

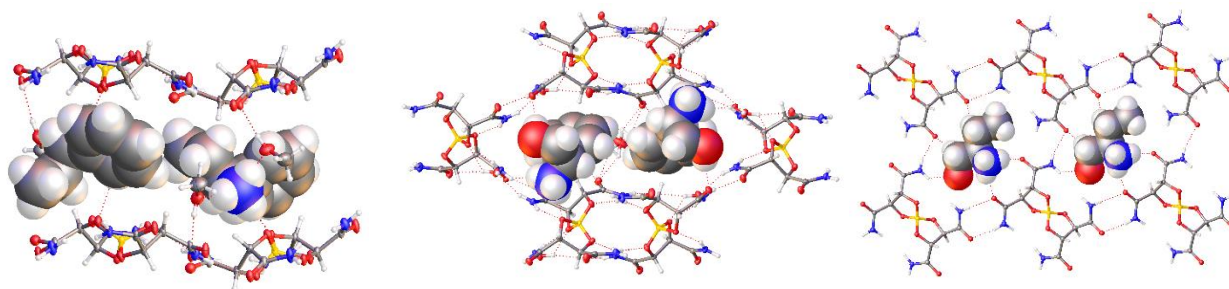
(Inorganic Chemistry)
Oral Abstract

Chiral Cationic Space formed in Spiroborates based on Tartramide [B(L-TarNH₂)₂] for Resolution

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The separation of chiral molecule from racemate has been studied for ages and still been explored in modern days. Preparation of spiroborate anions, bis(mandelato)borate [B(Man)₂]^{1,2} and bis(N,N'-diphenyltartramido)borate [B(L-Tar(NHPh)₂)₂]³ show effective separation of chiral cations with excess of 90% ee via one pot reaction or metathesis reaction. [B(L-TarNH₂)₂] shows a promising result as resolving agent by its extended H-bond connectivity. Different structures types are found by differentiate its reaction condition.



One of the building block of the self-segregation between [B(L-TarNH₂)₂] anion is the inter-amide bond N-H...O-C R₂² (8) synthons resulting in different chiral channel, layer or cavities for cations. The figures above show the layer, channel and cavities where R-Phenylpropylamine, S-Phenylglycinol and R-2-amino-1-butanol are successfully separate from its racemate.

We are grateful to the Research Grants Council of Hong Kong for funding of this work (grant 16306515).

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(Inorganic Chemistry) Oral Abstract

Bismuth drugs suppress SARS-CoV-2 replication and relieve virus-associated pneumonia in vitro and in vivo

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SARS-CoV-2 leads to a global pandemic of COVID-19 with high infectivity and mortality¹. Currently, therapeutic options targeting SARS-CoV-2 are very limited. Metal compounds are historic antimicrobial agents; however, their antiviral activities were barely explored. Here, we screened a set of metallodrugs and related compounds, and identified ranitidine bismuth citrate (Pylorid[®]), a drug in clinical use for the treatment of *Helicobacter pylori* infection, as a potent anti-SARS-CoV-2 agent both in vitro and in vivo. Pylorid exhibited low cytotoxicity and protected SARS-CoV-2-infected cells. Importantly, it suppressed SARS-CoV-2 replication with decreased viral loads in both upper and lower respiratory tracts, and relieved virus-associated pneumonia in a golden Syrian hamster model. Our mechanistic studies revealed that Pylorid and related compounds exhibited excellent inhibition towards both ATPase (IC₅₀=0.69 μM) and DNAunwinding (IC₅₀=0.70 μM) activity of SARS-CoV-2 helicase via an irreversible displacement of zinc(II) ions from the enzyme with bismuth(III) ions. Our findings suggest viral helicase as a druggable target and the high clinical potential of bismuth(III) or other metallodrugs for the treatment of SARS-CoV-2 infection.

We thank the Research Grants Council (RGC) of Hong Kong and Norman & Celia Yip Foundation for financial support.

