

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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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 H₂O 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 *cis*-RuL₂(NCS)₂ was to substitute the chloride ions with thiocyanate ions. The *cis*-RuL₂Cl₂ complex(0.19mmol) and KNCS (1.31mmol) were mixed in 3 mL H₂O, 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.

Proton	$\delta(\text{H})/\text{ppm}$
1	9.36
2	8.03
3	8.76
4	7.62
5	7.33
6	8.57

Figure 1: Cis-RuL₂(NCS)₂ Ruthenium Dye

Figure 2: table of ¹H NMR chemical shifts with proton allocation.

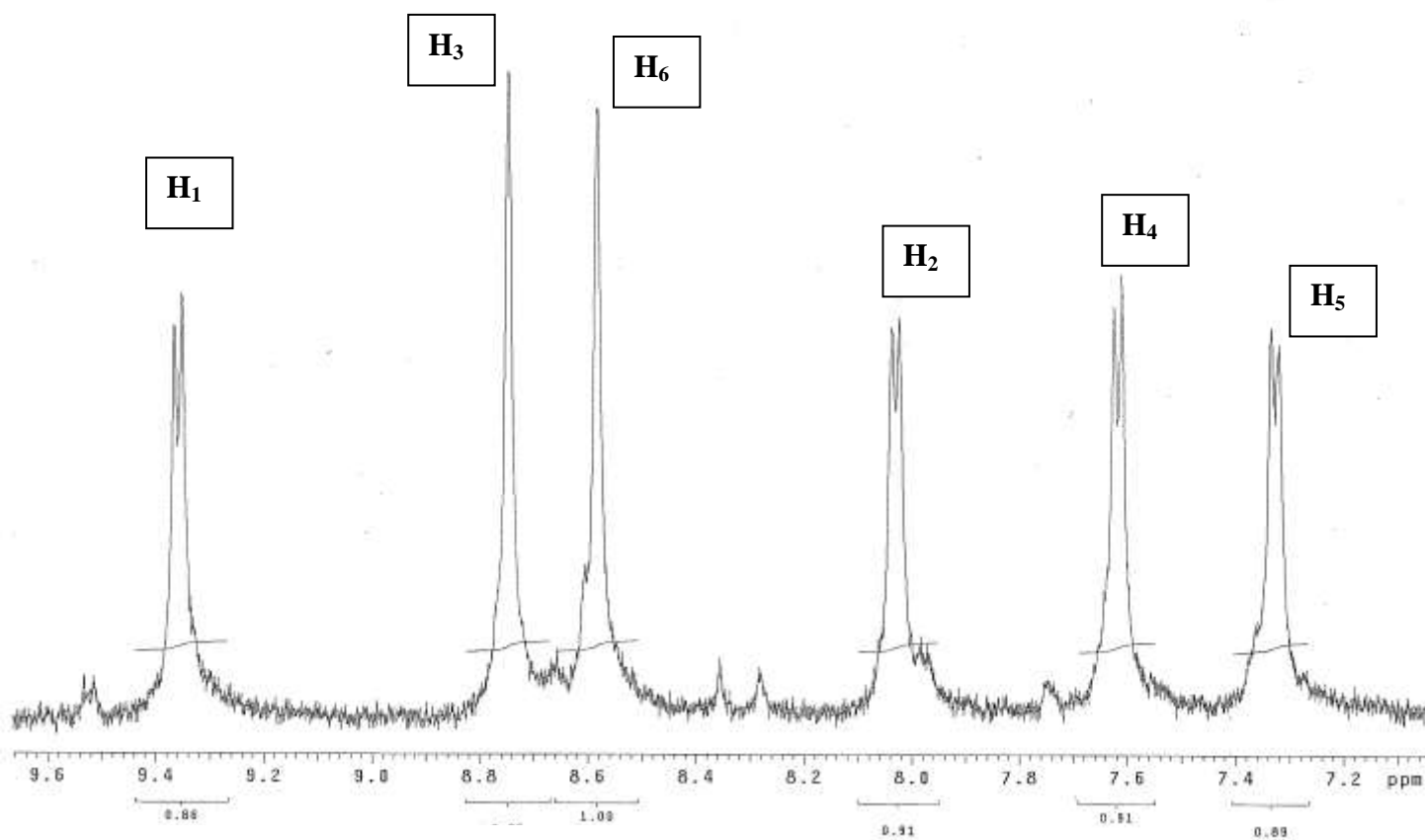


Figure 3: ¹H NMR of cis-RuL₂(NCS)₂

