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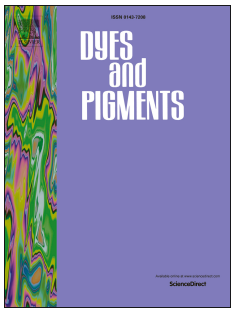

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PII: S0143-7208(18)30693-4

DOI: 10.1016/j.dyepig.2018.05.060

Reference: DYPI 6789

To appear in: *Dyes and Pigments*

Received Date: 6 April 2018

Revised Date: 23 May 2018

Accepted Date: 25 May 2018

Please cite this article as: Lyu S, Bertrand C, Hamamura T, Ducasse L, Toupance T, Olivier Cé, Molecular engineering of ruthenium-diacetylide organometallic complexes towards efficient green dye for DSSC, *Dyes and Pigments* (2018), doi: 10.1016/j.dyepig.2018.05.060.

Manuscript prepared for Dyes and Pigments

Molecular engineering of Ruthenium-diacetylide organometallic complexes towards efficient green dye for DSSC.

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Abstract

Three new dyes encompassing the organometallic [Ru(dppe)$_2$] (dppe = 1,2-bis(diphenylphosphino)ethane) fragment were designed and prepared for application in dye-sensitized solar cells. Introduction of the strong electron-withdrawing benzothiadiazole (BTD) unit as an additional acceptor in the attracting ligand led to original D–[M]–A–π–A' architectures. In particular the use of a thienyl-BTD motif led to a narrow bandgap sensitizer with deep-green coloration. The dye afforded 5.2 % power conversion efficiency in TiO_2-based DSSC device in the presence of the iodine/iodide couple as redox mediator. A joint experimental and theoretical study of the new dyes is reported.

Keywords

Dye-sensitized solar cells; Benzothiadiazole; Ruthenium-diacetylide complexes; DFT calculations; Organometallics; Photovoltaics.