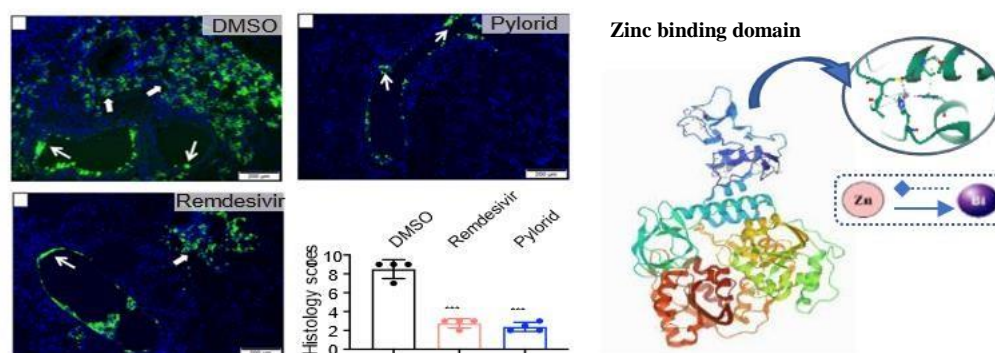


Figure 1. Viral N protein distribution in lung tissues section from groups of hamsters (Left) and the substitution of zinc(II) in SARS-CoV-2 helicase by bismuth(III) (Right).

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(Inorganic Chemistry)
Oral Abstract

Synthesis and Reactivity of Tantalum Alkyne Complexes Supported by Linked Cyclopentadienyl-Carboranyl Ligand

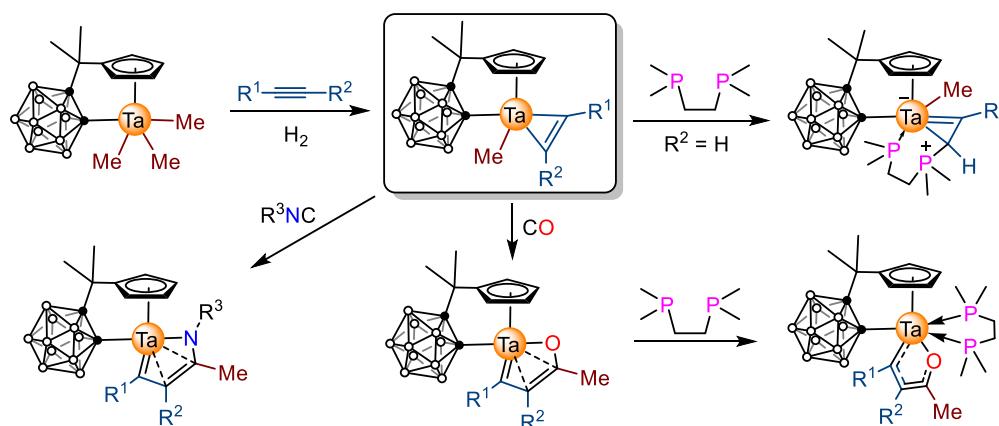
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Alkyne reagents have been applied as versatile ligands in organometallic chemistry. While alkynes readily form adducts with low-valent late transition metals, the early-transition-metal alkyne complexes are generally derived from reduction of a high-valent metal center in the presence of an alkyne.¹ Herein, we report a facile, one-pot method to synthesize a series of tantalum alkyne complexes from a Ta(V) alkyl complex, where using strong reducing agent is avoided. Such synthetic method is suitable for both terminal and internal alkynes bearing different functional groups.

Moreover, the reactivity of these tantalum alkyne complexes towards unsaturated molecules has been investigated. By treatment with carbon monoxide or isocyanides, these tantalum alkyne complexes produced nonplanar five-membered metallacycles. Interestingly, the chelation of a bidentate phosphine ligand could planarize the oxa five-membered ring and gave a six-electron metallafuran complex. On the other hand, direct reaction of the phosphine ligand with alkynylated tantalum compounds afforded η^2 -vinyl complexes. The structures of these novel tantalum complexes have been unambiguously characterized by single crystal X-ray analyses.



Acknowledgements

This work was supported by a grant from the Research Grant Council of HKSAR.

(Inorganic Chemistry)
Oral Abstract

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(Inorganic Chemistry)
Oral Abstract

