

Electronic Supplementary Information

New fluorescent bis dithienylethene (DTE)-based bipyridines as reverse interrupters: single vs double photochromism

Lucie Ordronneau,^a Julien Boixel,^a Vincent Aubert,^a Mattias S. Vidal,^b Sergio Moya,^b Pedro Aguirre,^c Loic Toupet,^d J. A. Gareth Williams,^e Hubert Le Bozec,^{*a} and Véronique Guerchais^{*a}

^aInstitut des Sciences Chimiques de Rennes UMR 6226 CNRS-Université de Rennes 1, Campus de Beaulieu, 35042 Rennes, France. Fax: 33223236939; Tel: 33223236544; E-mail: lebozec@univ-rennes1.fr, veronique.guerchais@univ-rennes1.fr.

^b Universidad de Santiago de Chile, Facultad de Química y Biología, Av. Libertador Bernardo O'Higgins 3363, Casilla 40, Correo 33, Santiago, Chile.

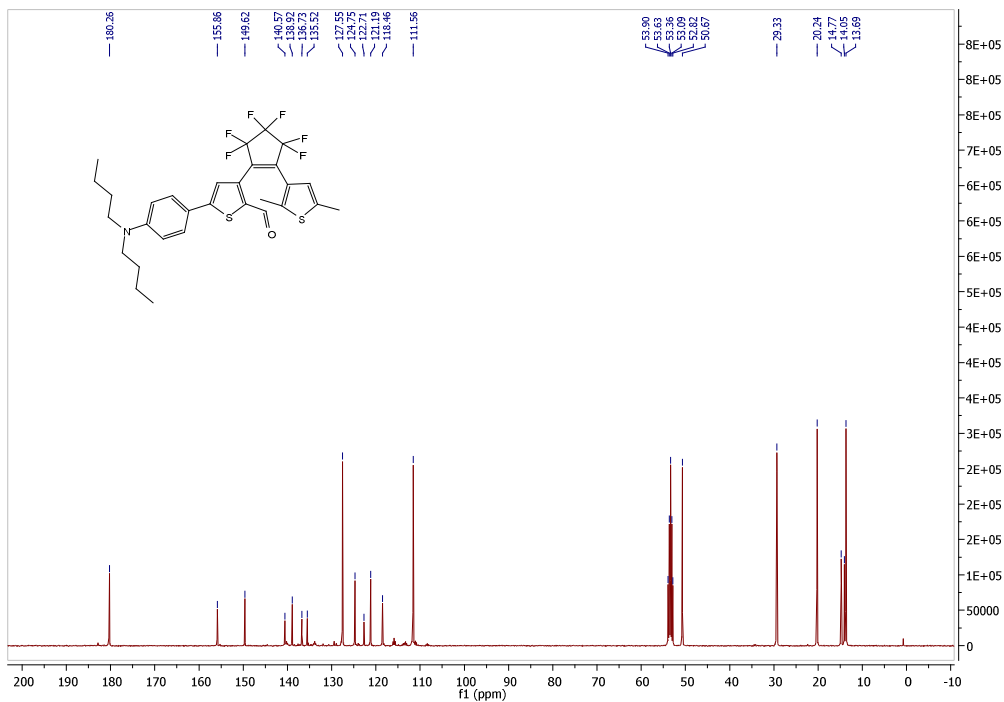
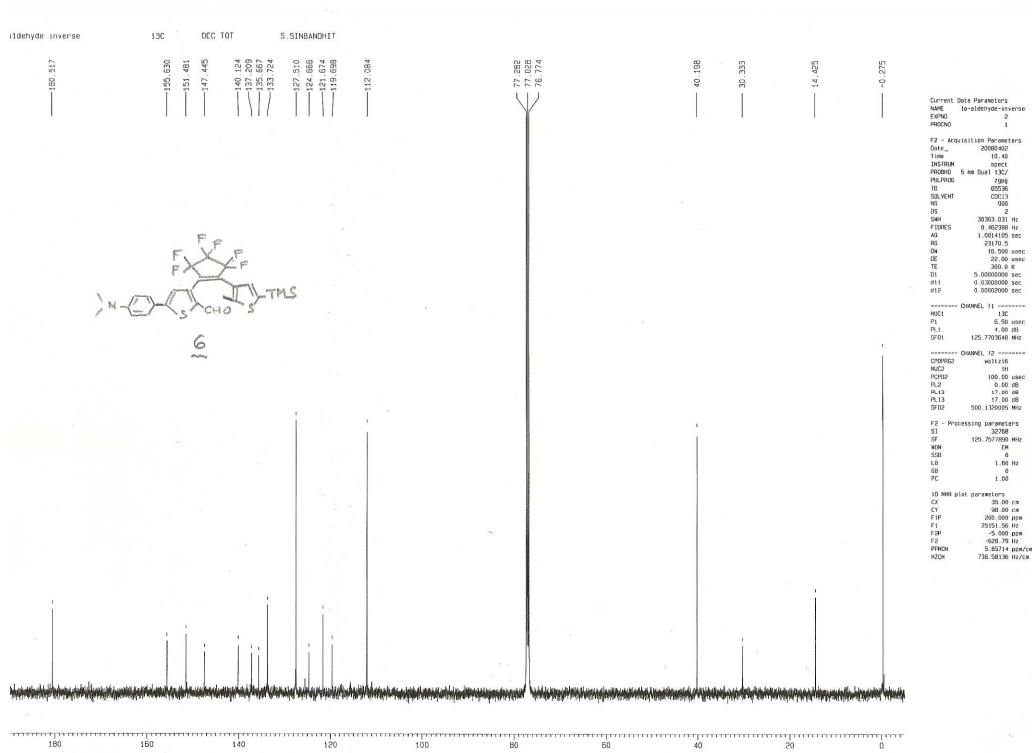
^c Universidad de Chile, Facultad de Ciencias Químicas y Farmacéuticas, Casilla 233, Santiago 1, Chile.

