

## Accepted Manuscript

Title: Interactions between thiocyanate-free bis-tridentate Ru complexes and iodide in dye-sensitized solar cells

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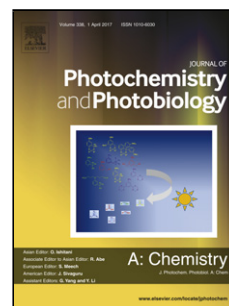
PII: S1010-6030(17)30290-3  
DOI: <http://dx.doi.org/doi:10.1016/j.jphotochem.2017.04.030>  
Reference: JPC 10619

To appear in: *Journal of Photochemistry and Photobiology A: Chemistry*

Received date: 7-3-2017  
Revised date: 13-4-2017  
Accepted date: 17-4-2017

Please cite this article as: H. Kusama, Interactions between thiocyanate-free bis-tridentate Ru complexes and iodide in dye-sensitized solar cells, *Journal of Photochemistry and Photobiology A: Chemistry* (2017), <http://dx.doi.org/10.1016/j.jphotochem.2017.04.030>

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# Interactions between thiocyanate-free bis-tridentate Ru complexes and iodide in dye-sensitized solar cells

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## ABSTRACT

The intermolecular interactions of thiocyanate-free Ru terpyridyl complexes containing a 2,6-disubstituted pyridine as a tridentate donor ligand (BTP, FT19, and TUS-29 dyes) with iodide ions are investigated using density functional theory. Similar to N749 dye with three thiocyanate ligands, the oxidized thiocyanate-free complexes mainly interact with  $I^-$  and  $I_2^-$  ions *via* the donor ligands. Oxidized BTP with a pyridine-2,6-ditetrazolyl ligand can be regenerated by three different mechanisms: (A) by one  $I^-$  through a one-step mechanism, (B) by two  $I^-$  ions *via* a two-step mechanism, or (C) by  $I_2^-$  *via* a one-step mechanism. Oxidized FT19 with a pyridine-2,6-dicarboxylate ligand can be regenerated *via* mechanism B or C. Although oxidized TUS-29 with a pyridine-2,6-dicarboxyamidato ligand can be reduced through mechanism C, the

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