Cellular Imaging Catalyzed by CeO₂: Right Shape Improves Fluorescence Intensity

Student: Zicong TAN (City U) Supervisor: Dr. Yung-Kang PENG

Abstract

It is important to choose a suitable material to achieve remarkable performance in biomedical applications. However, the shape of material itself shapes its performance as well. Although CeO₂ has been reported with phosphatase- and peroxidase-like activity, herein, we demonstrate the importance of choosing the right shape (e.g. octahedron and cube) of CeO₂ to improve its activity in mimicking phosphatase and peroxidase in cellular imaging. The imaging experiment shows that octahedron has higher phosphatase-like activity than cube (>17 times in k constant) in the dephosphorylation of the fluorogenic substrate (e.g. DHXP), which can enhance the fluorescence intensity (>8 times). On the other hand, compared with octahedron, cube is more active (>14 times in k constant) in mimicking peroxidase to catalyze the oxidation of the o-phenylenediamine (OPD) in the presence of H₂O₂ to generate stronger fluorescence (>3 times in intensity). According to the principle of heterogeneous catalysis, the catalytic conversion of the substrates occurs on the surface of different CeO₂ shapes, which contains the surface Ce atoms with different chemical states (i.e. electron density) playing a significant role in this shape-dependent activity. The probe-assisted nuclear magnetic resonance (NMR) is a sensitive surface characterization technique that can measure the chemical state (i.e. electron density) of surface Ce atom. The NMR result indicates that octahedron hosts the surface Ce atom with lower electron density than cube, which promotes the adsorption and dephosphorylation of phosphate substrate. On the other hand, the surface Ce atom on cube has higher electron density (cf. octahedron) facilitating the H₂O₂ reduction and OPD oxidation. We believe that this fundamental understanding of the CeO₂ surface is important to manipulate its catalytic activity and thus performance.

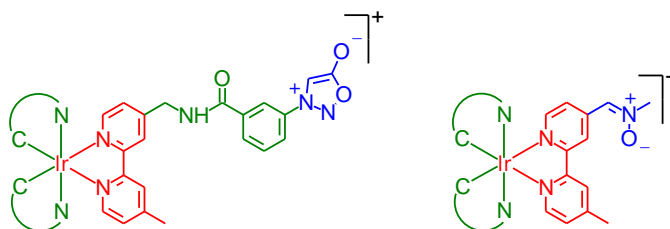
(Inorganic Chemistry) Oral Abstract

Rational Design of Bioorthogonal Reagents Derived from Photofunctional Cyclometalated Iridium(III) Polypyridine Complexes

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In the past two decades, the bioorthogonal chemical reporter approach has been developed as a versatile platform for the detection and visualization of biomolecules in their native environments without disrupting the biological processes. Although a large number of luminescent bioorthogonal probes have been developed, their use in cellular imaging often suffers from the problem of high retention of the unreacted probes inside the cells and thus strong background emission. Thus, the development of bioorthogonal probes with activatable emission has captured increasing attention. With our long-standing interest in the development of luminescent transition metal complexes as cellular probes, bioimaging reagents, and (photo)cytotoxic agents, in this presentation, the rational design of photofunctional cyclometalated iridium(III) polypyridine complexes as novel bioorthogonal reagents will be described. Our results demonstrated that the incorporation of a bioorthogonal group into complexes not only endow the complexes with excellent specificity but also a high degree of control of their emission properties and photocytotoxic activity, which enable the use of these complexes in targeted imaging and photodynamic therapy.



We thank Hong Kong Research Grants Council (Project No. CityU 11300017 and CityU 11300019) for financial support.

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(Inorganic Chemistry) Oral Abstract

Impressive near-infrared brightness and singlet oxygen generation from strategic lanthanide–porphyrin double-decker complexes in aqueous solution

Jing-Xiang Zhang, Wai-Lun Chan, Chen Xie, Yan Zhou, Ho-Fai Chau, Partha Maity, George T. Harrison,

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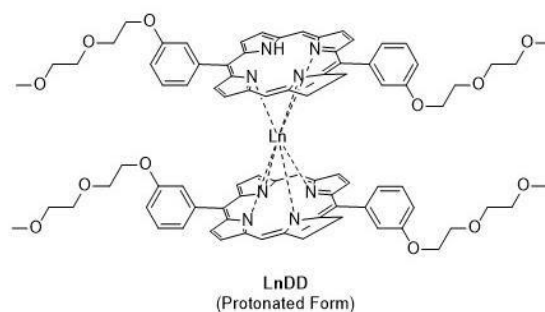
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Abstract

Although lanthanide double-decker complexes with hetero-macrocyclic ligands as functional luminescent and magnetic materials have promising properties, their inferior water solubility has negated their biomedical applications. Herein, four water-soluble homoleptic lanthanide (Ln = Gd, Er, Yb and La) sandwiches with diethylene-glycol-disubstituted porphyrins (**DD**) are reported, with their structures proven by both quantum chemical calculations and scanning tunneling microscopy. Our findings demonstrate that the near-infrared emission intensity and singlet oxygen ($^1\text{O}_2$) quantum yields of **YbDD** and **GdDD** in aqueous media are higher than those of the reported capped lanthanide monoporphyrinato analogues, **YbN¹** and **GdN²**; the brightness and luminescence lifetime in water of **YbDD** are greater than those of **YbN**. This work provides a new dimension for the future design and development of molecular theranostics-based water-soluble double-decker lanthanide bisporphyrinates.