^dInstitut de Physique de Rennes, UMR 6251 CNRS-Université de Rennes 1, Campus de Beaulieu, 35042 Rennes, France.

^eDepartment of Chemistry, Durham University, South Road, Durham, DH1 3LE, United Kingdom.

Table of contents

- S1.** ¹³C NMR of **6a** in CDCl₃
- S2.** ¹³C NMR of **6b** in CD₂Cl₂
- S3.** ¹³C NMR of **6c** in CDCl₃
- S4.** ¹³C NMR of **L^a** in CDCl₃
- S5.** ¹³C NMR of **L^b** in CD₂Cl₂
- S6.** ¹³C NMR of **L^c** in CDCl₃
- S7.** ¹³C NMR of **ReL^b** in CD₂Cl₂
- S8.** ¹³C NMR of **ZnL^b** in CD₂Cl₂
- S9.** Absorption (PSS) and emission (open form) spectra of **L^b** in cyclohexane



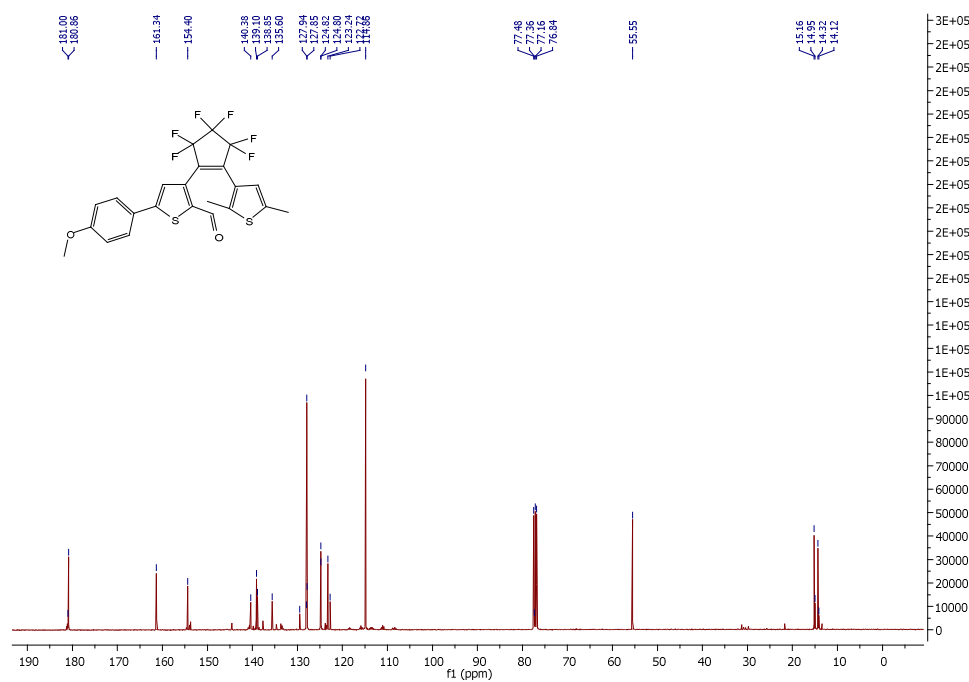


Figure S3. ^{13}C NMR of **6c** in CDCl_3

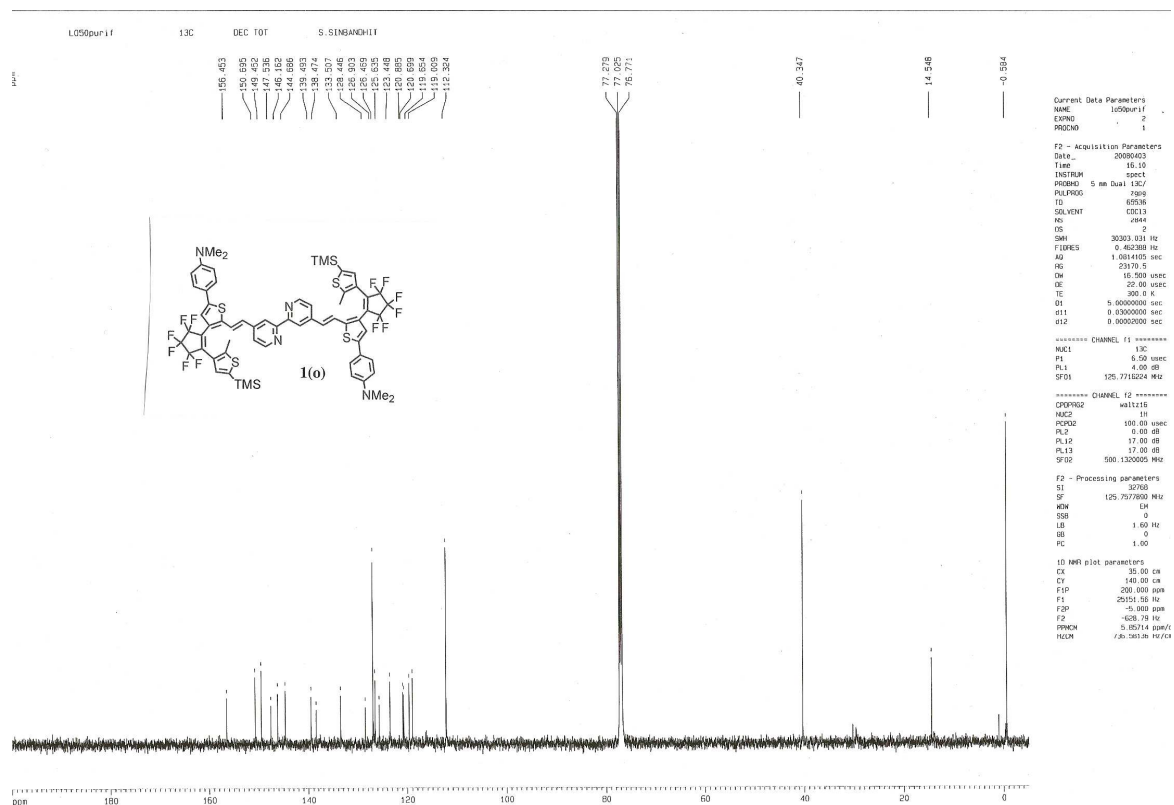
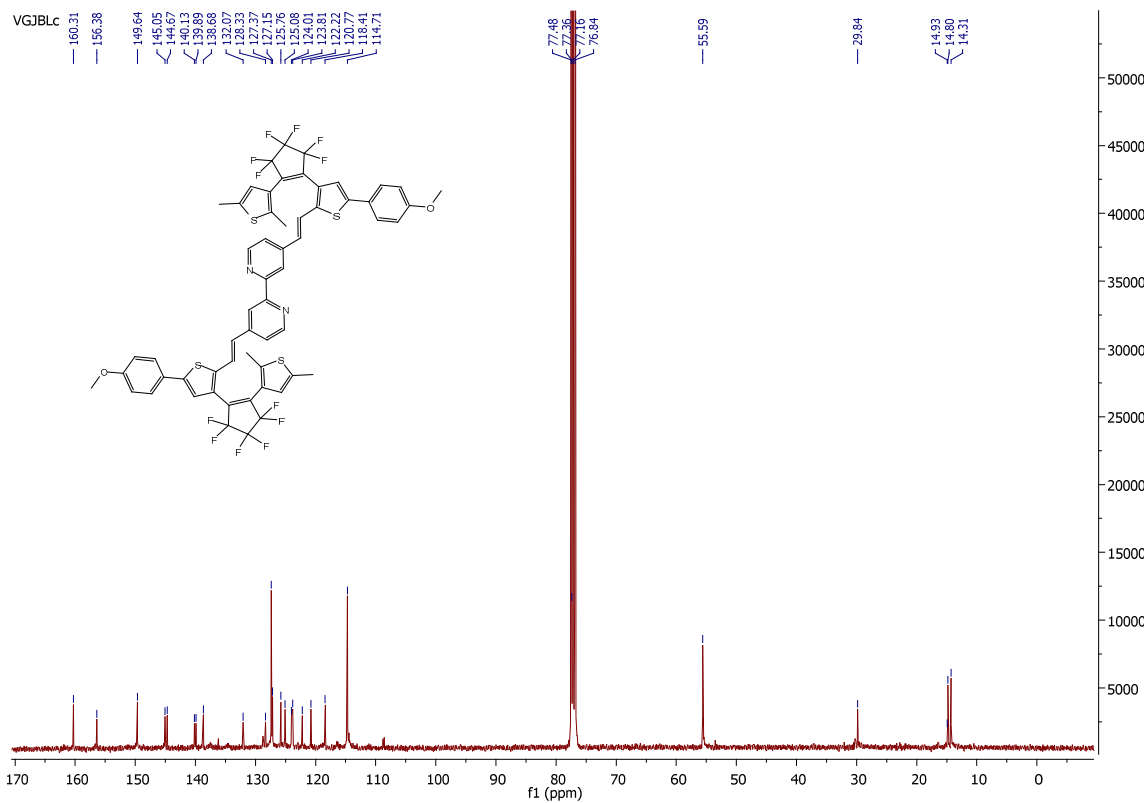
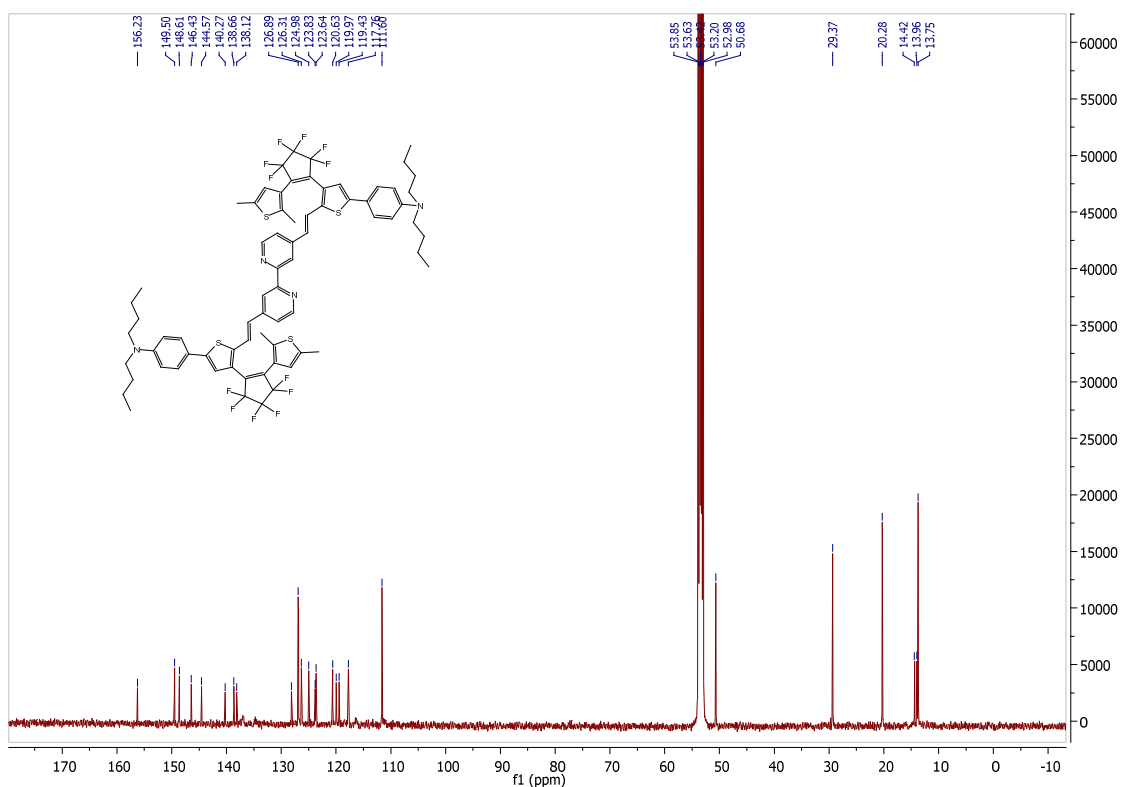


