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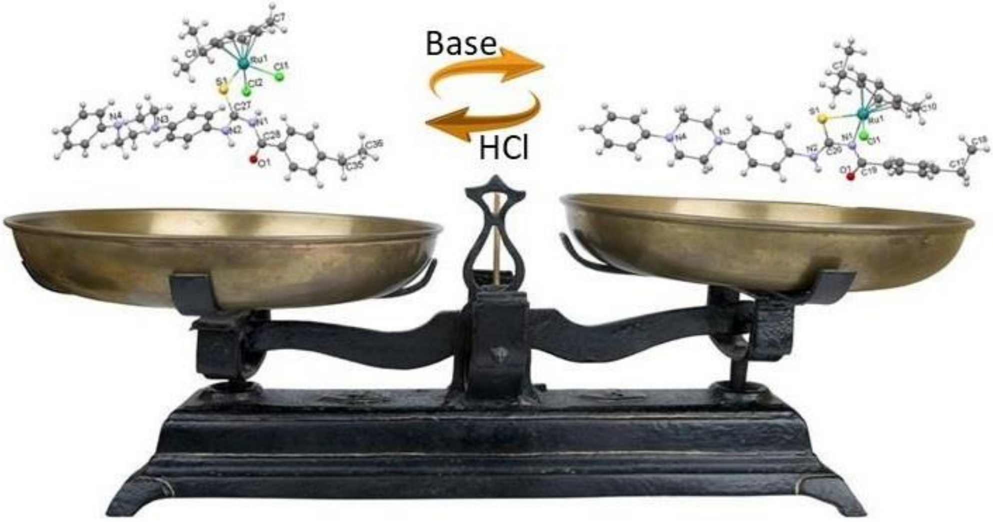
酸鹼控制的釕錯合物硫脲配位基鍵結模式「變身術」



想像一下，一種化學物質像變形金剛一樣，能在酸性或鹼性環境中「切換」自己的連接方式！這就是這篇論文的超酷發現。高雄醫學大學醫藥暨應用化學系無機合成化學研究團隊合成了一種新型的釕(Ru)金屬錯合物，使用「醯基硫脲」這種特別的配位基（ligand)。這個配位基就像一隻手，可以用「單牙」(只用一個點連接）或「雙牙」(用兩個點連接）的方式抓住釕金屬。

✧ **酸鹼當開關，配位基隨意變**

過去的釕錯合物通常固定一種連接方式，但這篇研究首次證明，只要加鹼(例如有機鹼或無機鹼)，就能讓配體從「單牙」變成「雙牙」；反過來，加酸（例如鹽酸）又能變回「單牙」。這就像用 pH 值遙控分子結構，超級方便！他們用紅外線光譜、核磁共振、質譜和 X 光晶體分析，清楚地確認這兩個形態的「身分證」。

✧ 結構小改變，效果大不同

單牙形態的錯合物比較鬆散，雙牙形態則更緊密。研究發現，N-甲基咪唑這種懸垂配體讓釕-氮鍵變短（2.066 Å），電子給得更多，錯合物更穩定。這對設計新催化劑或藥物很重要，因為結構決定功能。

✧ 未來應用超有潛力

這種「酸鹼可控」的錯合物，可以用來開發智能材料（例如感測 pH 變化）或抗癌藥物（釕錯合物本來就很有潛力）。更酷的是，這種動態切換讓科學家能更精準控制金屬-配位基間的互動，開啟生物啟發化學的新可能。

總之，這篇論文不只合成新東西，還發現了酸鹼切換配位基形態的魔法，讓金屬錯合物從「死板」變「靈活」，為未來化學與醫學應用注入新活力！

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【研究團隊】

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團隊簡介：許智能教授的研究團隊（Sodio Lab; 無機和成實驗室）致力於

1. 設計與合成仿生金屬配位化合物，模擬金屬蛋白的活性中心。
2. 探討金屬在生物反應中的角色，並以化學角度理解其機制。
3. 應用這些研究成果於藥物設計與催化劑開發。