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(Inorganic Chemistry)
Oral Abstract

The Geometric and Electronic Properties of Single-atom Catalysts for Enhanced Catalytic Performance

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Abstract

The application of metal-organic frameworks (MOFs) to host single atom has been developed nowadays.¹ In this research, the geometric and electronic properties of single atoms inside MOFs have been extensively studied. A series of mid-to-late 3d transition metal sites have been immobilised within the microporous cavity of UiO-66-NH₂. By employing Rietveld refinement of *new-generation* synchrotron diffraction, we not only identified the crystallographic and atomic parameters of the single atoms, but also elucidated the end-on coordination geometry with CO₂. A volcano trend in the Faradaic efficiencies (FEs) of CO has been observed. In particular, the confinement effect within rigid MOF can greatly facilitate redox hopping between the Cu SACs, rendering high FEs of CH₄ and C₂H₄ at the current density of -100 mA cm⁻². Despite only demonstrated in selected SACs within UiO-66-NH₂, this study sheds light towards the rational engineering of molecular interactions(s) with SACs for the sustainable provision of fine chemicals.

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<https://us04web.zoom.us/j/6593115461?pwd=bU50Y3o4SEkwbU1EYi8yT05LazZMUT09> (Meeting ID: 659 311 5461, Password: ivWY26)

(Inorganic Chemistry)

Oral Abstract

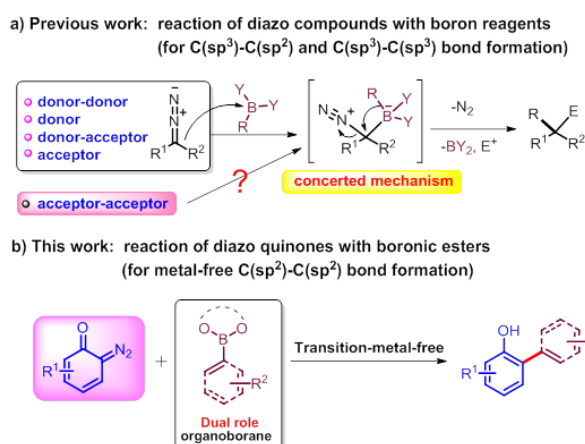
Transition-Metal-Free C(sp²)-C(sp²) Cross-Coupling of Diazo Quinones with Catechol Boronic Esters

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Abstract

Due to the constraints on the levels of trace metals permitted in pharmaceuticals, there is a growing interest in developing transition-metal-free C-C bond forming reactions. Among these reactions, diazo compounds with organoboranes are appealing because of their efficiency, mild conditions and diversity, as well as the availability of the substrates.^[1-3] Nonetheless, the extension of diazo compounds to less nucleophilic acceptor/acceptor type and construction of C(sp²)-C(sp²) bonds via the current methodology is challenging.



A transition-metal-free C(sp²)-C(sp²) bond formation reaction via the cross-coupling of diazo quinones with catechol boronic esters was developed. With this protocol, a variety of biaryls and alkenyl phenols were obtained in good to high yields under mild conditions. The reaction tolerates various functionalities and is applicable to the derivatization of pharmaceuticals and natural products. The synthetic utility of the method was demonstrated by the short synthesis of multi-substituted triphenylenes and three bioactive natural products, honokiol, moracin M and stemofuran A. Mechanistic studies and density functional theory (DFT) calculations revealed that the reaction involves attack of the boronic ester by a singlet quinone carbene followed by a 1,2-rearrangement via a stepwise mechanism.