Figure S4. ^{13}C NMR of **L^a** in CDCl_3



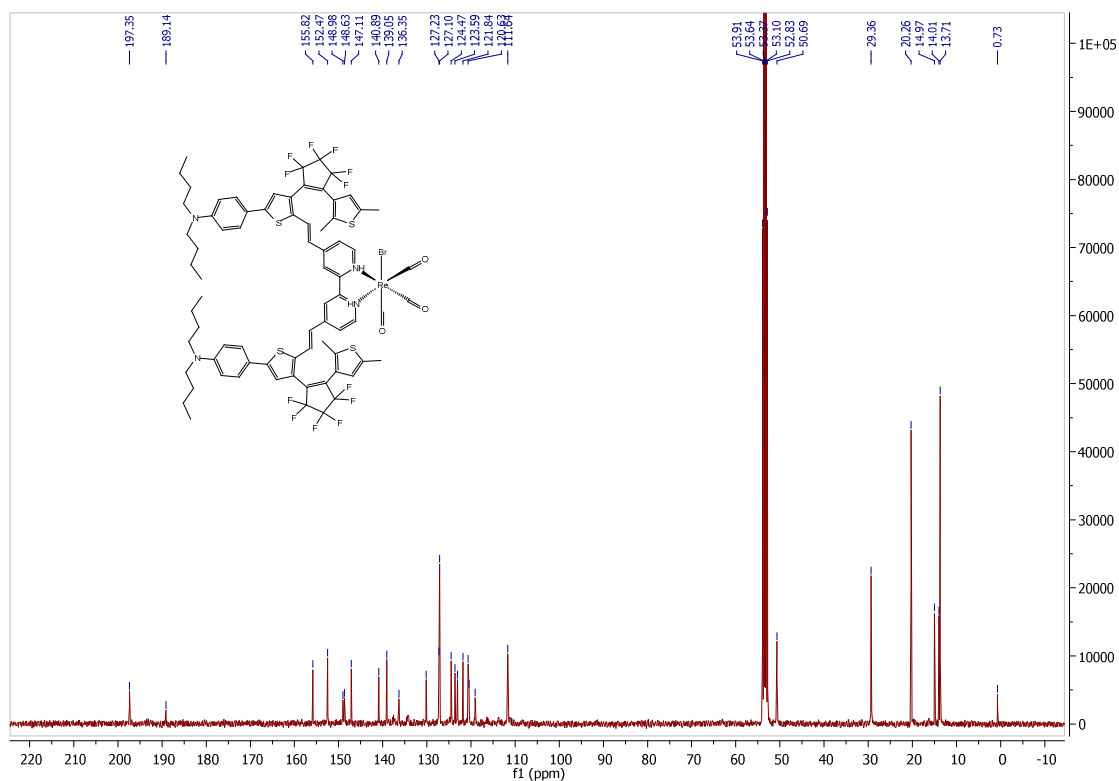


Figure S7. ¹³C NMR of **ReL^b** in CD₂Cl₂

Additional equations^(a) used in calculating the Förster critical radius R_0 and efficiency E of energy transfer:

$$R_0^6 = 8.79 \times 10^{23} (\kappa^2 n^{-4} Q_D J(\lambda)) \quad [\text{equation S1}]$$

where Q_D is the quantum yield of the donor (here we have used the value of the open–open form), n is the refractive index (1.42 for cyclohexane), and κ^2 is factor that takes into account the orientational dependence of the dipoles of donor and acceptor. For simplicity, we have assumed a value for κ^2 of 2/3, as found for random averaging in intermolecular energy transfer.

$$E = \frac{R_0^6}{R_0^6 + r^6} \quad [\text{equation S2}]$$

(a) See, for example, chapter 13 of J. R. Lakowicz, *Principles of Fluorescence Spectroscopy*, 3rd edition, Springer, 2006.