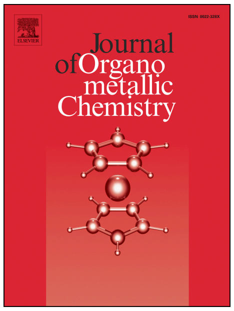

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Di(N-heterocyclic carbene) gold(III) imidate complexes obtained by oxidative addition of N-halosuccinimides

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Abstract. The reaction between the gold(I) dicarbene complexes $[Au_2(\mu^2\text{-MeIm}(CH_2)_n\text{ImMe})_2](PF_6)_2$ (Im = imidazol-2-ylidene, n = 1, 2, 3) and N-bromosuccinimide affords the gold(III) complexes $[\{AuBr(N\text{-suc})\}_2(\mu^2\text{-MeIm}(CH_2)_n\text{ImMe})_2](PF_6)_2$, in which both gold centres have a bromide and a N-succinimidate 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.