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(Inorganic Chemistry) Oral Abstract

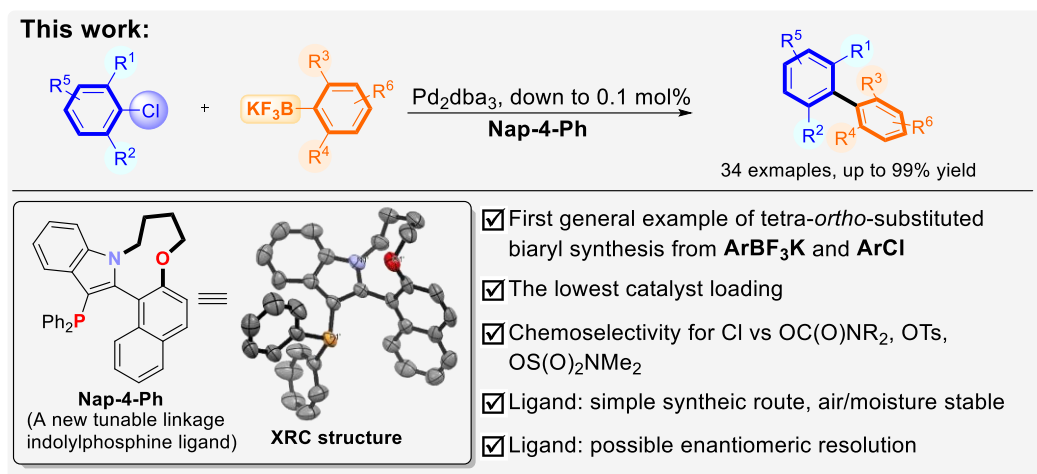
New Palladium complexes for facile assembly of highly steric hindered biaryls

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Abstract



The first general example of tetra-*ortho*-substituted biaryl synthesis *via* Suzuki-Miyaura cross coupling of potassium aryltrifluoroborates and (hetero)aryl chlorides is reported. Organotrifluoroborates often serve as a better coupling partner than arylboronic acids for Suzuki-coupling due to no association of uncertain amount of boroxine. The activity of this would be a concern and thus leads such transformation remains challenging. Herein, a new class of tailor-made indolylphosphine ligand-palladium complex bearing a tunable linkage is designed for tackling challenging tetra-*ortho*-substituted biaryl synthesis. With the metal complex of Pd₂dba₃/**Nap-4-Ph**, a wide range of sterically hindered chloroarenes coupled-well with steric bulky aryltrifluoroborates in good-to-excellent yields (up to 99%) with catalyst loading down to 0.1 mol%. The possible resolution strategies of **Nap-n-Ph** ligands in achieving optically pure form are also demonstrated.

(Inorganic Chemistry)
Oral Abstract

Mass cytometry-based approach for profiling B-cell acute lymphoblastic leukemia (B-ALL)

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Flow cytometry has been used clinically for B-cell acute lymphoblastic leukemia (B-ALL) diagnosis and prognosis. However, it suffers from some inherent limitations. Herein, by using mass cytometry combined with bioinformatic algorithms, we develop a streamlined platform, enabling cancer cells from B-ALL patients to be quantitatively distinguished from normal haematopoietic cells in an unsupervised data-driven manner. Specifically, evident decreases of CD38 and CD81, and overexpression of abnormal markers CD73, CD123, CD304 and CD66c were noted in the tested leukemic population. The panoramic view of leukemia associated immunophenotypes across the whole cell populations facilitates a more comprehensive understanding of leukemogenesis. The different cell subsets (CD34⁺CD10⁺CD38⁻, CD38⁺CD10⁻, CD73⁺, CD123⁺, CD304⁺, CD304⁺) shown in B-ALL cells provide a basis for B-ALL diagnosis, and the newly explored cell clusters by SPADE (CD123⁺CD34⁻CD10⁻CD38⁺, CD73⁺CD34⁺CD10⁺CD38⁻, CD304⁺CD34⁺CD10⁺CD38^{int}) may serve as additional biomarkers to facilitate the leukemia prognosis. Taken together, we demonstrate that mass cytometry based approach is more robust and precise, and may serve as a potential alternative of flow cytometry for B-ALL diagnosis and prognosis.

This work is supported by the Research Grants Council of Hong Kong (17307017, R7070-18), the Innovation and Technology Commission of Hong Kong (ITS/124/17), and the University of Hong Kong. Norman & Cecilia Yip Foundation is acknowledged for support. This work is also supported in part by a grant from the University of Macau (MYRG 2018-00033-FHS) to E.C. We would also like to acknowledge Kaeling Tan and Tiffany Nga-Teng Iu for their help with the Helios Mass Cytometer at the Genomics, Bioinformatics and Single Cell Analysis Core at Faculty of Health Sciences, University of Macau.