










RESEARCH ARTICLE

Pyridine-functionalized N-heterocyclic carbene gold(I) binuclear complexes as molecular electrocatalysts for oxygen evolution reactions

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N-heterocyclic carbene (NHC) complexes of gold(I/III) attained immense interest in catalytic organic transformations and as anticancer agents against several types of human cancers; however, their potential as electrocatalysts is scarce. The electrocatalytic oxygen evolution reaction was performed for the first time using pyridine-functionalized NHC gold(I) binuclear metallacycles (**8** and **9**) possessing aptly designed ligand field. Complexes were prepared by the transmetallation of corresponding silver(I) NHC complexes, which were prepared by in situ deprotonation of pyridine and aryl substituted 1,2,4-triazolium hexafluorophosphate salts (**6** and **7**) with Ag₂O under dark. Both triazolium salts and binuclear gold(I) metallacycles were thoroughly characterised by NMR and ATR-IR spectral and elemental analyses. A bromide salt **4** and a binuclear gold complex **9** were elucidated for structure by single crystal X-ray diffraction analysis. Complex **9** possesses distorted linear coordination geometry around the gold atoms by the coordination of carbene carbon and pyridine nitrogen atoms bearing close Au–Au interaction (3.251 Å). The binuclear gold complexes **8** and **9** (along with 10 wt% conductive mesoporous carbon) were investigated as molecular electrocatalysts in oxygen evolution reaction (OER), which evidenced an oxygen evolution overpotential of 2.422 and 2.370 V versus reversible hydrogen electrode (RHE), respectively, to attain a current density of 10 mA.cm⁻². The Tafel slope values of 40.9 and 30.4 mV dec⁻¹ for **8** and **9**, respectively, indicate the reaction mechanism involved and the suitability of these complexes as apt electrocatalysts for OER. The stability of the prepared molecular electrocatalysts was investigated by cyclic voltammetry and chronoamperometry techniques.

KEYWORDS

1,2,4-triazoles, molecular electrocatalyst, N-heterocyclic carbene, oxygen evolution reaction, X-ray diffraction