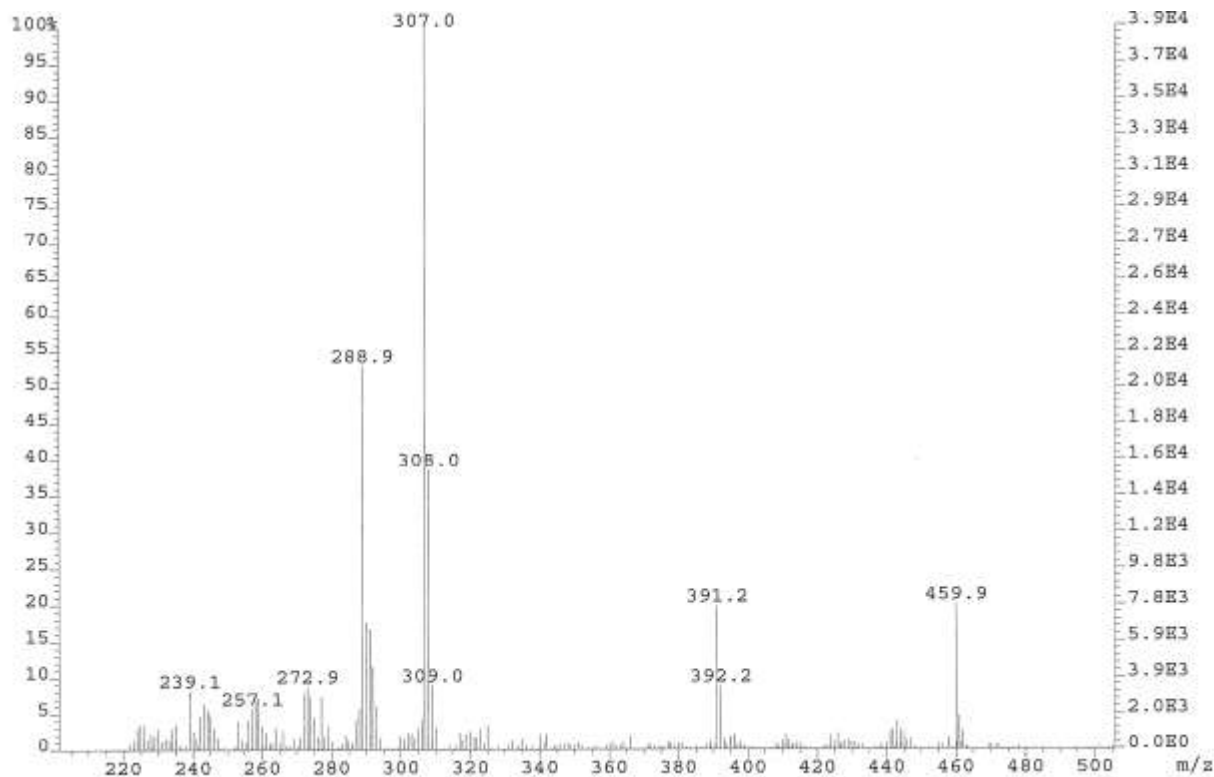


Figure 4: Mass Spec of cis-RuL₂(NCS)₂

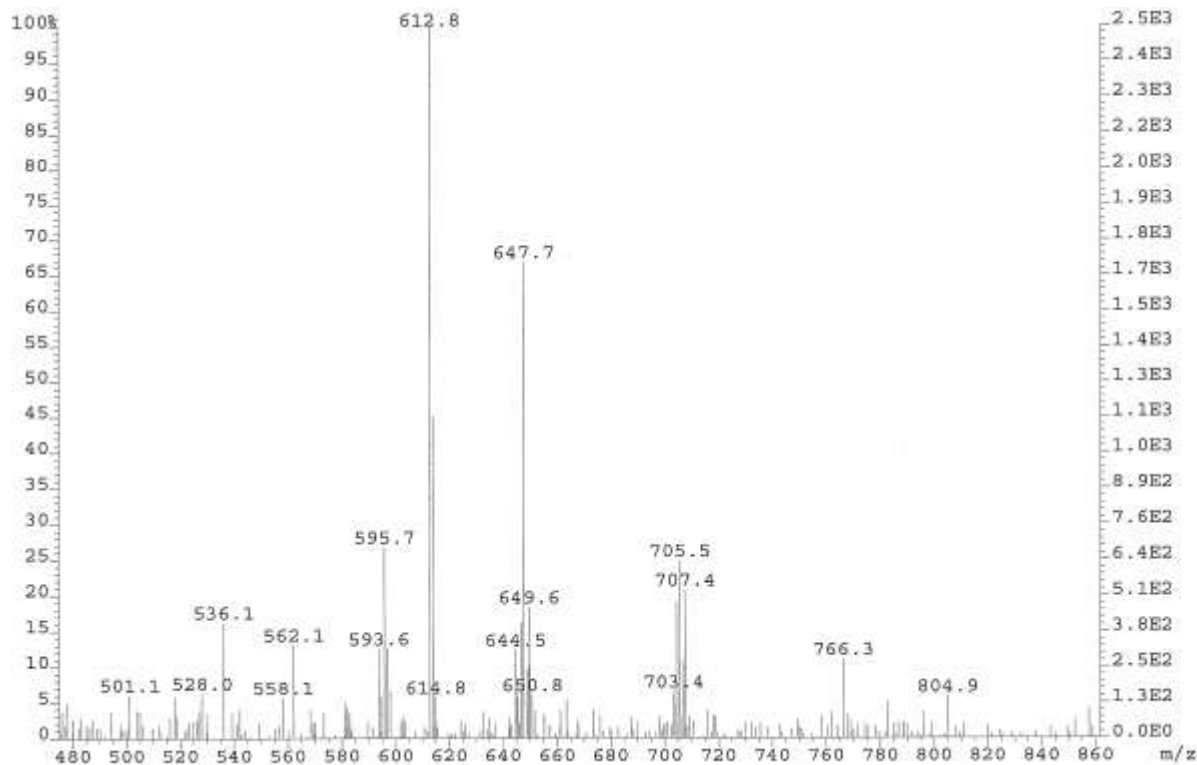


Figure 5: Mass Spec of cis-RuL₂(NCS)₂

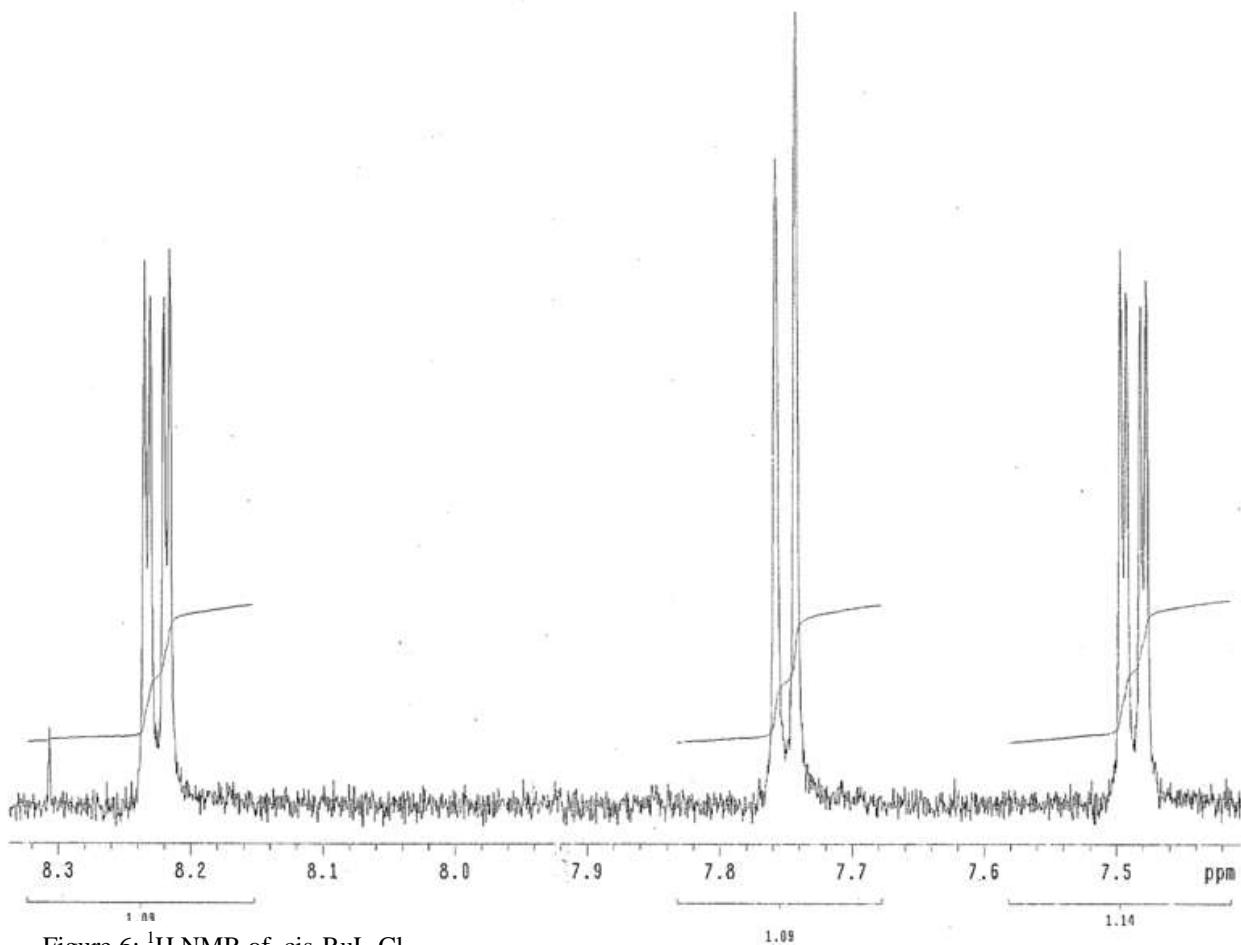


