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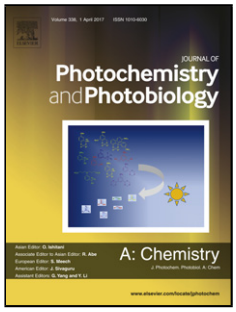

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Interactions between thiocyanate-free bis-tridentate Ru complexes and iodide in dye-sensitized solar cells

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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