Structrural and photophysical properties of [Cu(N^S)(P^P)][PF_6] complexes

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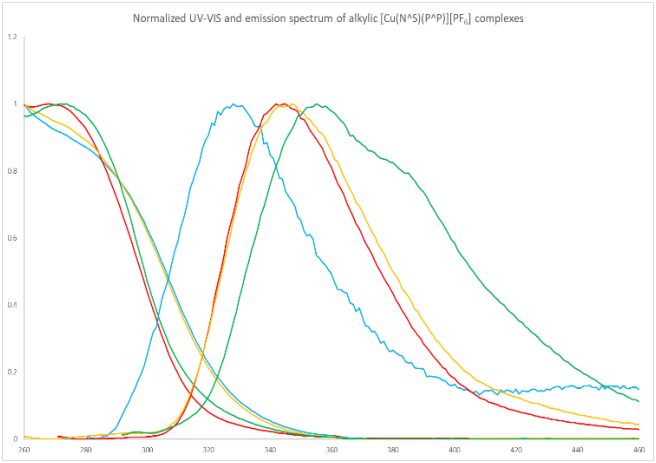
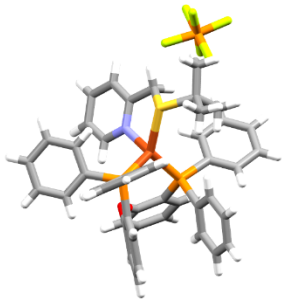
Heteroleptic copper complexes with P^P ligands exemplified by xanthphos or POP, and N^N ligands based on 2,2'-bipyridine have been known for some years. Their luminescent and structural properties have been investigated in detail.[1] Changing the substituents on the diimine ligand changes the overall photophysical properties of the complex and has an influence on the photoluminescence quantum yield and the lifetime of the complex.[2]

Another possibility to create a new set of copper(I) complexes is to adapt the ligand by introducing a different heteroatom. Sulfur has an affinity towards copper and stabilizing effects on the Cu(I) geometry have been observed and investigated.[3] However few heteroleptic Cu(I) complexes are known in which a bidentate N^S ligand binds with its both heteroatoms to the copper centre. Four complexes of the type [Cu(N^S)(P^P)][PF_6] where the N^S ligand is a 2-thioalkylpyridine have been prepared and structurally and photochemically investigated. These properties will be presented along with low temperature NMR spectroscopic data which demonstrate dynamic behaviour in the complexes.



Normalized solution absorption and emission spectra of a series of [Cu(N^S)(P^P)][PF_6] complexes



Crystal structure of one example of the series studied.

[1] Casadonte, D. J.; McMillin, D. R. *Inorg. Chem*. 1987, **26**, 3950-3952.
[2] Zhang Y.; Yu, X.; Lin, S.; Jin, Q.; Yang, Y.; Liu, M. Li, Z.; Zhang, C.; Xin, X. *Polyhedron*, 2017, **138**, 46-56.
[3] Braithwaite, A. C., *PhD-Thesis*, University of Auckland, 1974, https://researchspace.auckland.ac.nz/handle/2292/2066