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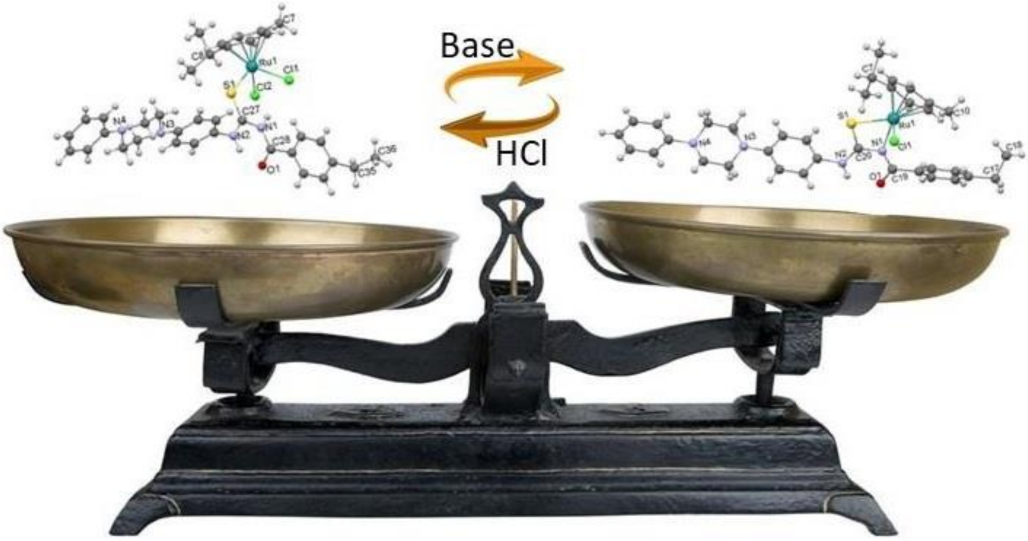
A Molecular Transformer: Ligand Switching via pH Control



Imagine a chemical compound that behaves like a Transformer—able to switch its bonding mode depending on whether it's in an acidic or basic environment. This is the fascinating discovery presented in this study. The Inorganic Synthetic Chemistry Research Team from the Department of Pharmaceutical and Applied Chemistry at Kaohsiung Medical University synthesized a novel ruthenium (Ru) complex using a thiourea-based ligand. This ligand can bind to the metal center in two distinct ways: Monodentate (single-point attachment) and Bidentate (dual-point attachment).

✧ Acids and Bases as Molecular Switches

Traditionally, ruthenium complexes exhibit fixed coordination patterns. This study is the first to demonstrate that the bonding mode of the thiourea ligand can be reversibly switched by simply adjusting the pH:

1. Adding a base (organic or inorganic) transforms the ligand into a bidentate form.
2. Adding an acid (e.g., hydrochloric acid) reverts it to a monodentate form.

This pH-responsive behavior was confirmed using a suite of analytical techniques, including infrared spectroscopy, nuclear magnetic resonance (NMR), mass spectrometry, and X-ray crystallography.

✧ Small Structural Shifts, Big Functional Impact

The study revealed that the monodentate complex is relatively loose, while the bidentate form is more compact and stable. Notably, the presence of a dangling N-methylimidazole ligand shortens the Ru–N bond to 2.066 Å, enhancing electron donation and overall stability. This structural flexibility is crucial for designing next-generation catalysts and metal-based drugs, where structure dictates function.

✧ Broad Potential for Smart Applications

This acid–base controllable ruthenium complex opens exciting possibilities for:

1. Smart materials that respond to pH changes.
2. Targeted anticancer therapies, leveraging the known bioactivity of ruthenium complexes.
3. Bio-inspired chemistry, enabling precise control over metal–ligand interactions.

Conclusion

This study not only introduces a novel ruthenium complex but also unveils a dynamic mechanism for switching ligand coordination via acid–base interactions. Such flexibility injects new life into the design of adaptive metal complexes, paving the way for innovative applications in chemistry, materials science, and medicine.

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【Concrete Results】

- **Academic Achievements:**

Acid–Base Controlled Transformation of the Bonding Mode of the Thiourea Ligand in a Ruthenium Wedge

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【Research Team】

Team Member: Amir Karim, Rahime Eshaghi Malekshah, Yu-Ting Chu, Sodio C.N. Hsu

Overview: Led by Professor Sodio C. N. Hsu, the Sodio Lab is dedicated to advancing the frontiers of bioinorganic and supramolecular chemistry through the following core research areas:

1. Design and Synthesis of Bioinspired Metal Coordination Complexes
2. Chemical Investigation of Metal Roles in Biological Systems
3. Application in Drug Design and Catalysis

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