

Development of Mononuclear and Dinuclear Ruthenium Complexes for Water Oxidation Catalysis

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Water oxidation is crucial for sustainable fuel generation in artificial photosynthesis. Dinuclear ruthenium complexes with closely spaced metal ions are promising catalysts for the $4e^-/4H^+$ transformation¹, and catalysts with ligands like 3,5-bis(pyridyl)pyrazolate (bpp) and 3,5-bis(bipyridyl)pyrazolate (bbp) stand out due to their stability and surface functionalization capabilities, making them suited for robust photoanodes^{2,3}. Complexes of the $\{(bpp)Ru_2\}$ type use the I2M mechanism, while $\{(bbp)Ru_2\}$ complexes undergo water nucleophilic attack (WNA)². Understanding the preference for these mechanisms remains unclear. We have now developed a novel dinuclear ruthenium complex with a pyridyl(bipyridyl) pyrazolate (pbp) ligand, combining features of both systems. The synthesis and water oxidation results of this complex, along with mononuclear ruthenium complexes, will be presented.

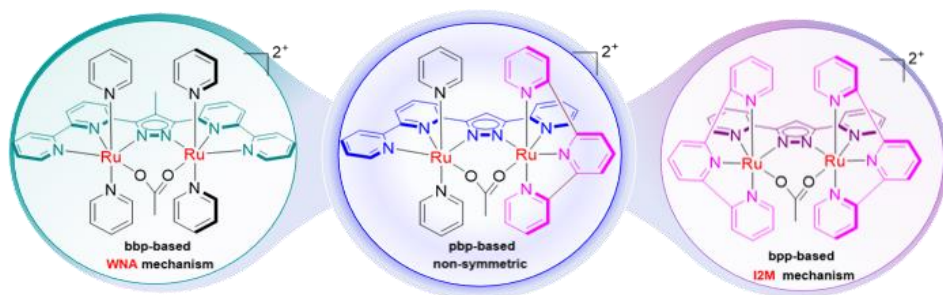


Figure 1: Pyrazolate-based dinuclear Ru-WOCs.

[1] Matheu, R.; et al. *Nature Reviews Chemistry* 2019, **3**, 331-341.10.1038/s41570-019-0096-0.

[2] (a)Sens, C.; et al. *JACS* 2004, **126**, 7798-7799,10.1021/ja0486824.(b)Neudeck, S.; et al. *JACS* 2014, **136**, 24-27,10.1021/ja409974b.

[3] (a) Odrobina, J.; et al. *ACS Catalysis* 2017, **7**, 6235-6244,10.1021/ja409974b (b) Odrobina, J.; et al. *ACS Catalysis* 2017, **7**, 2116-2125,10.1021/acscatal.6b02860; (c) Rajabi, S.; et al. *ACS Catalysis* 2020, **10**, 10614-10626,10.1021/acscatal.2c05175