

**SYSTEMATIC COORDINATION COMPOUNDS:
FROM FUNDAMENTALS TO APPLICATIONS**

By

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ABSTRACT

Coordination compounds (complexes) are formed as a result of coordinate bonds between Lewis bases (ligands) and Lewis acids with excess ligands bonded to the transition metal ions.

Comprehensive studies of complexes using basic physicochemical techniques involve varying substituents on ligands. The experimental data allow unbiased pronouncement on the complexes which are the fundamentals of coordination chemistry.

Various substituted ligands, their metal complexes and adducts were studied. The presence of outer-sphere coordinated β -diketone anion in copper R_3 -substituted β -diketonates and the varied bonding modes in the adducts were reported for the first time. A major contribution was the overriding importance of Lewis base concentration over the pKa/% enol consideration with two “outer-sphere anions” in 1:3 adducts of nickel. Similar “outer anions” in metal adducts were confirmed by x-ray crystallographic data and density functional theory. The various x-ray crystallographic data/structures clearly confirmed the interpretations of other experimental data in our studies on hydrazides and mixed ligand complexes.

Structure / activity relationship on the antimicrobial activities showed enhanced activities on coordinating ligand to metal e.g. nickel (II) hydrazide against *Staphylococcus* and *Pseudomonas* while activities of nickel complexes with N-donor heterocyclic ligands were better than gentamicin at 2 mg/mL and had stronger antifungal activity than ticonazole.

In our modest contribution on new materials, we published our studies on substituent and solvent effects on the luminescent properties of some imidazole/oxazole based heterocycles, hemilability of

imidazole/oxazole pyridine ligands and syntheses/evaluation of substituent effects on imidazole N-donor strengths for a new ligand series.

Our findings that oxazole derivatives could be explored for molecular sensing/signalling applications due to better photoluminescence efficiencies; brilliant, green solid-state photoluminescence of compound 3 suitable for organic lighting materials; imidazole donor strength influenced by carbon 2-position substituents modification, and effective conjugation between the imidazole ring and substituent aromatic groups was accountable for significant withdrawal of charge densities on the imidazole N-donor atom and vice versa will be useful in various industrial designs/applications.

In our contribution in two well-known catalytic processes, we confirmed that steric properties of coordinated organic framework were more important than electronic properties in determining catalyst efficiency in the monomer insertion step of norbornene polymerization. We also reported for the first time in the Suzuki-Miyaura C-C cross coupling catalysis that introduction of bulky units at the terminal ends of alkyl-based (sulphonamide) ligand system enabled construction of active palladium species with high turnover frequencies and yields of up to 91 % within 5 min with higher catalyst efficiency derivable from the preformed complexes. The extremely high TOF value of 18,000 h⁻¹ for the preformed complex *Pd-4E-2* confirmed its superiority over the *in situ* at a low catalyst loading of 0.05 mol % compared to the 0.2 mol % of Pd(AcO)₂ used for the *in situ*.

We recommended that UI should invest on human capital development by employing young promising UI graduates and Federal Government of Nigeria should set up the intended world class laboratories in six geopolitical zones.