Figure 6: ^1H NMR of $\text{cis-RuL}_2\text{Cl}_2$

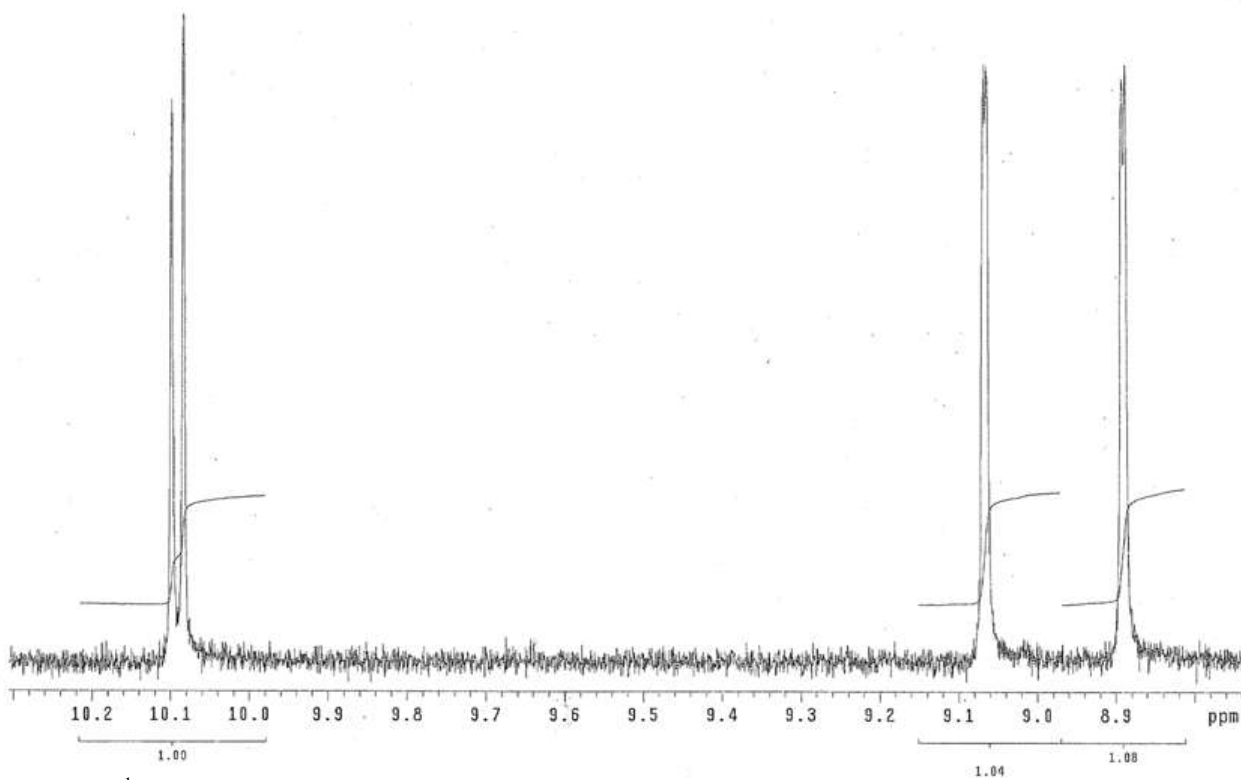


Figure 7: ^1H NMR of $\text{cis-RuL}_2\text{Cl}_2$

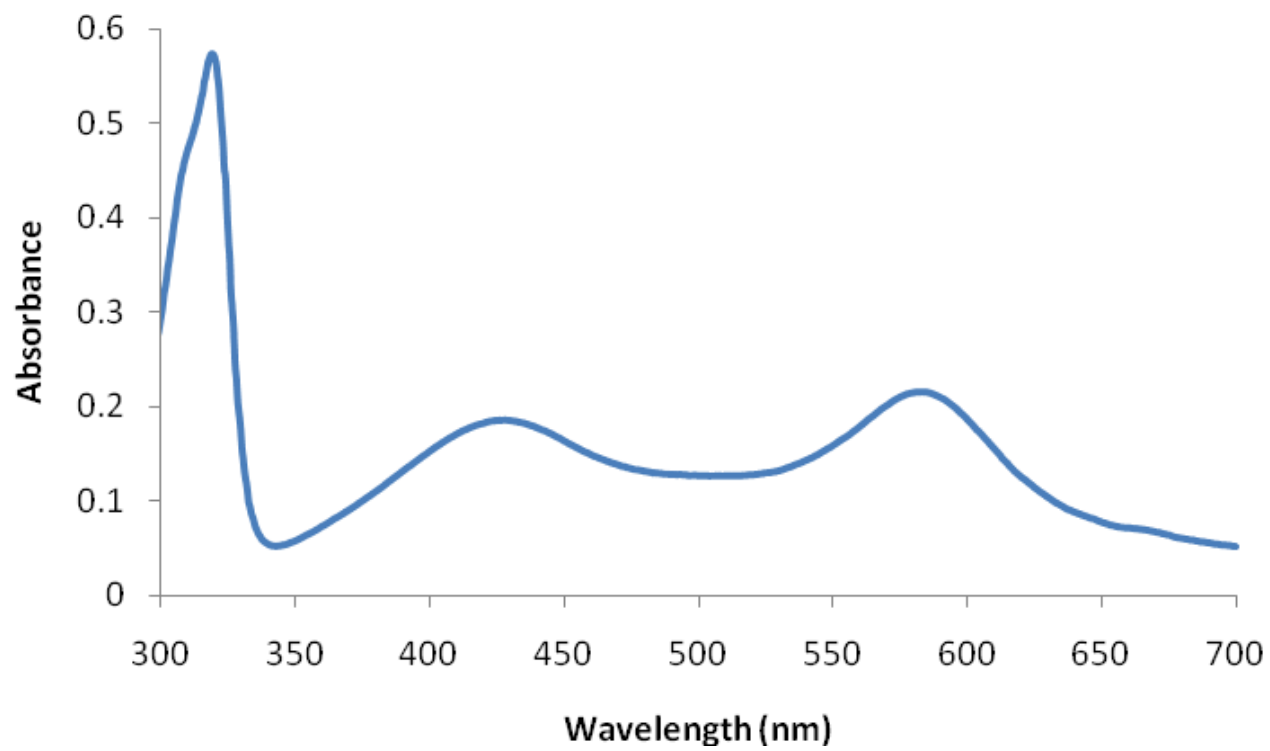


Figure 8: UV/Vis Spectra of *cis*-RuL₂Cl₂.