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Di(N-heterocyclic carbene) gold(III) imidate complexes obtained by oxidative addition of N-halosuccinimides

Marco Baron,^{*,a} Marco Dalla Tiezza,^a Alice Carlotto,^a Cristina Tubaro,^{*,a} Claudia Graiff,^b and Laura Orian^a

^a Dipartimento di Scienze Chimiche, Università degli Studi di Padova, via Marzolo 1, 35131 Padova, Italy.

^b Dipartimento di Scienze Chimiche, della Vita e della Sostenibilità Ambientale, Università degli Studi di Parma, Parco Area delle Scienze 17/A, 43124 Parma, Italy.

Corresponding authors. For M. B.: e-mail: marco.baron@unipd.it. For C. T.: cristina.tubaro@unipd.it

Abstract. The reaction between the gold(I) dicarbene complexes $[\text{Au}_2(\mu^2\text{-MeIm}(\text{CH}_2)_n\text{ImMe})_2](\text{PF}_6)_2$ (Im = imidazol-2-ylidene, $n = 1, 2, 3$) and N-bromosuccinimide affords the gold(III) complexes $[\{\text{AuBr}(\text{N-suc})\}_2(\mu^2\text{-MeIm}(\text{CH}_2)_n\text{ImMe})_2](\text{PF}_6)_2$, in which both gold centres have a bromide and a N-succinimide anion in the coordination sphere. In the case of the CH_2CH_2 bridge, two different conformers of the gold(III) complex are formed; the structure of the major species has been clarified by single crystal X-ray diffraction analysis, while the nature and the properties of the minor one have been investigated by means of DFT calculations. Compared to N-bromosuccinimide, oxidative additions are slower with the N-chloro- and faster with the N-iodosuccinimides. In both cases the reactions are scarcely selective and the products distribution markedly depends on halide size and reaction conditions.

Keywords: N-heterocyclic carbenes, gold complexes, oxidative addition, DFT calculations, N-halosuccinimides.

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