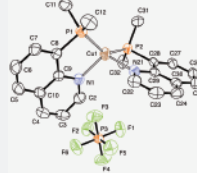
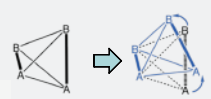


Flattening Distortion

Copper (I) Complex with Me₂Pqn



Rocking Distortion of Tetrahedral Complexes

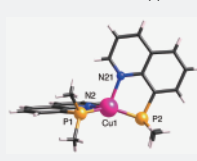


Copper (I) Complex with Me₂Pqn

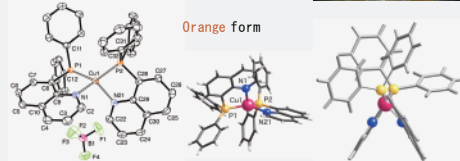
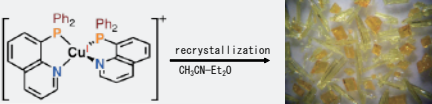


Steric interaction is expected with a larger substituents

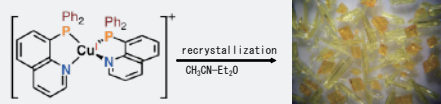
Plane[Cu1, P1, N2] vs. Cu1-P2 : 154.3°
Plane[Cu1, P2, N21] vs. Cu1-P1 : 119.2°
P1-Cu1-P2 : 138.21(6)°
N1-Cu1-N21 : 103.4(1)°



Copper (I) Complex with Ph₂Pqn

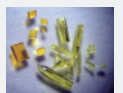


Copper (I) Complex with Ph₂Pqn

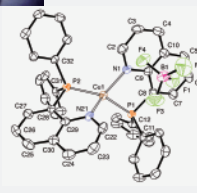
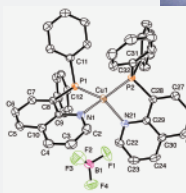


Copper (I) Complex with Ph₂Pqn

Orange form
triclinic, P 1
D_x = 1.442 Mg m⁻³



Yellow form
monoclinic, P2₁/c
D_x = 1.477 Mg m⁻³

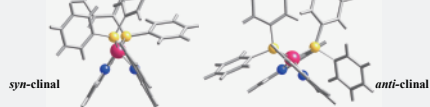
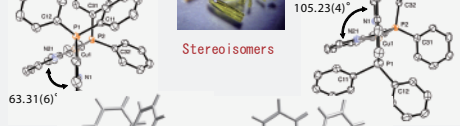


Copper (I) Complex with Ph₂Pqn

Orange form

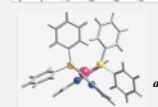
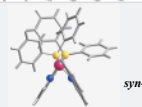
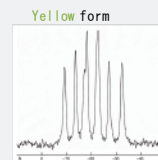
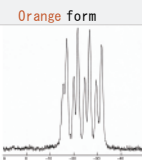


Yellow form



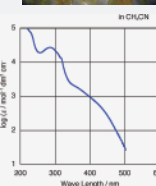
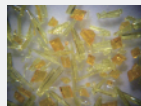
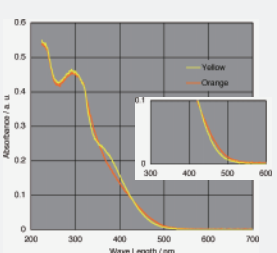
Copper (I) Complex with Ph₂Pqn

³¹P CP-MAS NMR Spectra

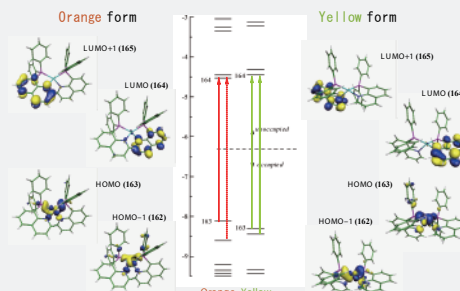


Copper (I) Complex with Ph₂Pqn

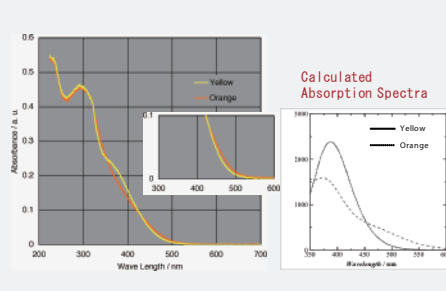
Diffuse Reflectance Spectra
(sample 1 mg, diluted with 1.00 g KBr)



TD-DFT Calculation of [Cu(Ph₂Pqn)₂]⁺



Absorption Spectra of [Cu(Ph₂Pqn)₂]⁺BF₄⁻



参考文献

Orange and yellow crystals of copper(I) complexes bearing 8-(diphenylphosphino)quinoline: a pair of distortion isomers of an intrinsic tetrahedral complex
Takayoshi Suzuki, Hiroshi Yamaguchi, Akira Hashimoto, Koichi Nozaki, Mototsugu Doi, Naoya Inazumi, Noriaki Ikeda, Satoshi Kawata, Masaaki Kojima, and Hideo D. Takagi
Inorganic chemistry (2011), 50(9), 3981-7.