Electronic Supplementary Information

Stereospecific microwave assisted conversion of a Ru(II)-p-cymene Complex to a solar cell dye in water

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1. Detailed Method
2. Allocated 1H NMR spectra of cis-RuL2NCS2.
4. 1H NMR spectra of cis-RuL2Cl2 (intermediate compound).
5. UV/Vis spectra of cis-RuL2Cl2.
Detailed Method:

CEM Discover Benchmate microwave unit was used for all microwave reactions. KNCS, The Ru(II)-p-cymene metal precursor, Scheme 1, and 4,4’-dicarboxylic acid-2,2’-bipyridine (dcbp) were all used as supplied by Dyesol. Hydrochloric acid (HCl) 32% supplied by Ajax Finechem was used as received. Analysis was carried out using the Perkin Elmer Spectrum One FTIR, the Varian Cary 50 UV-Vis and the Varian 400 HNMR spectrometer.

Ru-p-cymene (0.081mmol) and dcbpy (0.287mmol) were mixed in a solution of 1.5 mL H$_2$O and 1.5 mL HCl (32%) in a pressurised microwave vial. The solution was heated to 170°C using microwave heating for 60 minutes with a power of 300 W and a pressure of 10 bar. After cooling the solution, a black powder was isolated by suction filtration and washed with water.

The next step in the synthesis of \( \text{cis-RuL}_2(\text{NCS})_2 \) was to substitute the chloride ions with thiocyanate ions. The cis-RuL$_2$Cl$_2$ complex(0.19mmol) and KNCS (1.31mmol) were mixed in 3 mL H$_2$O, and the solution was heated to 170°C and irradiated with microwaves for 30 minutes with a power of 300 W and 10 bar. After cooling a black powder was vacuum filtered and washed with water.
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<th>Proton</th>
<th>δ(H)/ppm</th>
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<td>1</td>
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<tr>
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Figure 1: Cis-RuL₂(NCS)₂ Ruthenium Dye

Figure 2: Table of $^1$H NMR chemical shifts with proton allocation.

Figure 3: H NMR of cis-RuL₂(NCS)₂
Figure 4: Mass Spec of cis-RuL₂(NCS)₂

Figure 5: Mass Spec of cis-RuL₂(NCS)₂
Figure 6: $^1$H NMR of cis-RuL$_2$Cl$_2$

Figure 7: $^1$H NMR of cis-RuL$_2$Cl$_2$
Figure 8: UV/Vis Spectra of cis-RuL₂Cl₂.