Clean singlet oxygen production by a Re^I complex embedded in a flexible self-standing polymeric silsesquioxane film

Spada, Ramiro M.

Cepeda-Plaza, Marjorie

Gómez, María L.

Günther, Germán

Jaque, Pablo

Pizarro, Nancy

Palacios, Rodrigo E.

Vega, Andrés

Rhenium complexes are versatile molecular building blocks whose tunable photophysical properties are useful in diverse opto-related applications. Herein we report the synthesis and characterization of a novel Re^I tricarbonyldiimine complex, [(phen)Re(CO)<inf>3</inf>Br] (phen: 1,10-phenanthroline), which was found to be an efficient singlet oxygen [O<inf>2</inf>(¹Î"<inf>g</inf>)] photosensitizer in homogeneous solution [?<inf>O</inf><inf>2</inf>(¹Î"g) = 0.55 (dichloromethane) and 0.16 (dimethylformamide)]. The photophysical properties of [(phen)Re(CO)<inf>3</inf>Br] were thoroughly characterized in solution and modeled by means of density functional theory (DFT) and time-dependent (TD)-DFT quantum mechanical calculations. The Re complex was incorporated into a flexible polymeric silsesquioxane (SSO) film, which has excellent dopant compatibility, chemical resistance, and mechanical properties. When [(phen)Re(CO)<inf>3</in